Univerzita Komenského v Bratislave
Prírodovedecká fakulta

Mlynská dolina
Ilkovičova 6
842 15 Bratislava 4

Ústredná knižnica PRIF UK
(Evidencia publikačnej činnosti)

Prehľad publikačnej činnosti a ohlasov

doc. Ing. Tomáš Bučko, PhD.

Výstup ku dňu 26.10.2026

Výstup záznamov od roku 2022

P1 - Pedagogický výstup publikačnej činnosti ako celok
- spolu : **1**

2025 - spolu : **1**

P1_001: / Bučko, Tomáš (Autor) [UKOPRCFZ] (100%) (6,88 AH) - Mihalkovič, Marek (Recenzent) - Tunega, Daniel (Recenzent) : **Investigating chemical reactions with VASP** [elektronický dokument] : A practical guide. – 1. vyd. – Bratislava (Slovensko) : Univerzita Komenského v Bratislave, 2025. – 109 s. [6,88 AH] [online] : text, ilustr., tab. – ISBN (online) 978-80-223-6054-8
Počet všetkých autorov: 1
[učebnica pre vysoké školy]
Lit.: 75
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]

V3 - Vedecký výstup publikačnej činnosti z časopisu - spolu : **22**

2022 - spolu : **6**

V3_001: / Dib, Eddy (Autor) (7.154%) - Rey, Jerome (Autor) (7.142%) - Vicente, Aurelie (Autor) (7.142%) - Kunjir, Shrikant (Autor) (7.142%) - Awala, Hussein (Autor) (7.142%) - Komaty, Sarah (Autor) (7.142%) - Daouli, Ayoub (Autor) (7.142%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (7.142%) - El Siblani, Hussein (Autor) (7.142%) - Bedard, Robert (Autor) (7.142%) - Bricker, Jeffery (Autor) (7.142%) - Gilson, Jean-Pierre (Autor) (7.142%) - Badawi, Michael (Autor) (7.142%) - Mintova, Svetlana (Autor) (7.142%): **Access to sodalite cages in ion-exchanged nanosized FAU zeolites probed by hyperpolarized 129Xe NMR and DFT calculations**. – text, graf., tab. – [recenzované]. – DOI 10.1016/j.micromeso.2022.111965. – CCC ; WOS CC ; SCO.
In: *Microporous and Mesoporous Materials* [textový dokument (print)] [elektronický dokument] . – Amsterdam (Holandsko) : Elsevier. – ISSN 1387-1811. – ISSN (online) 1873-3093. – č. 338 (2022), art. no. 111965, s. [1-7] [tlačená forma] [online]
Počet všetkých autorov: 14
[článok]
Lit.: 36
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 5.2 - 2022
SNIP: 1,026 - 2022

SJR: 0,922 - 2022
CiteScore: 9,6 - 2022
AIS: 0.664 - 2022
Kvartil Q:
2022, AIS - Chemistry, applied - Q1; **2022, AIS** - Chemistry, physical - Q2; **2022, AIS** - Materials science, multidisciplinary - Q2; **2022, AIS** - Nanoscience & nanotechnology - Q3; **2022, JCI** - Chemistry, applied - Q1; **2022, JCI** - Chemistry, physical - Q2; **2022, JCI** - Materials science, multidisciplinary - Q2; **2022, JCI** - Nanoscience & nanotechnology - Q2; **2022, JIF** - Chemistry, applied - Q1; **2022, JIF** - Chemistry, physical - Q2; **2022, JIF** - Materials science, multidisciplinary - Q2; **2022, JIF** - Nanoscience & nanotechnology - Q2; **2022, Scimago** - Chemistry (miscellaneous) - Q1; **2022, Scimago** - Condensed matter physics - Q1; **2022, Scimago** - Materials science (miscellaneous) - Q1; **2022, Scimago** - Mechanics of materials - Q1; **2022, Scimago** - Nanoscience and nanotechnology - Q2

Ohlasy (9):

2025 [01/20] / **DEU** - Reyes Villegas, Víctor Alfredo - De León Ramirez, Jesús Isaías - Pérez-Cabrera, Luis - Pérez-Sicairos, Sergio - Yocupicio-Gaxiola, Rosario Isidro - Chávez-Méndez, José Román - Huerta-Arcos, Lázaro - Petranovskii, Vitalii. **Sonochemical post-synthesis modification of Y zeolite with iron species** [elektronický dokument]. DOI 10.1016/j.matchemphys.2024.130199 In: **Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2025, Roč. 331, art. no. 130199 [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 130199

2025 [01/20] / **NLD** - Lee, Kang Min - Song, Minseok - Lim, Wootaek - Cho, Hae Sung - Jo, Changbum. **Aminoethanethiol-assisted capture of ppm-level Hg2+ by FAU zeolites for water purification** [elektronický dokument]. DOI 10.1016/j.seppur.2025.131485 In: **Separation and Purification Technology**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 361, art. no. 131485 [tlačená forma] [online]. ISSN 1383-5866. ISSN (online) 1873-3794. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 131485

2025 [01/20] / **USA** - Gao, Xu - Feng, Aihu - Mi, Le - Yu, Yang - Zhang, Liangmiao - Yu, Yun. **Molecular dynamics simulation study on the adsorption mechanism of VOCs by NaY zeolite under low-pressure conditions** [elektronický dokument]. DOI 10.1007/s10853-025-11783-9 In: **Journal of Materials Science**. Norwell: Springer Nature. Springer International Publishing AG, 2025, Roč. 60, č. 47, s. 24313-24325 [tlačená forma] [online]. ISSN 0022-2461. ISSN (online) 1573-4803. - SCO ; CCC ; WOS CC ; SCIE, s. 24313 - 24325

2025 [01/20] / **JPN** - Hiraishi, Masatoshi - Utsuno, Kaito - Takei, Tomoki - Ishihara, Misaki - Ohishi, Kazuki - Kojima, Kenji M. - Nakano, Takehito. **Metal–Insulator Transition in the Na-Loaded Zeolite Low Silica X Probed by Muon Knight Shift Measurement and DFT Calculations** [elektronický dokument]. DOI 10.7566/JPSJ.94.094708 In: **Journal of the Physical Society of Japan**. Tokio: The Physical Society of Japan, 2025, Roč. 94, č. 9, art. no. 094708 [tlačená forma] [online]. ISSN 0031-9015. ISSN (online) 1347-4073. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 094708

2023 [01/20] / **BGR** - Stanimirova, Tsveta - Kirov, Georgi. **Modification of zeolite Na-X, sodalite and cancrinite in salt melts** [elektronický dokument]. DOI 10.52321/GeolBalc.52.3.41 In: **Geologica Balcanica**. Sofia: Balgarska akademiya na naukite. Geological Institute "Strashimir Dimitrov", 2023, Roč. 52, č. 3, s. 41-49 [tlačená forma] [online]. ISSN 03240894. ISSN (online) 25351060. - SCO, s. 41 - 49

2023 [01/20] / **NLD** - Boycheva, Silviya - Szegedi, Ágnes - Lázár, Károly - Popov, Cyril - Popova, Margarita. **Advanced high-iron coal fly ash zeolites for low-carbon emission catalytic combustion of VOCs** [elektronický dokument]. DOI 10.1016/j.cattod.2023.114109 In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2023, Roč. 418, art. no. 114109 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; CCC ; WOS CC, s. art. no. 114109

2023 [01/20] / **GBR** - Hong, Zhe - Li, Lei - Miao, Lei - Zhao, Guoqing - Zhu, Zhirong. **Opening sodalite cages of X zeolite for boosting toluene side-chain alkylation performance** [elektronický dokument]. DOI 10.1039/d2cy01970a In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 7, s. 1991-1995 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 1991 - 1995

2023 [01/20] / **GBR** - Equbal, Asif - Mewis, Ryan E. **Hyperpolarisation techniques**. DOI 10.1039/BK9781837672455-00146 In: **Nuclear Magnetic Resonance**. Cambridge: The Royal Society of Chemistry, 2023, s. 146-176. ISBN 978-1-83767-190-8. ISBN 978-1-83767-245-5. - SCO, s. 146 - 176

2022 [01/20] / **NLD** - Khalili, Roya - Kantola, Anu M. - Komulainen, Sanna - Selent, Anne - Selent, Marcin - Vaara, Juha - Larsson, Anna Carin - Lantto, Perttu - Telkki, Ville Veikko. **¹²⁹Xe NMR analysis of pore structures and adsorption phenomena in rare-earth element phosphates** [elektronický dokument]. DOI 10.1016/j.micromeso.2022.112209 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 344, art. no. 112209 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. art. no. 112209

V3_002: / Herzog, Basile (Autor) (12.5%) - da Silva, Mauricio Chagas (Autor) (12.5%) - Casier, Bastien (Autor) (12.5%) - Badawi, Michael (Autor) (12.5%) - Pascale, Fabien (Autor) (12.5%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (12.5%) - Lebegue, Sebastien (Autor) (12.5%) - Rocca, Dario (Autor) (12.5%): **Assessing the Accuracy of Machine Learning Thermodynamic Perturbation Theory: Density Functional Theory and Beyond**. – text, graf., tab. – [recenzované]. – DOI 10.1021/acs.jctc.1c01034. – SCO ; OA ; CCC ; WOS CC.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 18, č. 3 (2022), s. 1382-1394 [tlačená forma] [online]
Počet všetkých autorov: 8
[článok]
Lit.: 71
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 5.5 - 2022
SNIP: 1,512 - 2022
SJR: 1,665 - 2022
CiteScore: 10,9 - 2022
AIS: 1.448 - 2022
Kvartil Q:
2022, AIS - Chemistry, physical - Q2; **2022, AIS** - Physics, atomic, molecular & chemical - Q1; **2022, JCI** - Chemistry, physical - Q1; **2022, JCI** - Physics, atomic, molecular & chemical - Q1; **2022, JIF** - Chemistry, physical - Q2; **2022, JIF** - Physics, atomic, molecular & chemical - Q1; **2022, Scimago** - Computer science applications - Q1; **2022, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (9):
2025 [01/20] / **DEU** - Bocus, Massimo - Vandenhaute, Sander - Van Speybroeck, Veronique. **The Operando Nature of Isobutene Adsorbed in Zeolite H−SSZ−13 Unraveled by Machine Learning Potentials Beyond DFT Accuracy** [elektronický dokument]. DOI 10.1002/anie.202413637 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 64, č. 1, art. no. e202413637 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **USA** - Jahan, Zarak - Kanishka, S. - Rahul, B. - Kavinn, S. - Palanisamy, T. - Senthil Kumar, T. - Srinidhi, K. - Bharanidhar, R. K. **Detection and classification of Early Parkinson's Disease Identification using Machine Learning Algorithms**. DOI 10.1109/ICOIICS67115.2025.11390330 In: **2025 International Conference on Intelligent Computing, Information and Control Systems (ICOIICS)**. New York: Institute of Electrical and Electronics Engineers, 2025, s. 1370-1381 [tlačená forma]. ISBN [9798331598976]. - SCO, s. 1370 - 1381

2025 [01/20] / **NLD** - Demirel, Yasar - Gerbaud, Vincent. **Nonequilibrium Thermodynamics Transport and Rate Processes in Physical Chemical and Biological Systems** [textový dokument (print)] [elektronický dokument] . Amsterdam: Elsevier. Elsevier Science, 2025. 5. vyd. ISBN [9780443221507, 9780443221491]. - SCO, s. 1 - 963

2025 [01/20] / **GBR** - Vacek, Jaroslav - Vrška, Dávid - Manna, Debashree - Lo, Rabindranath - Hobza, Pavel. **Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches** [elektronický dokument]. DOI 10.1039/D5SC06336A In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 48, s. 23129-23138 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; WOS CC ; CCC ; SCIE ; Nature Index ; OA, s. 23129 - 23138

2023 [01/20] / **GBR** - Van Speybroeck, Veronique. **Challenges in modelling dynamic processes in realistic nanostructured materials at operating conditions** [elektronický dokument]. DOI 10.1098/rsta.2022.0239 In: **Philosophical Transactions of the Royal Society A**: Mathematical, Physical & Engineering Sciences. Londýn: Royal Society, 2023, Roč. 381, č. 2250, art. no. 20220239 [tlačená forma] [online]. ISSN 1364-503X. ISSN (online) 1471-2962. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **USA** - Rizzi, Andrea - Carloni, Paolo - Parrinello, M. **Free energies at QM accuracy from force fields via multimap targeted estimation** [elektronický dokument]. DOI 10.1073/pnas.2304308120 In: **Proceedings of the National Academy of Sciences of the United States of America**. Washington: National Academy of Sciences of the United States of America, 2023, Roč. 120, č. 46, art. no. 4308120 [tlačená forma] [online]. ISSN 0027-8424. ISSN (online) 1091-6490. - SCO ; CCC ; WOS CC, s.

2022 [01/20] / **USA** - Giese, Timothy J. - Zeng, Jinzhe - York, Darrin M. **Multireference Generalization of the Weighted Thermodynamic Perturbation Method** [elektronický dokument]. DOI 10.1021/acs.jpca.2c06201 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2022, Roč. 126, č. 45, s. 8519-8533 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO, s. 8519 - 8533

V3_003: / Said, Halima (Autor) (50%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (50%): **Effect of molecular impurities on properties of clean and cesiated Mo(001) surface: A DFT study of the low coverage limit**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1016/j.apsusc.2022.154706. – SCO ; CCC ; WOS CC.
In: *Applied Surface Science* [textový dokument (print)] [elektronický dokument] : a journal devoted to applied physics and

chemistry of surfaces and interfaces. – Amsterdam (Holandsko) : Elsevier. – ISSN 0169-4332. – ISSN (online) 1873-5584. – č. 605 (2022), art. no. 154706, s. [1-12] [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
Lit.: 57
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 6.7 - 2022
SNIP: 1,259 - 2022
SJR: 1,187 - 2022
CiteScore: 12,7 - 2022
AIS: 0.867 - 2022
Kvartil Q:
2022, AIS - Chemistry, physical - Q2; **2022, AIS** - Materials science, coatings & films - Q1; **2022, AIS** - Physics, applied - Q2; **2022, AIS** - Physics, condensed matter - Q2; **2022, JCI** - Chemistry, physical - Q1; **2022, JCI** - Materials science, coatings & films - Q1; **2022, JCI** - Physics, applied - Q1; **2022, JCI** - Physics, condensed matter - Q1; **2022, JIF** - Chemistry, physical - Q2; **2022, JIF** - Materials science, coatings & films - Q1; **2022, JIF** - Physics, applied - Q1; **2022, JIF** - Physics, condensed matter - Q1; **2022, Scimago** - Chemistry (miscellaneous) - Q1; **2022, Scimago** - Condensed matter physics - Q1; **2022, Scimago** - Physics and astronomy (miscellaneous) - Q1; **2022, Scimago** - Surfaces and interfaces - Q1; **2022, Scimago** - Surfaces, coatings and films - Q1

Ohlasy (6):
2025 [01/20] / **NLD** - Ma, Yubo - Li, Wei - Hu, Jun - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Geng, Shaofei - Liu, Haifeng - Wang, Xianqu - Huang, Jie - Liu, Hai - Cheng, Jun - Tang, Changjian. **Investigating the stability and work function effects of Ba atoms adsorption on the Mo (110) surface** [elektronický dokument]. DOI 10.1016/j.nme.2025.101984 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2025, Roč. 45, art. no. 101984 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101984

2025 [01/20] / **NLD** - Zhang, Xin - Li, Heng - Tsumori, Katsuyoshi - Xu, Yuhong - Isobe, Mitsutaka - Lei, Guangjiu - Liu, Sanqiu - Osakabe, Masaki - Nakano, Haruhisa - Shimizu, Akihiro - Okamura, Shoichi - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Liu, Xiaoqiao - Zheng, Huaqing - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Chen, Jun. **The influence of hydrogen and impurities on the work function of multilayer Cs atoms on the plasma grid: An ab-initio molecular dynamics study about negative hydrogen ion sources for neutral beam injection systems** [elektronický dokument]. DOI 10.1016/j.nme.2025.101897 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2025, Roč. 42, art. no. 101897 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101897

2025 [01/20] / **USA** - Schaefer-Dalmau, Diego - Martínez-Alonso, Carmen - Llorca, Javier - Vassilev-Galindo, Valentin. **Computational Study to Assess the Influence of Elastic Strains on the Catalytic Activity of Au Surfaces for the HER and ORR Including the Effect of Coverage** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c01962 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 38, s. 17036-17048 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 17036 - 17048

2024 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Tsumori, Katsuyoshi - Nakano, Haruhisa - Osakabe, Masaki - Isobe, Mitsutaka - Okamura, Shoichi - Shimizu, Akihiro - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Zheng, Huaqing - Liu, Xiaoqiao - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **Effect of oxygen or copper impurities on the work function of cesiated surfaces under co-existence with hydrogen: A study about negative hydrogen ion sources for neutral beam injection systems** [elektronický dokument]. DOI 10.1016/j.nme.2024.101792 In: **Nuclear Materials and**

Energy. Amsterdam: Elsevier, 2024, Roč. 41, art. no. 101792 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC, s. art. no. 101792

2024 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Tsumori, Katsuyoshi - Nakano, Haruhisa - Osakabe, Masaki - Isobe, Mitsutaka - Okamura, Shoichi - Shimizu, Akihiro - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Zheng, Huaqing - Liu, Xiaoqiao - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **Effect of metal impurities on the adsorption energy of cesium and work function of the cesiated Mo (0 0 1) surface** [elektronický dokument]. DOI 10.1016/j.nme.2024.101619 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2024, Roč. 38, art. no. 101619 [online]. ISSN (online) 2352-1791. - SCO ; WOS CC, s. art. no. 101619

2023 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Tsumori, Katsuyoshi - Nakano, Haruhisa - Osakabe, Masaki - Isobe, Mitsutaka - Okamura, Shoichi - Shimizu, Akihiro - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Zheng, Huaqing - Liu, Xiaoqiao - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **Effect of H atoms and O impurities on the adsorption stability and work function of the cesiated Mo(0 0 1) surface: A study about negative hydrogen ion sources for neutral beam injection systems** [elektronický dokument]. DOI 10.1016/j.nme.2023.101550 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2023, Roč. 37, art. no. 101550 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC, s. art. no. 101550

V3_004: / Gešvandtnerová, Monika (Korešpondenčný autor) [Interný doktorand] [UKOPRCFZ] (25%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (25%) - Raybaud, Pascal (Autor) (25%) - Chizallet, Celine (Autor) (25%): **Monomolecular mechanisms of isobutanol conversion to butenes catalyzed by acidic zeolites: Alcohol isomerization as a key to the production of linear butenes**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1016/j.jcat.2022.07.025. – SCO ; CCC ; WOS CC ; OA.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – č. 413 (2022), s. 786-802 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 75
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 7.3 - 2022
SNIP: 1,313 - 2022
SJR: 1,776 - 2022
CiteScore: 12,7 - 2022
AIS: 1.450 - 2022
Kvartil Q:
2022, AIS - Chemistry, physical - Q2; **2022, AIS** - Engineering, chemical - Q1; **2022, JCI** - Chemistry, physical - Q1; **2022, JCI** - Engineering, chemical - Q1; **2022, JIF** - Chemistry, physical - Q1; **2022, JIF** - Engineering, chemical - Q1; **2022, Scimago** - Catalysis - Q1; **2022, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (8):
2025 [01/20] / **USA** - Hernandez, Eric D. - Bhave, Dipti - Jentoft, Friederike C. **Spectroscopic summation of surface species as a measure of zeolite hydride transfer activity** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115917 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2025, Roč. 443, art. no. 115917 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 115917

2025 [01/20] / **USA** - Hadi, Ghassan Jasim - Alibak, Ali Hosin. **Ethanol Conversion to Linear Olefin Over Phosphorus-Modified Beta Zeolite Catalysts** [elektronický dokument]. DOI 10.1007/s10562-025-05116-3 In: **Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2025, Roč. 155, č. 9, art. no.. 288 [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCO ; CCC ; WOS CC ; SCIE, s. art. no.. 288

2025 [01/20] / **USA** - Hao, Fengting - Liu, Zhaochun - Huang, Pengcheng - Fu, Wenqian - Ren, Jie - Fan, Lu - Chen, Wei - Tang, Tiandi. **Shape-selective zeolite catalysis for the tandem reaction of aromatic alcohol dehydration isomerization to internal alkene** [elektronický dokument]. DOI 10.1016/j.jcat.2025.116221 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2025, Roč. 449, art. no. 116221 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 116221

2024 [01/20] / **USA** - Zikrata, Oksana V. - Larina, Olga V. - Balakin, Dmytro Yu - Nychiporuk, Yurii M. - Khalakhan, Ivan - Švegovec, Marija - Volavšek, Janez - Yaremov, Pavlo S. - Soloviev, Sergiy O. - Orlyk, Svitlana M. **Influence of Acid-Base Characteristics of Different Structural-Type Zeolites (FER, MFI, FAU, BEA) on Their Activity and Selectivity in Isobutanol Dehydration** [elektronický dokument]. DOI 10.1002/cctc.202400068 In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2024, Roč. 16, č. 15, art. no. e202400068 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Liu, Qiang - van Bokhoven, Jeroen A. **Water structures on acidic zeolites and their roles in catalysis** [elektronický dokument]. DOI 10.1039/d3cs00404j In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 53, č. 6, s. 3065-3095 [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO ; CCC ; WOS CC, s. 3065 - 3095

2024 [01/20] / **GBR** - Potter, Matthew E. - Spiske, Lucas - Plessow, Philipp N. - McShane, Evangeline B. - Carravetta, Marina - Oakley, Alice E. - Bere, Takudzwa - Carter, James H. - Vandegehuchte, Bart D. - Kaźmierczak, Kamila M. - Studt, Felix - Raja, Robert. **Combining computational and experimental studies to gain mechanistic insights for n-butane isomerisation with a model microporous catalyst** [elektronický dokument]. DOI 10.1039/d4cy01035c In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 24, s. 7140-7151 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 7140 - 7151

2023 [01/20] / **NLD** - Dubois, Jean Luc - Segondy, Sandra - Postole, Georgeta - Auroux, Aline. **Isobutanol to isobutene: Processes and catalysts** [elektronický dokument]. DOI 10.1016/j.cattod.2023.114126 In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2023, Roč. 418, art. no. 114126 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; CCC ; WOS CC, s. art. no. 114126

2023 [01/20] / **USA** - Chen, Wei - Huang, Mengdi - Yi, Xianfeng - Hui, Yu - Gao, Pan - Hou, Guangjin - Stepanov, Alexander G. - Qin, Yucai - Song, Lijuan - Liu, Shang Bin - Chen, Zhongfang - Zheng, Anmin. **Protonated methylcyclopropane is an intermediate providing complete 13C-label scrambling at C4 olefin isomerization in zeolite** [elektronický dokument]. DOI 10.1016/j.checat.2022.100503 In: **Chem Catalysis**. Philadelphia: Elsevier, 2023, Roč. 3, č. 2, art. no. 100503 [tlačená forma] [online]. ISSN 2667-1107. ISSN (online) 2667-1093. - SCO ; WOS CC, s. art. no. 100503

V3_005: / Schweitzer, Jean-Marc (Autor) (10%) - Rey, Jerome (Autor) (10%) - Bignaud, Charles (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (10%) - Raybaud, Pascal (Autor) (10%) - Moscovici-Mirande, Mailys (Autor) (10%) - Portejoie, Frederic (Autor) (10%) - James, Christophe (Autor) (10%) - Bouchy, Christophe (Autor) (10%) - Chizallet, Celine (Autor) (10%): **Multiscale Modeling as a Tool for the Prediction of Catalytic Performances: The Case of n-Heptane Hydroconversion in a Large- Pore Zeolite**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1021/acscatal.1c04707. – SCO ;

CCC ; WOS CC ; OA.
In: *ACS Catalysis* [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN (online) 2155-5435. – Nordic list level 2 - 2021 koeficient 6. – Nordic list level 1 - 2022 koeficient 4. – Roč. 12, č. 2 (2022), s. 1068-1081 [online]
Počet všetkých autorov: 10
[článok]
Lit.: 65
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 12.9 - 2022
SNIP: 2,134 - 2022
SJR: 4,195 - 2022
CiteScore: 20,6 - 2022
AIS: 3.152 - 2022
Kvartil Q:
2022, AIS - Chemistry, physical - Q1; **2022, JCI** - Chemistry, physical - Q1; **2022, JIF** - Chemistry, physical - Q1; **2022, Scimago** - Catalysis - Q1; **2022, Scimago** - Chemistry (miscellaneous) - Q1

Ohlasy (23):
2025 [01/20] / **USA** - Liu, Bangjian - Yang, Hong - Ren, Limin - Song, Zhaoyang - Liu, Quanjie - Hou, Shuandi - Zhang, Anfeng - Guo, Xinwen. **Rapid Synthesis of ZSM-50 Zeolites for Effective n-Heptane Hydroisomerization** [elektronický dokument]. DOI 10.1021/acs.chemmater.5c00735 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2025, Roč. 37, č. 16, s. 6182-6192 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC ; SCIE, s. 6182 - 6192

2025 [01/20] / **CHE** - Wei, Lisha - Wang, Hui - Dong, Qi - Li, Yongwang - Xiang, Hongwei. **A Review on the Research Progress of Zeolite Catalysts for Heavy Oil Cracking**. DOI 10.3390/catal15040401 In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 4, art. no. 401 [online]. ISSN 2073-4344. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 401

2025 [01/20] / **GBR** - Kolganov, Alexander A. - Pidko, Evgeny A. **Computational Chemistry in Zeolite Catalysis**. DOI 10.1039/9781837676859-00312 In: **Zeolites from Fundamentals to Emerging Applications**. London: The Royal Society of Chemistry, 2025, s. 312-369 [tlačená forma] [online]. ISBN [9781837675456, 9781837676859]. - SCO, s. 312 - 369

2024 [01/20] / **GBR** - Ke, Jun - Wang, Yang Dong - Wang, Chuan Ming - Xie, Zai Ku. **Microkinetic simulations of ketene conversion to olefins in H-SAPO-34 zeolite for bifunctional catalysis** [elektronický dokument]. DOI 10.1039/d4cy00405a In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 13, s. 3728-3738 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 3728 - 3738

2024 [01/20] / **CHE** - Chen, Zhengyu - Zhao, Xiangyu - Wu, Jian - Xu, Chunming - Zhang, Linzhou. **Recent progress toward molecular-level kinetic model for complex hydrocarbon conversion processes** [elektronický dokument]. DOI 10.1016/j.cej.2024.150462 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2024, č. 487, art. no. 150462 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 150462

2024 [01/20] / **USA** - Sotelo-Boyás, Rogelio - Smolikov, Mikhail D. - Shkurenok, Violetta A. - Lavrenov, Alexander V. - González-Garay, Andrés - Rosas-Trigueros, Jorge L. - Cázares-Marroquín, José Francisco. **Prediction of Alkyl Carbenium Ion Concentrations and Octane Number Increase in Heptane Hydroisomerization over a Pt/WO3/ZrO2 Catalyst** [elektronický dokument]. DOI 10.1021/acs.iecr.3c02647 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2024, Roč. 63, č. 4, s. 1784-1801 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO ; CCC ; WOS CC, s. 1784 - 1801

2024 [01/20] / **GBR** - He, Guangyuan - Mei, Donghai. **The critical role of the active [GaH]2+ site in n-heptane dehydrocyclization over Ga/H-ZSM-5 zeolite** [elektronický dokument]. DOI 10.1039/d4cy00648h In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 18, s. 5450-5463 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 5450 - 5463

2024 [01/20] / **USA** - He, Guangyuan - Mei, Donghai. **Deciphering reaction mechanism network of n-heptane dehydrocyclization over H-ZSM-5 zeolite** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115623 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 436, art. no. 115623 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Van Speybroeck, Veronique. **Challenges in modelling dynamic processes in realistic nanostructured materials at operating conditions** [elektronický dokument]. DOI 10.1098/rsta.2022.0239 In: **Philosophical Transactions of the Royal Society A**: Mathematical, Physical & Engineering Sciences. Londýn: Royal Society, 2023, Roč. 381, č. 2250, art. no. 20220239 [tlačená forma] [online]. ISSN 1364-503X. ISSN (online) 1471-2962. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Yasumura, Shunsaku - Saita, Kenichiro - Miyakage, Takumi - Nagai, Ken - Kon, Kenichi - Toyao, Takashi - Maeno, Zen - Taketsugu, Tetsuya - Shimizu, Ken ichi. **Designing main-group catalysts for low-temperature methane combustion by ozone** [elektronický dokument]. DOI 10.1038/s41467-023-39541-y In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2023, Roč. 14, č. 1, art. no. 3926 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s. art. no. 3926

2023 [01/20] / **USA** - Gueci, Laura - Bertini, Marco - Nania, Chiara - Ferrante, Francesco - Duca, Dario. **DFT Study of Pt Particle Growth inside β-Zeolite Cages** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c02957 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 30, s. 14765-14775 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 14765 - 14775

2023 [01/20] / **CHN** - Feng, Wei Wei - Qian, Ye Gui - Wang, Ting Hai - Cui, Qing Yan - Yue, Yuan Yuan - Yuan, Pei - Bao, Xiao Jun. **Impacts of support properties on the vacuum residue slurry-phase hydrocracking performance of Mo catalysts** [elektronický dokument]. DOI 10.1016/j.petsci.2023.02.029 In: **Petroleum Science**. Peking: KEAI publishing, 2023, Roč. 20, č. 4, s. 2575-2584 [tlačená forma] [online]. ISSN 16725107. ISSN (online) 19958226. - SCO ; WOS CC, s. 2575 - 2584

2023 [01/20] / **GBR** - Shakor, Zaidoon M. - Al-Shafei, Emad N. **The mathematical catalyst deactivation models: a mini review** [elektronický dokument]. DOI 10.1039/d3ra02912c In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 32, s. 22579-22592 [online]. ISSN (online) 2046-2069. - SCO ; CCC ; WOS CC, s. 22579 - 22592

2023 [01/20] / **USA** - Ke, Jun - Hu, Wen De - Du, Yu Jue - Wang, Yang Dong - Wang, Chuan Ming - Xie, Zai Ku. **Microkinetic Simulations of Methanol-to-Olefin Conversion in H-SAPO-34: Dynamic Distribution and Evolution of the Hydrocarbon Pool and Implications for Catalytic Performance** [elektronický dokument]. DOI 10.1021/acscatal.3c02140 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 13, s. 8642-8661 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 8642 - 8661

2023 [01/20] / **CHE** - Al-Zaidi, Bashir Y. - Al-Shathr, Ali - Shehab, Amal K. - Shakor, Zaidoon M. - Majdi, Hasan Sh - AbdulRazak, Adnan A. - McGregor, James. **Hydroisomerisation and Hydrocracking of n-Heptane: Modelling and Optimisation Using a Hybrid Artificial Neural Network–Genetic Algorithm (ANN–GA)**. DOI 10.3390/catal13071125 In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 7, art. no. 1125 [online]. ISSN 2073-4344. - SCO ; CCC ; WOS CC, s. art. no. 1125

2023 [01/20] / **NLD** - Shostak, Vladyslav - Redekop, Evgeniy - Olsbye, Unni. **Parametric sensitivity analysis of the transient adsorption-diffusion models for hydrocarbon transport in microporous materials** [elektronický dokument]. DOI 10.1016/j.cattod.2022.05.050 In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2023, Roč. 417, art. no. 113785 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; CCC ; WOS CC, s. art. no. 113785

2023 [01/20] / **CHE** - Yang, Fan - Zhou, Qiuming - Wang, Jia - Ding, Hongxin - Zhu, Xuedong - Zhu, Kake - Fan, Weibin. **Conquering the solubility barrier of di-n-octylamine as structure-directing agent in hierarchical silicoaluminophosphate synthesis by using phase-transfer synthesis** [elektronický dokument]. DOI 10.1016/j.cej.2023.141887 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2023, č. 461, art. no. 141887 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 141887

2023 [01/20] / **GBR** - Yasumura, Shunsaku - Kato, Taisetsu - Toyao, Takashi - Maeno, Zen - Shimizu, Ken Ichi. **An automated reaction route mapping for the reaction of NO and active species on Ag4 clusters in zeolites** [elektronický dokument]. DOI 10.1039/d2cp04761f In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 12, s. 8524-8531 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 8524 - 8531

2023 [01/20] / **NLD** - Cheng, Gong - Wang, Xin Xin - Zhang, Shuai Hui - Zhu, Ka Ke - Sui, Zhi Jun - Zhou, Xing Gui - Chen, De - Zhu, Yi An. **On the product and transition-state shape selectivities in 2-heptene isomerization** [elektronický dokument]. DOI 10.1016/j.cplett.2022.140263 In: **Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2023, Roč. 812, art. no. 140263 [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCO ; CCC ; WOS CC, s. art. no. 140263

2022 [01/20] / **GBR** - Liu, Peng - Liu, Qian - Liu, Wei - Peng, Shaozhong - Mei, Donghai. **Mechanistic insights into positional and skeletal isomerization of cyclohexene in the H-BEA zeolite** [elektronický dokument]. DOI 10.1039/d2cp02310e In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s.

2022 [01/20] / **USA** - Agarwal, Umang - Rigutto, Marcello S. - Zuidema, Erik - Jansen, A. P.J. - Poursaeidesfahani, Ali - Sharma, Shrinjay - Dubbeldam, David - Vlugt, Thijs J.H. **Kinetics of zeolite-catalyzed heptane hydroisomerization and hydrocracking with CBMC-modeled adsorption terms: Zeolite Beta as a large pore base case** [elektronický dokument]. DOI 10.1016/j.jcat.2022.09.026 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2022, Roč. 415, s. 37-50 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 37 - 50

2022 [01/20] / **USA** - Zhang, Mingwei - Liu, Linlin - Wang, Li - Zhang, Xiangwen - Li, Guozhu. **Four-Carbon Segmented Discrete Hydrocracking of Long-Chain Paraffins in MTT Channels Following a Pore-Mouth Mechanism** [elektronický dokument]. DOI 10.1021/acscatal.2c03090 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 16, s. 10313-10325 [online]. ISSN (online) 2155-5435. - SCO, s. 10313 - 10325

2022 [01/20] / **GBR** - Nakhaei Pour, Ali - Mohammadi, Ali. **Effect of ZSM-5 zeolite porosity on catalytic cracking of n-heptane** [elektronický dokument]. DOI 10.1039/d2nj03251a In: **New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2022, Roč. 46, č. 32, s. 15585-15595 [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCO, s. 15585 - 15595

V3_006: / Jaykhedkar, Namrata (Autor) [Interný doktorand] [UKOPRCAM] (25%) - Bystrický, Roman (Autor) [UKOPRCAM] (25%) - Sýkora, Milan (Autor) [UKOPRCAM] (25%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (25%): **Understanding the structure-band gap relationship in SrZrS3 at elevated temperatures: a detailed NPT MD study**. – text, ilustr., graf., tab. – [recenzované]. – DOI 10.1039/d2tc02253b. – CCC ; SCO ; WOS CC ; SCIE ; OA.

In: *Journal of Materials Chemistry C* [textový dokument (print)] [elektronický dokument] : Materials for Optical, Magnetic and Electronic Devices. – Londýn (Veľká Británia) : The Royal Society of Chemistry. – ISSN 2050-7526. – ISSN (online) 2050-7534. – Roč. 10, č. 33 (2022), s. 12032-12042 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 68
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 6.4 - 2022
SNIP: 1,229 - 2022
SJR: 1,534 - 2022
CiteScore: 11,8 - 2022
AIS: 1.166 - 2022
Kvartil Q:
2022, AIS - Materials science, multidisciplinary - Q2; **2022, AIS** - Physics, applied - Q1; **2022, JCI** - Materials science, multidisciplinary - Q1; **2022, JCI** - Physics, applied - Q1; **2022, JIF** - Materials science, multidisciplinary - Q1; **2022, JIF** - Physics, applied - Q1; **2022, Scimago** - Chemistry (miscellaneous) - Q1; **2022, Scimago** - Materials chemistry - Q1

Ohlasy (11):
2025 [01/20] / **GBR** - Amuthan, R. - Mohamed Jibri, K. P. - Archana, J. - Navaneethan, M. - KrishnaMohan, M. **Superior thermoelectric power factor in BiCuSeO enabled by a ferromagnetic metallic phase and spin entropy effect** [elektronický dokument]. DOI 10.1088/1361-6463/ada4b9 In: **Journal of Physics D**: Applied Physics. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 58, č. 12, art. no. 125502 [tlačená forma] [online]. ISSN 0022-3727. ISSN (online) 1361-6463. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 125502

2025 [01/20] / **USA** - Khan, Irum Shahid - Gul, Iftikhar Hussain. **Exploring barium ferrite (BaFe2O4) nanoparticle's functioning under the influence of manganese (Mn) on structural, magnetic, electric, and optical properties for photovoltaic (PV) applications** [elektronický dokument]. DOI 10.1007/s10971-025-06924-0 In: **Journal of Sol-Gel Science and Technology**. New York: Springer Nature, 2025, Roč. 116, č. 2, s. 1358-1388 [tlačená forma] [online]. ISSN 0928-0707. ISSN (online) 1573-4846. - SCO ; CCC ; WOS CC ; SCIE, s. 1358 - 1388

2025 [01/20] / **GBR** - Wang, Ziqi - Kenry. **Explainable ensemble learning to predict anisotropic nanomaterial band gap using atomic-scale structural descriptors** [elektronický dokument]. DOI 10.1039/d5qm00559k In: **Materials chemistry frontiers**. Londýn: The Royal Society of Chemistry, 2025, Roč. 9, č. 22, s. 3339-3348 [online]. ISSN (online) 2052-1537. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 3339 - 3348

2025 [01/20] / **USA** - Khan, Irum Shahid - Gul, Iftikhar Hussain. **Tunable properties of silver (Ag) substituted BaFe2O4 nanoparticles for photovoltaic (PV) applications** [elektronický dokument]. DOI 10.1186/s11671-025-04261-3 In: **Discover Nano**. New York: Springer Nature, 2025, Roč. 20, č. 1, art. no. 80 [online]. ISSN (online) 2731-9229. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 80

2025 [01/20] / **GBR** - Eya, Henry I. - Patterson, Robert - Dzade, Nelson Y. **Bandgap engineering of SrZrS3 chalcogenide perovskite via substitutional doping for photovoltaic applications: a first-principles DFT study** [elektronický dokument]. DOI 10.1039/d5cp02689j In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 45, s. 24195-24210 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - WOS CC ; CCC ; SCO, s. 24195 - 24210

2025 [01/20] / **CHE** - Li, Qingyu - Wu, Helong - Li, Weiguo - Zhang, Jiming - Sa, Rongjian. **Computational Discovery of Novel Chalcogenide Perovskites YbMX3 (M = Zr, Hf; X = S, Se) for Optoelectronics** [elektronický dokument]. DOI 10.3390/molecules30071468 In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 30, č. 7, art.

no. 1468 [online]. ISSN (online) 1420-3049. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 1468

2025 [01/20] / **NLD** - Kumar, Satyajeet - Allam, Likhita - Bharadwaj, Soumya - Barman, Biswajit. **Enhancing SrZrS3 perovskite solar cells: A comprehensive SCAPS-1D analysis of inorganic transport layers** [elektronický dokument]. DOI 10.1016/j.jpcs.2024.112378 In: **Journal of Physics and Chemistry of Solids**: an International Journal. Amsterdam: Elsevier, 2025, Roč. 196, art. no. 112378 [tlačená forma]. ISSN (online) 0022-3697. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 112378

2024 [01/20] / **NLD** - Qin, Mutian - Xing, Huilin - Dou, Kunpeng - Tan, Yuyang - Yan, Weichao - Wang, Jianchao - Jin, Zongwei - Hu, Zhongwen. **Estimation of antigorite wave velocities in subduction conditions based on first-principles thermoelasticity**. DOI 10.1016/j.tecto.2024.230444 In: **Tectonophysics**: The International Journal of Integrated Solid Earth Sciences. Amsterdam: Elsevier, 2024, Roč. 887, art. no. 230444 [tlačená forma] [online]. ISSN 0040-1951. - SCO ; CCC ; WOS CC, s. art. no. 230444

2023 [01/20] / **GBR** - Liu, Diwen - Zeng, Huihui - Peng, Huan - Sa, Rongjian. **Computational study of the fundamental properties of Zr-based chalcogenide perovskites for optoelectronics** [elektronický dokument]. DOI 10.1039/d3cp01522j In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s.

2023 [01/20] / **USA** - Koocher, Nathan Z. - Rondinelli, James M. **Effect of Octahedral Connectivity on the Negative Thermal Expansion of SrZrS3** [elektronický dokument]. DOI 10.1021/acs.inorgchem.3c01232 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2023, Roč. 62, č. 28, s. 11134-11141 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 11134 - 11141

2023 [01/20] / **USA** - Jansen, Thies - Brocks, Geert - Bokdam, Menno. **Phase transitions of LaMnO3 and SrRuO3 from DFT+U based machine learning force fields simulations** [elektronický dokument]. DOI 10.1103/PhysRevB.108.235122 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 108, č. 23, art. no. 235122 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 235122

2023 - **spolu** : **3**

V3_007: / Amsler, Jonas (Korešpondenčný autor) (20%) - Plessow, Philipp N. (Autor) (20%) - Studt, Felix (Autor) (20%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (40%): **Anharmonic Correction to Free Energy Barriers from DFT-Based Molecular Dynamics Using Constrained Thermodynamic Integration**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1021/acs.jctc.3c00169. – SCO ; CCC ; WOS CC.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 19, č. 9 (2023), s. 2455-2468 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 100
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 5.7 - 2023
SNIP: 1,433 - 2023
SJR: 1,457 - 2023

CiteScore: 9,9 - 2023
AIS: 1.425 - 2023
Kvartil Q:
2023, AIS - Chemistry, physical - Q1; **2023, AIS** - Physics, atomic, molecular & chemical - Q1; **2023, JCI** - Chemistry, physical - Q1; **2023, JCI** - Physics, atomic, molecular & chemical - Q1; **2023, JIF** - Chemistry, physical - Q2; **2023, JIF** - Physics, atomic, molecular & chemical - Q1; **2023, Scimago** - Computer science applications - Q1; **2023, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (3):
2025 [01/20] / **CHE** - Tran, Vu Hung Anh - Lims, S. Cathrin - Anwar, Nadia - Ahmed, Muqarrab - Iram, Nazia - Ponnusamy, Vinoth Kumar - Pham, Phuong V. **Atomic layer deposition of metal and metal oxides: Mechanisms, challenges, and future prospects** [elektronický dokument]. DOI 10.1016/j.jallcom.2025.183864 In: **Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2025, Roč. 1041, art. no. 183864 [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 183864

2025 [01/20] / **USA** - Pieck, Fabian - Tonner-Zech, Ralf. **Computational Ab Initio Approaches for Area-Selective Atomic Layer Deposition: Methods, Status, and Perspectives** [elektronický dokument]. DOI 10.1021/acs.chemmater.4c03477 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2025, Roč. 37, č. 9, s. 2979-3021 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 2979 - 3021

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

V3_008: / Jaykhedkar, Namrata (Korešpondenčný autor) [Interný doktorand] [UKOPRCAM] (25%) - Bystrický, Roman (Autor) [UKOPRCAM] (25%) - Sýkora, Milan (Autor) [UKOPRCAM] (25%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (25%): **How the Temperature and Composition Govern the Structure and Band Gap of Zr-Based Chalcogenide Perovskites: Insights from ML Accelerated AIMD**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1021/acs.inorgchem.3c01696. – SCO ; SCIE ; CCC ; WOS CC.
In: *Inorganic Chemistry* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 0020-1669. – ISSN (online) 1520-510X. – Roč. 62, č. 31 (2023), s. 12480-12492 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 66
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 4.3 - 2023
SNIP: 0,894 - 2023
SJR: 0,928 - 2023
CiteScore: 7,6 - 2023
AIS: 0.692 - 2023
Kvartil Q:
2023, AIS - Chemistry, inorganic & nuclear - Q1; **2023, JCI** - Chemistry, inorganic & nuclear - Q1; **2023, JIF** - Chemistry,

inorganic & nuclear - Q1; **2023, Scimago** - Chemistry (miscellaneous) - Q1; **2023, Scimago** - Inorganic chemistry - Q1; **2023, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (13):
2025 [01/20] / **USA** - Kayastha, Prakriti - Fransson, Erik - Erhart, Paul - Whalley, Lucy. **Octahedral Tilt-Driven Phase Transitions in BaZrS3 Chalcogenide Perovskite** [elektronický dokument]. DOI 10.1021/acs.jpclett.4c03517 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2025, Roč. 16, č. 8, s. 2064-2071 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 2064 - 2071

2025 [01/20] / **GBR** - Dai, Meng Yao - Wen, Xue - Xia, Rui - Zheng, Yi Min - Wei, Lai - Zhang, Li Li - Liang, Xiao Hui - Huang, Yi Neng. **First-principles calculations of the photocatalytic performance of ZnO-MX2 (M = Mo, W; X = S, Se) heterojunctions** [elektronický dokument]. DOI 10.1039/d5ra03215f In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 15, č. 29, s. 23489-23498 [online]. ISSN (online) 2046-2069. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 23489 - 23498

2025 [01/20] / **USA** - Riva, Stefania - Johansson, Fredrik O.L. - Butorin, Sergei M. - Comparotto, Corrado - Donzel-Gargand, Olivier - Thakur, Pardeep K. - Lee, Tien Lin - Nameirakpam, Henry - Kamalakar, M. Venkata - Mukherjee, Soham - Scragg, Jonathan J.S. - Rensmo, Håkan. **Surface Processing and Characterization of Stoichiometry-Varied BaZrS3Thin Films** [elektronický dokument]. DOI 10.1021/acsaem.5c01766 In: **ACS Applied Energy Materials**. Washington: American Chemical Society. ACS Publications, 2025, Roč. 8, č. 16, s. 12281-12293. ISSN (online) 2574-0962. - SCO ; OA, s. 12281 - 12293

2025 [01/20] / **GBR** - Soni, Ritika - Soni, Vatika - Lokhande, P. E. - Kumar, Deepak - Mubarak, Nabisab Mujawar - Praveenkumar, Seepana - Kumar, Raj - Singh, Kulwinder - Rednam, Udayabhaskar - Aepuru, Radhamanohar - Shanmugaraj, Krishnamoorthy. **Recent advances in lead-free carbon supported perovskites based on Z-scheme and S-scheme heterojunctions for photocatalytic energy conversion** [elektronický dokument]. DOI 10.1039/d4mh01516a In: **Materials Horizons**. Londýn: The Royal Society of Chemistry, 2025, Roč. 12, č. 10, s. 3234-3266 [tlačená forma] [online]. ISSN 2051-6347. ISSN (online) 2051-6355. - SCO ; CCC ; WOS CC ; SCIE, s. 3234 - 3266

2025 [01/20] / **CHE** - Mahanti, Moumita - Mukherjee, Sutirtha - Shirahata, Naoto - Ghosh, Batu. **Design and Simulation of Thermally Stable Lead-Free BaHfSe3 Perovskite Solar Cells: Role of Interface Barrier Height and Temperature**. DOI 10.3390/eng6120345 In: **Eng**. Basel: Multidisciplinary Digital Publishing Institute, 2025, Roč. 6, č. 12, art. no. 345 [online]. ISSN 2673-4117. - SCO ; WOS CC ; ESCI ; OA, s. art. no. 345

2025 [01/20] / **CHE** - Pang, Guowang - Wen, Xue - Zhang, Lili - Huang, Yineng. **First-Principles Study of Biaxial Strain Effects on Schottky Barrier Modulation in Graphene/ZnSe Heterostructures** [elektronický dokument]. DOI 10.3390/nano15231816 In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 23, art. no. 1816 [online]. ISSN (online) 2079-4991. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 1816

2025 [01/20] / **GBR** - Paşca, Laura Bianca - Liu, Yuanbin - Anker, Andy S. - Steier, Ludmilla - Deringer, Volker L. **Machine-learning-driven modelling of amorphous and polycrystalline BaZrS3** [elektronický dokument]. DOI 10.1039/d5ta04536c In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2025, s. 35447-35454 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 35447 - 35454

2025 [01/20] / **NLD** - Zhao, Yihang - Li, Yunxiu - Xi, Jinyang - Yang, Jiong. **Significant temperature tunability of the band gap in two-dimensional materials** [elektronický dokument]. DOI 10.1016/j.commt.2024.100019 In: **Computational Materials Today**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 5, art. no. 100019 [online]. ISSN (online) 29504635. - SCO ; OA, s. art. no. 100019

2024 [01/20] / **NLD** - Abolade, Simeon A. - Akinpelu, Shittu B. - Obada, David O. - Kumar R, Syam - Akande, Akinlolu. **Insights into the band gap anomalies of certain bismuth-based chalcogenides through ab initio calculations of structural and electronic properties** [elektronický dokument]. DOI 10.1016/j.rinp.2024.107891 In: **Results in Physics**: The new online only, open access journal in Physics. Amsterdam: Elsevier, 2024, Roč. 64, art. no. 107891 [online]. ISSN (online) 2211-3797. - SCO, s. art. no. 107891

2024 [01/20] / **USA** - Timmerman, Lucas R. - Kumar, Shashikant - Suryanarayana, Phanish - Medford, Andrew J. **Overcoming the Chemical Complexity Bottleneck in on-the-Fly Machine Learned Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jctc.4c00474 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 14, s. 5788-5795 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 5788 - 5795

2024 [01/20] / **USA** - Adhikari, Surajit - Johari, Priya. **Photovoltaic properties of AB Se3 chalcogenide perovskites (A = Ca, Sr, Ba; B = Zr, Hf)** [elektronický dokument]. DOI 10.1103/PhysRevB.109.174114 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2024, Roč. 109, č. 17, art. no. 174114 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 174114

2024 [01/20] / **GBR** - Pradhan, Apurva A. - Agarwal, Shubhanshu - Vincent, Kiruba Catherine - Hayes, Daniel C. - Peterson, Jonas M. - Turnley, Jonathan W. - Spilker, Robert M. - Uible, Madeleine C. - Bart, Suzanne C. - Huang, Libai - Kisslinger, Kim - Agrawal, Rakesh. **Emergence of Ruddlesden-Popper phases and other pitfalls for moderate temperature solution deposited chalcogenide perovskites** [elektronický dokument]. DOI 10.1039/d4qm00441h In: **Materials chemistry frontiers**. Londýn: The Royal Society of Chemistry, 2024, Roč. 8, č. 20, s. 3358-3372 [online]. ISSN (online) 2052-1537. - SCO ; CCC ; WOS CC, s. 3358 - 3372

2024 [01/20] / **USA** - Jaiswal, Ankit - Sakharov, Konstantin A. - Lekina, Yulia - Kamonsuangkasem, Krongthong - Tomm, Yvonne - Wei, Fengxia - White, Timothy J. **High-Temperature Polymorphism and Band-Gap Evolution in BaZrS3** [elektronický dokument]. DOI 10.1021/acs.inorgchem.4c03895 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2024, Roč. 63, č. 51, s. 24157-24166 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO, s. 24157 - 24166

V3_009: / Eisa, Mohamed (Autor) (15.835%) - Ragauskaite, Dovile (Autor) (15.833%) - Shi, Jingming (Autor) (15.833%) - Shimizu, Seishi (Autor) (15.833%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (5%) - Williams, Clinton (Autor) (15.833%) - Baltrušaitis, Jonas (Autor) (15.833%): **Interactions of Urea Surfaces with Water as Relative Humidity Obtained from Dynamic Vapor Sorption Experiments, In Situ SingleParticle Raman Spectroscopy, and Ab Initio Calculations**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1021/acsearthspacechem.3c00210. – SCO ; OA ; SCIE ; CCC ; WOS CC.
In: *ACS Earth and Space Chemistry* [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN (online) 2472-3452. – Roč. 7, č. 10 (2023), s. 2139-2153 [online]
Počet všetkých autorov: 7
[článok]
Lit.: 99
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 2.9 - 2023
SNIP: 0,769 - 2023
SJR: 0,773 - 2023
CiteScore: 5,3 - 2023
AIS: 0.916 - 2023

Kvartil Q:
2023, AIS - Chemistry, multidisciplinary - Q2; **2023, AIS** - Geochemistry & geophysics - Q2; **2023, JCI** - Chemistry, multidisciplinary - Q2; **2023, JCI** - Geochemistry & geophysics - Q2; **2023, JIF** - Chemistry, multidisciplinary - Q2; **2023, JIF** - Geochemistry & geophysics - Q2; **2023, Scimago** - Atmospheric science - Q2; **2023, Scimago** - Geochemistry and petrology - Q2; **2023, Scimago** - Space and planetary science - Q2

Ohlasy (4):
2025 [01/20] / **CHE** - Hosney, Ahmed - Kundrotaitė, Algimanta - Drapanauskaitė, Donata - Urbonavičius, Marius - Varnagiris, Šarūnas - Ullah, Sana - Barčauskaitė, Karolina. **Green Synthesis of Chitosan Silver Nanoparticle Composite Materials: A Comparative Study of Microwave and One-Pot Reduction Methods** [elektronický dokument]. DOI 10.3390/polym17212960 In: **Polymers**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 17, č. 21, art. no. 2960 [online]. ISSN (online) 2073-4360. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 2960

2025 [01/20] / **CHE** - Altoé, Fernanda Sossai - Santos, Dulce Maria - Vilas-Boas, Sérgio M. - da Costa, Mariana Conceição. **Insights on the Separation of Kraft Lignin from Betaine-Based Eutectic Solvents: A Liquid–Liquid Equilibrium and Partitioning Study** [elektronický dokument]. DOI 10.3390/pr13123784 In: **Processes**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 13, č. 12, art. no. 3784 [online]. ISSN (online) 2227-9717. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 3784

2025 [01/20] / **CHE** - Cao, Yuechao - Qu, Haibin - Wan, Xuxing - Guo, Shengzheng - Li, Kangli - Wu, Songgu - Gong, Junbo. **Spherical cocrystal as a fertilizer slow-release platform for improved nitrogen cycle management** [elektronický dokument]. DOI 10.1016/j.cej.2025.160288 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2025, Roč. 506, art. no. 160288 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 160288

2024 [01/20] / **DEU** - Mojica Sepúlveda, Ruth D. - Mendoza Herrera, Luis J. - Muñoz, Mercedes - Grumel, Eduardo E. - Tebaldi, Myrian. **Study of hygroscopic properties of the mixture of porous and non-porous materials by using optical techniques** [elektronický dokument]. DOI 10.1007/s00340-024-08263-4 In: **Applied Physics B**: Lasers and Optics. Berlín: Springer Nature. Springer International Publishing AG, 2024, Roč. 130, č. 7, art. no. 126 [tlačená forma]. ISSN 0946-2171. ISSN (online) 1432-0649. - SCO ; CCC ; WOS CC, s. art. no. 126

2024 - spolu : **8**

V3_010: / Herzog, Basile (Autor) (12.5%) - Gallo, Alejandro (Autor) (12.5%) - Hummel, Felix (Autor) (12.5%) - Badawi, Michael (Autor) (12.5%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (12.5%) - Lebegue, Sebastien (Autor) (12.5%) - Grüneis, Andreas (Korešpondenčný autor) (12.5%) - Rocca, Dario (Korešpondenčný autor) (12.5%): **Coupled cluster finite temperature simulations of periodic materials via machine learning**. – text, graf., tab. – [recenzované]. – DOI 10.1038/s41524-024-01249-y. – SCO ; WOS CC ; SCIE.
In: *npj Computational Materials* [elektronický dokument] . – Londýn (Veľká Británia) : Springer Nature. Nature Publishing Group. – ISSN (online) 2057-3960. – Roč. 10, č. 1 (2024), art. no. 68, s. [1-7] [online]
Počet všetkých autorov: 8
[článok]
Lit.: 61
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 11.9 - 2024
SNIP: 2,444 - 2024

SJR: 2,835 - 2024
CiteScore: 16,3 - 2024
AIS: 3.169 - 2024
Kvartil Q:
2024, AIS - Chemistry, physical - Q1; **2024, AIS** - Materials science, multidisciplinary - Q1; **2024, JCI** - Chemistry, physical - Q1; **2024, JCI** - Materials science, multidisciplinary - Q1; **2024, JIF** - Chemistry, physical - Q1; **2024, JIF** - Materials science, multidisciplinary - Q1; **2024, Scimago** - Computer science applications - Q1; **2024, Scimago** - Materials science (miscellaneous) - Q1; **2024, Scimago** - Mechanics of materials - Q1; **2024, Scimago** - Modeling and simulation - Q1

Ohlasy (6):
2025 [01/20] / **DEU** - Temmerman, Wim - Goeminne, Ruben - Rawat, Kuber Singh - Van Speybroeck, Veronique. **Computational Modeling of Reticular Materials: The Past, the Present, and the Future** [elektronický dokument]. DOI 10.1002/adma.202412005 In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 37, č. 52, art. no. 2412005 [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **CHN** - Yin, Chang - Li, Zhenyu - Yang, Jinlong. **Electronic structure calculation methods for surface catalysis** [elektronický dokument]. DOI 10.1360/CSB-2025-5618 In: **Chinese science bulletin**. Peking: Chung-Kuo Hsueh Ysan, 2025, Roč. 70, č. 34, s. 5810-5825 [tlačená forma] [online]. ISSN 0023-074X. ISSN (online) 2095-9419. - SCO ; WOS CC ; SCIE ; OA, s. 5810 - 5829

2025 [01/20] / **GBR** - Poul, Marvin - Huber, Liam - Neugebauer, Jörg. **Automated generation of structure datasets for machine learning potentials and alloys** [elektronický dokument]. DOI 10.1038/s41524-025-01669-4 In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 11, č. 1, art. no. 174 [online]. ISSN (online) 2057-3960. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 174

2025 [01/20] / **USA** - Willman, Jonathan T. - Perriot, Romain - Ticknor, Christopher. **An atomic cluster expansion (ACE) potential for water under extreme conditions** [elektronický dokument]. DOI 10.1063/5.0293523 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 20, art. no. 204306 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 204306

2025 [01/20] / **USA** - Mészáros, Bence Balázs - Szabó, András - Daru, János. **Short-Range Δ-Machine Learning: A Cost-Efficient Strategy to Transfer Chemical Accuracy to Condensed Phase Systems** [elektronický dokument]. DOI 10.1021/acs.jctc.5c00367 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 11, s. 5372-5381 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 5372 - 5381

2025 [01/20] / **GBR** - Vacek, Jaroslav - Vrška, Dávid - Manna, Debashree - Lo, Rabindranath - Hobza, Pavel. **Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches** [elektronický dokument]. DOI 10.1039/D5SC06336A In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 48, s. 23129-23138 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; WOS CC ; CCC ; SCIE ; Nature Index ; OA, s. 23129 - 23138

V3_011: / Grumet, Manuel (Autor) (25%) - Scarpatetti, Clara von (Autor) (25%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (25%) - Egger, David A. (Korešpondenčný autor) (25%): **Delta Machine Learning for Predicting Dielectric Properties and Raman Spectra**. – text, graf. – [recenzované]. – DOI 10.1021/acs.jpcc.4c00886. – SCO ; WOS CC ; SCIE.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 128, č. 15 (2024), s. 6464-6470 [tlačená forma] [online]

Počet všetkých autorov: 4
[článok]
Lit.: 60
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 3.2 - 2024
SNIP: 0,801 - 2024
SJR: 0,914 - 2024
CiteScore: 6,2 - 2024
AIS: 0.690 - 2024
Kvartil Q:
2024, AIS - Chemistry, physical - Q2; **2024, AIS** - Materials science, multidisciplinary - Q2; **2024, AIS** - Nanoscience & nanotechnology - Q2; **2024, JCI** - Chemistry, physical - Q3; **2024, JCI** - Materials science, multidisciplinary - Q3; **2024, JCI** - Nanoscience & nanotechnology - Q3; **2024, JIF** - Chemistry, physical - Q3; **2024, JIF** - Materials science, multidisciplinary - Q3; **2024, JIF** - Nanoscience & nanotechnology - Q3; **2024, Scimago** - Electronic, optical and magnetic materials - Q1; **2024, Scimago** - Energy (miscellaneous) - Q2; **2024, Scimago** - Nanoscience and nanotechnology - Q2; **2024, Scimago** - Physical and theoretical chemistry - Q1; **2024, Scimago** - Surfaces, coatings and films - Q1

Ohlasy (15):
2025 [01/20] / **GBR** - Han, Bowen - Okabe, Ryotaro - Chotrattanapituk, Abhijatmedhi - Cheng, Mouyang - Li, Mingda - Cheng, Yongqiang. **AI-powered exploration of molecular vibrations, phonons, and spectroscopy** [elektronický dokument]. DOI 10.1039/d4dd00353e In: **Digital Discovery**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 4, č. 3, s. 584-624. ISSN (online) 2635098X. - SCO ; WOS CC ; ESCI ; OA, s. 584 - 624

2025 [01/20] / **USA** - Yang, Mengxin - Wang, Shiyu - Song, Guanli - Cheng, Longhui - Ren, Haisheng. **CBH-BDC Enhanced Δ-ML for Predicting the Accurate Standard Enthalpy of Formation** [elektronický dokument]. DOI 10.1021/acs.jpca.5c03134 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2025, Roč. 129, č. 26, s. 5901-5910 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO ; CCC ; WOS CC ; SCIE, s. 5901 - 5910

2025 [01/20] / **GBR** - Frolov, Dmitry - Ibraev, Ilya - Sedov, Igor. **Quantum chemical properties of chlorinated polycyclic aromatic hydrocarbons for delta machine learning** [elektronický dokument]. DOI 10.1038/s41597-025-05383-0 In: **Scientific data**. London: Springer Nature. Nature Publishing Group, 2025, Roč. 12, č. 1, art. no. 1059 [online]. ISSN (online) 2052-4463. - SCO ; WOS CC ; SCIE ; OA, s. art. no. 1059

2025 [01/20] / **GBR** - Pérez-Soto, Raúl - Popescu, Mihai V. - Kumar, Sabari - A. Gomes, Leticia - Lee, Changyeob - Shore, Elijah - Lopez, Steven A. - Paton, Robert S. - Kim, Seonah. **A fragment based approach towards curating, comparing and developing machine learning models applied in photochemistry** [elektronický dokument]. DOI 10.1039/d5sc05615b In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 46, s. 21874-21886 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 21874 - 21886

2025 [01/20] / **USA** - Ben Mahmoud, Chiheb - Rosset, Louise A.M. - Yates, Jonathan R. - Deringer, Volker L. **Graph-neural-network predictions of solid-state NMR parameters in silica from spherical tensor decomposition** [elektronický dokument]. DOI 10.1063/5.0274240 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 2, art. no. 024118 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 024118

2025 [01/20] / **USA** - Paul, Atanu - Grinberg, Ilya. **Atomistic Approach for Modeling of Polarizability and Raman Scattering of Water Clusters and Liquid Water** [elektronický dokument]. DOI 10.1021/acs.jctc.5c00452 In: **Journal of**

Chemical Theory and Computation. Washington: American Chemical Society, 2025, Roč. 21, č. 14, s. 7017-7026 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 7017 - 7026

2025 [01/20] / **USA** - Chaudhry, Imran - Bronson, Mark J. - Jensen, Lasse. **Δ-Machine Learning of Polarizability Tensors Using a Dipole Interaction Model** [elektronický dokument]. DOI 10.1021/acs.jctc.5c00752 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 14, s. 7040-7050 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 7040 - 7050

2025 [01/20] / **GBR** - Malenfant-Thuot, Olivier - Shaaban Kabakibo, Dounia - Blackburn, Simon - Rousseau, Bruno - Côté, Michel. **Large scale Raman spectrum calculations in defective 2D materials using deep learning** [elektronický dokument]. DOI 10.1088/1361-648X/ada106 In: **Journal of Physics**: Condensed Matter. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 37, č. 11, art. no. 115903 [tlačená forma] [online]. ISSN 0953-8984. ISSN (online) 1361-648X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 115903

2025 [01/20] / **USA** - Bandyopadhyay, Prasanta - Isamura, Bienfait K. - Popelier, Paul L.A. **Accurate prediction of electron correlation energies of topological atoms by delta learning from the Müller approximation** [elektronický dokument]. DOI 10.1063/5.0252228 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 162, č. 7, art. no. 074102 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 074102

2025 [01/20] / **USA** - Omodemi, Oluwaseun - Kaledin, Martina. **First-Principles Molecular Dynamics Simulations of Infrared and Raman Vibrational Spectra of H5O2+, D5O2+, DH4O2+, and D4HO2+from 50 to 300 K** [elektronický dokument]. DOI 10.1021/acs.jpca.5c05184 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2025, Roč. 129, č. 43, s. 9921-9929 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 9921 - 9929

2025 [01/20] / **GBR** - Allec, Sarah I. - Ziatdinov, Maxim. **Active and transfer learning with partially Bayesian neural networks for materials and chemicals** [elektronický dokument]. DOI 10.1039/d5dd00027k In: **Digital Discovery**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 4, č. 5, s. 1284-1297. ISSN (online) 2635098X. - SCO ; WOS CC ; ESCI ; OA, s. 1284 - 1297

2025 [01/20] / **USA** - Paul, Atanu - Samala, Nagaprasad Reddy - Grinberg, Ilya. **Generalized bond polarizability model for more accurate atomistic modeling of Raman spectra** [elektronický dokument]. DOI 10.1063/5.0246427 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 162, č. 5, art. no. 054711 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 054711

2024 [01/20] / **USA** - Sowa, Jakub K. - Rossky, Peter J. **A Bond-Based Machine Learning Model for Molecular Polarizabilities and A Priori Raman Spectra** [elektronický dokument]. DOI 10.1021/acs.jctc.4c01086 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 22, s. 10071-10079 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 10071 - 10079

2024 [01/20] / **GBR** - Chen, Yongxing - Long, Peng - Liu, Bin - Wang, Yi - Wang, Junlong - Ma, Tian - Wei, Huilin - Kang, Yue - Ji, Haining. **Development and application of Few-shot learning methods in materials science under data scarcity** [elektronický dokument]. DOI 10.1039/d4ta06452f In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2024, Roč. 12, č. 44, s. 30249-30268 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 30249 - 30268

2024 [01/20] / **USA** - Berger, Ethan - Niemelä, Juha - Lampela, Outi - Juffer, André H. - Komsa, Hannu Pekka. **Raman Spectra of Amino Acids and Peptides from Machine Learning Polarizabilities** [elektronický dokument]. DOI 10.1021/acs.jcim.4c00077 In: **Journal of Chemical Information and Modeling**. Washington, D.C.: American Chemical

Society, 2024, Roč. 64, č. 12, s. 4601-4612 [tlačená forma] [online]. ISSN 1549-9596. ISSN (online) 1549-960X. - SCO ; WOS CC, s. 4601 - 4612

V3_012: / Gešvandtnerová, Monika (Autor) [Interný doktorand] [UKOPRCFZ] (25%) - Raybaud, Pascal (Autor) (25%) - Chizallet, Celine (Autor) (25%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (25%): **Importance of Dynamic Effects in Isobutanol to Linear Butene Conversion Catalyzed by Acid Zeolites Assessed by AIMD**. – text, ilustr., graf., tab. – [recenzované]. – DOI 10.1021/acscatal.4c00736. – SCO ; WOS CC ; CCC.
In: *ACS Catalysis* [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN (online) 2155-5435. – Nordic list level 2 - 2021 koeficient 6. – Nordic list level 1 - 2022 koeficient 4. – Roč. 14, č. 10 (2024), s. 7478-7491 [online]
Počet všetkých autorov: 4
[článok]
Lit.: 63
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 13.1 - 2024
SNIP: 2,031 - 2024
SJR: 3,782 - 2024
CiteScore: 19,5 - 2024
AIS: 2.833 - 2024
Kvartil Q:
2024, AIS - Chemistry, physical - Q1; **2024, JCI** - Chemistry, physical - Q1; **2024, JIF** - Chemistry, physical - Q1; **2024, Scimago** - Catalysis - Q1; **2024, Scimago** - Chemistry (miscellaneous) - Q1

Ohlasy (5):
2025 [01/20] / **DEU** - Göltl, Florian. **Exploring Quality Criteria for the Computational Modeling of Heterogeneous Catalysts** [elektronický dokument]. DOI 10.1002/cphc.202401123 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 11, art. no. e202401123 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC, s.

2025 [01/20] / **GBR** - Kolganov, Alexander A. - Pidko, Evgeny A. **Computational Chemistry in Zeolite Catalysis**. DOI 10.1039/9781837676859-00312 In: **Zeolites from Fundamentals to Emerging Applications**. London: The Royal Society of Chemistry, 2025, s. 312-369 [tlačená forma] [online]. ISBN [9781837675456, 9781837676859]. - SCO, s. 312 - 369

2025 [01/20] / **NLD** - Song, Hanyao - Guo, Xiaoyu - He, Yingluo - Li, Yanbing - Liu, Guangbo - Yang, Guohui - Tsubaki, Noritatsu. **Highly selective and efficient isobutanol dehydration over WO3-modified mesoporous alumina catalysts** [elektronický dokument]. DOI 10.1016/j.cattod.2025.115476 In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 460, art. no. 115476 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 115476

2025 [01/20] / **USA** - Cheng, Xiaoxue - Li, Chenchen - Ling, Qifan - Wang, Xinyu - Zhang, Jiangshan - Zhang, Kexin - Kasetsomboon, Naparat - Wang, Shuang - Jiang, Ding. **Solvent-Mediated and Interface-Engineered Ni/NiO@CN Catalysis for the Conversion of Vanillin into Drug Intermediates Vanillonitrile** [elektronický dokument]. DOI 10.1021/acssuschemeng.5c06559 In: **ACS Sustainable Chemistry & Engineering**. Washington: American Chemical Society, 2025, Roč. 13, č. 39, s. 16554-16566 [online]. ISSN (online) 2168-0485. - SCO ; CCC ; WOS CC ; SCIE, s. 16554 - 16566

2024 [01/20] / **GBR** - Kumar, Dipanshu - Sauer, Joachim - Airi, Alessia - Bordiga, Silvia - Galimberti, Daria Ruth. **Assignment of IR spectra of ethanol at Brønsted sites of H-ZSM-5 to monomer adsorption using a Fermi resonance model** [elektronický dokument]. DOI 10.1039/d4cp03861d In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2024, Roč. 27, č. 1, s. 550-563 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 550 - 563

V3_013: / Jaykhedkar, Namrata (Autor) [Interný doktorand] [UKOPRCAM] (25%) - Bystrický, Roman (Autor) [UKOPRCAM] (25%) - Sýkora, Milan (Autor) [UKOPRCAM] (25%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (25%): **Investigating the role of dispersion corrections and anharmonic effects on the phase transition in SrZrS3: A systematic analysis from AIMD free energy calculations**. – text, graf., obr. – [recenzované]. – DOI 10.1063/5.0185319. – MEDLINE® ; CCC ; WOS CC ; SCO.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 160, č. 1 (2024), art. no. 014710 , s. [1-10] [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 84
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 3.1 - 2024
SNIP: 0,911 - 2024
SJR: 0,819 - 2024
CiteScore: 5,3 - 2024
Nordic List: 1 - 2024
AIS: 0.908 - 2024
Kvartil Q:
2024, AIS - Chemistry, physical - Q2; **2024, AIS** - Physics, atomic, molecular & chemical - Q1; **2024, JCI** - Chemistry, physical - Q2; **2024, JCI** - Physics, atomic, molecular & chemical - Q1; **2024, JIF** - Chemistry, physical - Q3; **2024, JIF** - Physics, atomic, molecular & chemical - Q2; **2024, Scimago** - Medicine (miscellaneous) - Q2; **2024, Scimago** - Physical and theoretical chemistry - Q1; **2024, Scimago** - Physics and astronomy (miscellaneous) - Q1

Ohlasy (1):
2025 [01/20] / **GBR** - Banerjee, Swastika - Tkatchenko, Alexandre. **Non-local interactions determine local structure and lithium diffusion in solid electrolytes** [elektronický dokument]. DOI 10.1038/s41467-025-56662-8 In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 16, č. 1, art. no. 1672 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 1672

V3_014: / Rey, Jerome (Autor) (20%) - Badawi, Michael (Autor) (20%) - Rocca, Dario (Autor) (20%) - Chizallet, Céline (Autor) (20%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (20%): **Machine learning thermodynamic perturbation theory offers accurate activation free energies at the RPA level for alkene isomerization in zeolites**. – text, graf., tab. – [recenzované]. – DOI 10.1039/d4cy00548a. – SCO ; WOS CC ; SCIE.
In: *Catalysis Science and Technology* [textový dokument (print)] [elektronický dokument] . – Cambridge (Veľká Británia) : The Royal Society of Chemistry. – ISSN 2044-4753. – ISSN (online) 2044-4761. – Roč. 14, č. 18 (2024), s. 5314-5323 [tlačená forma] [online]

Počet všetkých autorov: 5
[článok]
Lit.: 85
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 4.3 - 2024
SNIP: 0,812 - 2024
SJR: 1,026 - 2024
CiteScore: 8 - 2024
AIS: 0.805 - 2024
Kvartil Q:
2024, AIS - Chemistry, physical - Q2; **2024, JCI** - Chemistry, physical - Q2; **2024, JIF** - Chemistry, physical - Q2; **2024, Scimago** - Catalysis - Q2

Ohlasy (3):
2025 [01/20] / **DEU** - Bocus, Massimo - Vandenhaute, Sander - Van Speybroeck, Veronique. **The Operando Nature of Isobutene Adsorbed in Zeolite H−SSZ−13 Unraveled by Machine Learning Potentials Beyond DFT Accuracy** [elektronický dokument]. DOI 10.1002/anie.202413637 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 64, č. 1, art. no. e202413637 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **DEU** - Huber, Philipp - Plessow, Philipp N. **Accurate and Efficient Description of Acidic Zeolites with Plane-Wave Density Functional Theory Using Range-Separated Hybrid Functionals** [elektronický dokument]. DOI 10.1002/cphc.202500147 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 15, art. no. e202500147 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **USA** - Liang, Yu Hsuan - Zhang, Xing - Chan, Garnet Kin Lic - Berkelbach, Timothy C. - Ye, Hong Zhou. **Efficient Implementation of the Random Phase Approximation with Domain-Based Local Pair Natural Orbitals** [elektronický dokument]. DOI 10.1021/acs.jctc.4c01540 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 6, s. 2918-2927 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 2918 - 2927

V3_015: / O'Leary, Willis (Autor) (16.67%) - Grumet, Manuel (Autor) (16.666%) - Kaiser, Waldemar (Autor) (16.666%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (16.666%) - Rupp, Jennifer L. M. (Korešpondenčný autor) (16.666%) - Egger, David A. (Korešpondenčný autor) (16.666%): **Rapid Characterization of Point Defects in Solid-State Ion Conductors Using Raman Spectroscopy, Machine-Learning Force Fields, and Atomic Raman Tensors**. – text, graf., tab. – [recenzované]. – DOI 10.1021/jacs.4c07812. – SCO ; WOS CC ; SCIE ; Nature Index.
In: *Journal of the American Chemical Society* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 0002-7863. – ISSN 1943-2984. – ISSN (online) 1520-5126. – Roč. 146, č. 39 (2024), s. 26863-26876 [tlačená forma] [CD-ROM] [online]
Počet všetkých autorov: 6
[článok]
Lit.: 127
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]

Indikátor časopisu:
IF: 15.7 - 2024
SNIP: 2,61 - 2024
SJR: 5,554 - 2024
CiteScore: 22,5 - 2024
AIS: 3.808 - 2024
Kvartil Q:
2024, AIS - Chemistry, multidisciplinary - Q1; **2024, JCI** - Chemistry, multidisciplinary - Q1; **2024, JIF** - Chemistry, multidisciplinary - Q1; **2024, Scimago** - Biochemistry - Q1; **2024, Scimago** - Catalysis - Q1; **2024, Scimago** - Chemistry (miscellaneous) - Q1; **2024, Scimago** - Colloid and surface chemistry - Q1

Ohlasy (4):
2025 [01/20] / **USA** - Park, Heung Sik - Cheon, Semin - Kwon, Yong Jun - Kang, Minho - Suh, Jeonghun - Park, Sang Youn - Yang, Yongsoo - Yang, Chan Ho. **Quantitative Control of Oxygen Non-Stoichiometry and Negative Raman Chemical Shift During Topotactic Phase Transition in a Ca-Doped BiFeO3 Thin-Film** [elektronický dokument]. DOI 10.1002/advs.202502439 In: **Advanced Science**. Hoboken: John Wiley & Sons. Wiley Blackwell, 2025, Roč. 12, č. 40, art. no. e02439 [online]. ISSN (online) 2198-3844. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. e02439

2025 [01/20] / **USA** - He, Yucheng - Huang, Yan - Xiao, Hengyu - Jiang, Jun - Wang, Song. **Infrared spectroscopy–based zero-shot learning for identifying reaction intermediates in unseen systems** [elektronický dokument]. DOI 10.1073/pnas.2506834122 In: **Proceedings of the National Academy of Sciences of the United States of America**. Washington: National Academy of Sciences of the United States of America, 2025, Roč. 122, č. 32, art. no. 2506834122 [tlačená forma] [online]. ISSN 0027-8424. ISSN (online) 1091-6490. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **GBR** - Fang, Yilin - Wang, Jintao - Jiang, Zexin - Gao, Ning - Zhou, Rui - Guo, Wanxiao - Wang, Tao - Li, Rusong. **First-principles study of the properties of plutonium oxides and their interfaces based on machine learning** [elektronický dokument]. DOI 10.1016/j.mtcomm.2025.112372 In: **Materials today. Communications.**. Oxford: Elsevier, 2025, Roč. 45, art. no. 112372 [online]. ISSN (online) 2352-4928. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 112372

2025 [01/20] / **USA** - Kumar, Neelesh - Najimu, Musa O. - Cho, Yoon Jin - Gilliard-AbdulAziz, Kandis Leslie - Nikolla, Eranda - Wu, Zili - Wachs, Israel E. **Probing Surface/Bulk Structural Chemistry of Key Components of Solid Oxide Electrochemical Cells with In Situ/Operando Raman Spectroscopy** [elektronický dokument]. DOI 10.1021/acs.chemrev.5c00222 In: **Chemical Reviews**. Washington: American Chemical Society, 2025, Roč. 125, č. 18, s. 8921-8955 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 8921 - 8955

V3_016: / Rey, Jerome (Autor) (20%) - Chizallet, Céline (Korešpondenčný autor) (20%) - Rocca, Dario (Autor) (20%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (20%) - Badawi, Michael (Korešpondenčný autor) (20%): **Reference-Quality Free Energy Barriers in Catalysis from Machine Learning Thermodynamic Perturbation Theory**. – text, graf. – [recenzované]. – DOI 10.1002/anie.202312392. – SCO ; WOS CC ; SCIE ; Nature Index.
In: *Angewandte Chemie* [textový dokument (print)] [elektronický dokument] : International Edition. – Weinheim (Nemecko) : John Wiley & Sons. Wiley-VCH. – ISSN 1433-7851. – ISSN (online) 1521-3773. – Roč. 63, č. 6 (2024), art no. e202312392, s. [1-8] [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 78
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]

Indikátor časopisu:
IF: 17.0 - 2024
SNIP: 2,465 - 2024
SJR: 5,55 - 2024
CiteScore: 27,6 - 2024
AIS: 3.524 - 2024
Kvartil Q:
2024, AIS - Chemistry, multidisciplinary - Q1; **2024, JCI** - Chemistry, multidisciplinary - Q1; **2024, JIF** - Chemistry, multidisciplinary - Q1; **2024, Scimago** - Catalysis - Q1; **2024, Scimago** - Chemistry (miscellaneous) - Q1

Ohlasy (5):
2025 [01/20] / **USA** - Plessow, Philipp N. **Anharmonic Adsorption Free Energies and Apparent Activation Barriers for Mobile Reactants Based on Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jctc.5c01100 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 17, s. 8518-8532 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 8518 - 8532

2025 [01/20] / **DEU** - Bocus, Massimo - Vandenhaute, Sander - Van Speybroeck, Veronique. **The Operando Nature of Isobutene Adsorbed in Zeolite H−SSZ−13 Unraveled by Machine Learning Potentials Beyond DFT Accuracy** [elektronický dokument]. DOI 10.1002/anie.202413637 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 64, č. 1, art. no. e202413637 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **DEU** - Huber, Philipp - Plessow, Philipp N. **Accurate and Efficient Description of Acidic Zeolites with Plane-Wave Density Functional Theory Using Range-Separated Hybrid Functionals** [elektronický dokument]. DOI 10.1002/cphc.202500147 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 15, art. no. e202500147 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **GBR** - Wu, Hongjing - Xie, Shangkang - Li, Xurui - Zhao, Yashuang - Guo, Lixia - Tu, Xinlei - Feng, Feiyu - Wang, Qingtao - Lyu, Jinghui - Feng, Feng - Lu, Chunshan - Fang, Rubo - Zhang, Qunfeng - Li, Xiaonian. **Machine learning for catalysis: Bridging data-driven discovery and physical insight** [elektronický dokument]. DOI 10.1016/j.mtchem.2025.103051 In: **Materials today. Chemistry**. Londýn: Elsevier, 2025, Roč. 49, art. no. 103051 [online]. ISSN (online) 2468-5194. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 103051

2024 [01/20] / **USA** - Sauer, Joachim. **The future of computational catalysis** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115482 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 433, art. no. 115482 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s.

V3_017: / Vrška, Dávid (Autor) [Interný doktorand] [UKOPRCFZ] (33.334%) - Pitoňák, Michal (Autor) [UKOPRCFZ] (33.333%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (33.333%): **Thermodynamics of the gas-phase dimerization of formic acid: Fully anharmonic finite temperature calculations at the CCSD(T) and many DFT levels**. – text, ilustr., graf., tab. – [recenzované]. – DOI 10.1063/5.0205448. – MEDLINE® ; WOS CC ; SCO ; CCC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 160, č. 17 (2024), art. no. 174106, s. [1-9] [tlačená forma] [online]
Počet všetkých autorov: 3

[článok]
Lit.: 85
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 3.1 - 2024
SNIP: 0,911 - 2024
SJR: 0,819 - 2024
CiteScore: 5,3 - 2024
Nordic List: 1 - 2024
AIS: 0.908 - 2024
Kvartil Q:
2024, AIS - Chemistry, physical - Q2; **2024, AIS** - Physics, atomic, molecular & chemical - Q1; **2024, JCI** - Chemistry, physical - Q2; **2024, JCI** - Physics, atomic, molecular & chemical - Q1; **2024, JIF** - Chemistry, physical - Q3; **2024, JIF** - Physics, atomic, molecular & chemical - Q2; **2024, Scimago** - Medicine (miscellaneous) - Q2; **2024, Scimago** - Physical and theoretical chemistry - Q1; **2024, Scimago** - Physics and astronomy (miscellaneous) - Q1

Ohlasy (1):
2025 [01/20] / **GBR** - Ylivainio, Kim Jonas - Sufyan, Ali - Andreas Larsson, J. **A quantitative relationship between electron localization function and the strength of physical binding** [elektronický dokument]. DOI 10.1088/1361-648X/adcc70 In: **Journal of Physics**: Condensed Matter. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 37, č. 20, art. no. 205502 [tlačená forma] [online]. ISSN 0953-8984. ISSN (online) 1361-648X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 205502

2025 - spolu : **4**

V3_018: / Skladanová, Katarína (Autor) [Interný doktorand] [UKOPRCFZ] (50%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (50%): **Adsorption of benzene on graphene studied by ML-accelerated ab initio molecular dynamics simulations**. – text, graf., tab. – [recenzované]. – DOI 10.1063/5.0280806. – SCO ; SCIE ; CCC ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 163 (2025), art. no. 124703 , s. [1-10] [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
Lit.: 74
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 3,7 - 2025
SNIP: 0,962 - 2025
SJR: 0,877 - 2025
CiteScore: 5,3 - 2025
Nordic List: 1 - 2025
AIS: 0,946 - 2025
Kvartil Q:
2025, AIS - Chemistry, physical - Q2; **2025, AIS** - Physics, atomic, molecular & chemical - Q1; **2025, JCI** - Chemistry, physical - Q2; **2025, JCI** - Physics, atomic, molecular & chemical - Q1; **2025, JIF** - Chemistry, physical - Q3; **2025, JIF** - Physics, atomic, molecular & chemical - Q1; **2025, Scimago** - Medicine (miscellaneous) - Q2; **2025, Scimago** - Physical and

theoretical chemistry - Q1; **2025, Scimago** - Physics and astronomy (miscellaneous) - Q1

V3_019: / Huynh, Thanh-Nam (Autor) (20%) - Mounssef Jr, Bassim (Autor) (20%) - Sharapa, Dmitry I. (Autor) (20%) - Studt, Felix (Korešpondenčný autor) (20%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (20%): **Anharmonic Correction to the Adsorption Free Energy of Oxygen-Containing Intermediates on Pt(111) by Machine-Learned Force Field-Based Thermodynamic Integrations**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1021/acs.jpcc.5c03465. – CCC ; WOS CC ; SCO ; SCIE.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 129, č. 37 (2025), s. 16742-16755 [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 58
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 3,4 - 2025
SNIP: 0,747 - 2025
SJR: 0,82 - 2025
CiteScore: 5,7 - 2025
Nordic List: 1 - 2025
AIS: 0,625 - 2025
Kvartil Q:
2025, AIS - Chemistry, physical - Q2; **2025, AIS** - Materials science, multidisciplinary - Q2; **2025, AIS** - Nanoscience & nanotechnology - Q2; **2025, JCI** - Chemistry, physical - Q3; **2025, JCI** - Materials science, multidisciplinary - Q3; **2025, JCI** - Nanoscience & nanotechnology - Q3; **2025, JIF** - Chemistry, physical - Q3; **2025, JIF** - Materials science, multidisciplinary - Q3; **2025, JIF** - Nanoscience & nanotechnology - Q3; **2025, Scimago** - Electronic, optical and magnetic materials - Q1; **2025, Scimago** - Energy (miscellaneous) - Q2; **2025, Scimago** - Nanoscience and nanotechnology - Q2; **2025, Scimago** - Physical and theoretical chemistry - Q1; **2025, Scimago** - Surfaces, coatings and films - Q1

Ohlasy (1):
2025 [01/20] / **USA** - Smith, Logan E. - Briega-Martos, Valentín - Yang, Yao - Hammes-Schiffer, Sharon. **Isotope Effects for Water at Pt(111) Computed with Nuclear−Electronic Orbital Theory** [elektronický dokument]. DOI 10.1021/acs.jpclett.5c03144 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2025, Roč. 16, s. 13054-13061 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC ; SCIE, s. 13054 - 13061

V3_020: / Gešvandtnerová, Monika (Autor) [Interný doktorand] [UKOPRCFZ] (25%) - Chizallet, Celine (Autor) (25%) - Badawi, Michael (Autor) (25%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (25%): **Linear versus branched products: How dynamical effects influence the transformations of isobutanol catalyzed by acidic zeolites**. – text, graf., tab. – [recenzované]. – DOI 10.1016/j.jcat.2025.116501. – CCC ; WOS CC ; SCO.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – Roč. 453 (2025), art. no. 116501, s. [1-10] [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 41
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:

IF: 6 - 2025
SNIP: 1,119 - 2025
SJR: 1,293 - 2025
CiteScore: 10,4 - 2025
AIS: 1,095 - 2025
Kvartil Q:
2025, AIS - Chemistry, physical - Q2; **2025, AIS** - Engineering, chemical - Q1; **2025, JCI** - Chemistry, physical - Q2; **2025, JCI** - Engineering, chemical - Q1; **2025, JIF** - Chemistry, physical - Q2; **2025, JIF** - Engineering, chemical - Q1; **2025, Scimago** - Catalysis - Q1; **2025, Scimago** - Physical and theoretical chemistry - Q1

V3_021: / Egger, David A. (Korešpondenčný autor) (33.334%) - Grumet, Manuel (Autor) (33.333%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (33.333%): **Machine Learning Accelerates Raman Computations from Molecular**. – text, graf., obr. – [recenzované]. – DOI 10.1063/5.0287358. – SCIE ; CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 163, č. 12 (2025), art. no. 120901, s. [1-11] [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 113
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
IF: 3,7 - 2025
SNIP: 0,962 - 2025
SJR: 0,877 - 2025
CiteScore: 5,3 - 2025
Nordic List: 1 - 2025
AIS: 0,946 - 2025
Kvartil Q:
2025, AIS - Chemistry, physical - Q2; **2025, AIS** - Physics, atomic, molecular & chemical - Q1; **2025, JCI** - Chemistry, physical - Q2; **2025, JCI** - Physics, atomic, molecular & chemical - Q1; **2025, JIF** - Chemistry, physical - Q3; **2025, JIF** - Physics, atomic, molecular & chemical - Q1; **2025, Scimago** - Medicine (miscellaneous) - Q2; **2025, Scimago** - Physical and theoretical chemistry - Q1; **2025, Scimago** - Physics and astronomy (miscellaneous) - Q1

2026 - **spolu** : **1**

V3_022: / Skladanová, Katarína (Autor) [Interný doktorand] [UKOPRCFZ] (14.29%) - Gešvandtnerová, Monika (Autor) [Skrátený úväzok] [UKOPRCFZ] (14.285%) - Sola, Emeline (Autor) (14.285%) - Chizallet, Céline (Autor) (14.285%) - Pigeon, Thomas (Autor) (14.285%) - Badawi, Michael (Autor) (14.285%) - Bučko, Tomáš (Korešpondenčný autor) [UKOPRCFZ] (14.285%): **Isobutanol dehydration catalyzed by bridging OH groups at the (100) surface of ferrierite: From static DFT to machine learning accelerated molecular dynamics**. – text, graf., tab. – [recenzované]. – DOI 10.1016/j.jcat.2026.117024. – CCC ; WOS CC ; SCO ; SCIE.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – Roč. 461 (2026), art. no. 117024, s. [1-15] [tlačená forma] [online]
Počet všetkých autorov: 7
[článok]
Lit.: 65
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]

Indikátor časopisu:
IF: 6.5 - 2024
SNIP: 1,243 - 2024
SJR: 1,558 - 2024
CiteScore: 10,9 - 2024
AIS: 1.234 - 2024
Kvartil Q:
2024, AIS - Chemistry, physical - Q2; **2024, AIS** - Engineering, chemical - Q1; **2024, JCI** - Chemistry, physical - Q2; **2024, JCI** - Engineering, chemical - Q1; **2024, JIF** - Chemistry, physical - Q2; **2024, JIF** - Engineering, chemical - Q1; **2024, Scimago** - Catalysis - Q1; **2024, Scimago** - Physical and theoretical chemistry - Q1

Výstup záznamov do roku 2021

ADC - Vedecké práce v zahraničných karentovaných časopisoch - spolu : **72**

2002 - spolu : **1**

ADC_001: / Bučko, Tomáš (Autor) (25%) - Benco, Ľubomír (Autor) (25%) - Demuth, Th. (Autor) (25%) - Hafner, Jürgen (Autor) (25%): **Ab initio density functional investigation of the (001) surface of mordenite**. – CCC ; SCO ; WOS CC ; SCIE.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 117, č. 15 (2002), s. 7295-7305 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 3199
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (35):
2025 [01/20] / **USA** - Deng, Xiangyang - Ma, Huan - Liu, Jinjia - Guo, Wenping - Wen, Xiaodong. **A Benchmark Framework for the Fast and Reliable Evaluation of Zeolite Surface Stability** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c05668 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 50, s. 21975-21984 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 21975 - 21984

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Ithisuphalap, Kemakorn - Nolen, Michelle A. - Monroe, Hanna - Kwon, Stephanie. **Kinetic, Spectroscopic, and Theoretical Study of Toluene Alkylation with Ethylene on Acidic Mordenite Zeolite** [elektronický dokument]. DOI 10.1021/acscatal.3c04315 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 24, s. 16012-16031 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 16012 - 16031

2023 [01/20] / **USA** - Jarrin, Thomas - de Bruin, Theodorus - Chizallet, Céline. **Stability and Acidity of Sites at the External Surface and at Point Defects of Faujasite** [elektronický dokument]. DOI 10.1002/cctc.202201302 In:

ChemCatChem: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2023, Roč. 15, č. 3, art. no. e202201302 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Xiong, Zhiping - Qi, Guodong - Zhan, Ensheng - Chu, Yueying - Xu, Jun - Wei, Jiake - Ta, Na - Hao, Aijing - Zhou, Yan - Deng, Feng - Shen, Wenjie. **Experimental identification of the active sites over a plate-like mordenite for the carbonylation of dimethyl ether** [elektronický dokument]. DOI 10.1016/j.chempr.2022.09.002 In: **Chem**. Cambridge, MA: Elsevier. Cell Press, 2023, Roč. 9, č. 1, s. 76-92 [tlačená forma] [online]. ISSN 2451-9308. ISSN (online) 2451-9294. - SCO ; CCC ; WOS CC, s. 76 - 92

2022 [01/20] / **USA** - Chizallet, Céline. **Achievements and Expectations in the Field of Computational Heterogeneous Catalysis in an Innovation Context** [elektronický dokument]. DOI 10.1007/s11244-021-01489-y In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, s. 69-81 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 69 - 81

2021 [01/20] / **NLD** - Rubes, M. - Koudelkova, E. - Vaculik, J. - Trachta, M. - Bulanek, R. - Bludsky, O. **Analysis of the BAS OH band reveals a non-statistical incorporation of Al into the MOR framework** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2021, Roč. 317, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 110994

2020 [01/12] / **USA** - Khalil, I. - Celis-Cornejo, C.M. - Thomas, K. - Bazin, P. - Travert, A. - Perez-Martinez, D.J. - Baldovino-Medrano, V.G. - Paul, J.F. - Mauge, F. **In Situ IR-ATR Study of the Interaction of Nitrogen Heteroaromatic Compounds with HY Zeolites: Experimental and Theoretical Approaches** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2020, Roč. 12, č. 4, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 1095 - 1108

2020 [01/12] / **USA** - Treps, L. - Gomez, A. - Bruin, T.D. - Chizallet, C. **Environment, Stability and Acidity of External Surface Sites of Silicalite-1 and ZSM-5 Micro and Nano Slabs, Sheets, and Crystals** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 5, [online]. ISSN (online) 2155-5435. - SCO, s. 3297 - 3312

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2019 [01/12] / **NLD** - Thang, H.V. - Vaculik, J. - Prech, J. - Kubu, M. - Cejka, J. - Nachtigall, P. - Bulanek, R. - Grajciar, L. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2019, Roč. 282, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 121 - 132

2019 [01/12] / Hernandez-Tamargo, C. - Roldan, A. - de Leeuw, N.H. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 13. - SCIE ; WOS CC, s. 7604 - 7614

2019 [01/12] / **USA** - Gutierrez-Acebo, E. - Rey, J. - Bouchy, C. - Schuurman, Y. - Chizallet, C. **In: ACS Catalysis**. Washington: American Chemical Society, 2019, Roč. 9, č. 3, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1692 - 1704

2019 [01/12] / **USA** - Carnahan, S.L. - Lampkin, B.J. - Naik, P. - Hanrahan, M.P. - Slowing, I.I. - VanVeller, B. - Wu, G. - Rossini, A.J. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2019, Roč. 141, č. 1, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 441 - 450

2019 [01/12] / **NLD** - Vorontsov, A.V. - Valdes, H. - Smirniotis, P.G. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2019, Roč. 1166, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. Art. No. UNSP

2018 [01/12] / **NLD** - Ho, T.V. - Nachtigall, P. - Grajciar, L. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2018, Roč. 304, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 12 - 21

2018 [01/12] / **NLD** - Chen, F.Y. - Zhang, L.J. - Feng, G. - Wang, X.W. - Zhang, R.B. - Liu, J.W. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 433, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 627 - 638

2017 [01/12] / **USA** - Rey, J. - Raybaud, P. - Chizallet, C. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2176 - 2185

2017 [01/12] / **USA** - Lari, G.M. - Chen, Z.P. - Mondelli, C. - Perez-Ramirez, J. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2195 - 2202

2017 [01/12] / **USA** - Zhai, D. - Liu, Y. - Zheng, H.M. - Zhao, L. - Gao, J.S. - Xu, C.M. - Shen, B.J. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 352, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 627 - 637

2016 [01/12] / Perez-Beltran, S. - Balbuena, P.B. - Ramirez-Caballero, G.E. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 32. - SCIE ; WOS CC, s. 18105 - 18114

2016 [01/12] / Pedevilla, P. - Cox, S.J. - Slater, B. - Michaelides, A. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 12. - SCIE ; WOS CC, s. 6704 - 6713

2016 [01/12] / **NLD** - Hernandez-Tamargo, C.E. - Roldan, A. - de Leeuw, N.H. **In: Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2016, Roč. 237, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCIE ; WOS CC, s. 192 - 203

2014 [01/12] / Lukyanov, D.B. - Vazhnova, T. - Cherkasov, N. - Casci, J.L. - Birtill, J.J. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 41. - SCIE ; WOS CC, s. 23918 - 23929

2014 [01/12] / **USA** - Shi, C.M. - Qin, H.W. - Zhang, Y.J. - Hu, J.F. - Ju, L. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2014, Roč. 115, č. 5, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 053907

2013 [01/12] / Vazhnova, T. - Lukyanov, D.B. **In: Analytical Chemistry**: an Indian Journal, 2013, Roč. 85, č. 23. - SCIE ; WOS CC, s. 11291 - 11296

2012 [01/12] / **USA** - Huo, H. - Peng, L.M. - Gan, Z.H. - Grey, C.P. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2012, Roč. 134, č. 23, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 9708 - 9720

2011 [01/12] / **USA** - Leydier, F. - Chizallet, C. - Chaumonnot, A. - Digne, M. - Soyer, E. - Quoineaud, A.A. - Costa, D. - Raybaud, P. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2011, Roč. 284, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 215 - 229

2010 [01/12] / **NLD** - Gil, B. - Kosova, G. - Cejka, J. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2010, Roč. 129, č. 1-2, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 256 - 266

2010 [01/12] / **USA** - Hansen, N. - Kerber, T. - Sauer, J. - Bell, A.T. - Keil, F.J. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2010, Roč. 132, č. 33, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 11525 - 11538

2008 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kuznicki, S.M. - Kovalenko, A. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 17. - SCIE ; WOS CC, s. 6794 - 6810

2007 [01/12] / Lercher, J.A. - Jentys, A. **In: Introduction to Zeolite Science and Practice**, 2007, Roč. 168. - SCIE ; WOS CC, s. 435 - 476

2006 [01/12] / Sholl, D.S. **In: Chemical Modelling: Applications and Theory**, 2006, Roč. 4. - SCIE ; WOS CC, s. 108 - 160

2005 [01/12] / **NLD** - Nikolakis, V. **In: Current Opinion in Colloid & Interface Science**. Amsterdam: Elsevier, 2005, Roč. 10, č. 5-6, [tlačená forma]. ISSN 1359-0294. - SCIE ; WOS CC, s. 203 - 210

2004 [01/12] / **USA** - Astala, R. - Auerbach, S.M. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2004, Roč. 126, č. 6, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 1843 - 1848

2003 - **spolu** : **1**

ADC_002: / Bučko, Tomáš (Autor) (33.333%) - Benco, Ľubomír (Autor) (33.334%) - Hafner, Jürgen (Autor) (33.333%): **Defect sites at the (001) surface of mordenite: An ab initio study**. – CCC ; SCO ; WOS CC ; SCIE.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 118, č. 18 (2003), s. 8437-8445 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 39142
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (21):
2025 [01/20] / **USA** - Deng, Xiangyang - Ma, Huan - Liu, Jinjia - Guo, Wenping - Wen, Xiaodong. **A Benchmark Framework for the Fast and Reliable Evaluation of Zeolite Surface Stability** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c05668 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 50, s. 21975-21984 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 21975 - 21984

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s.

6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **GBR** - Prodinger, Sebastian - Berdiell, Izar Capel - Cordero-Lanzac, Tomas - Bygdnes, Odd Reidar - Solemsli, Bjørn Gading - Kvande, Karoline - Arstad, Bjørnar - Beato, Pablo - Olsbye, Unni - Svelle, Stian. **Cation-induced speciation of port-size during mordenite zeolite synthesis** [elektronický dokument]. DOI 10.1039/d3ta03444e In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2023, Roč. 11, č. 40, s. 21884-21894 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 21884 - 21894

2022 [01/20] / **USA** - Huber, P. - Studt, F. - Plessow, P.N. **Reactivity of Surface Lewis and Bronsted Acid Sites in Zeolite Catalysis: A Computational Case Study of DME Synthesis Using H-SSZ-13** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 13. - SCO, s. 5896 - 5905

2022 [01/20] / **USA** - Chizallet, Céline. **Achievements and Expectations in the Field of Computational Heterogeneous Catalysis in an Innovation Context** [elektronický dokument]. DOI 10.1007/s11244-021-01489-y In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, s. 69-81 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 69 - 81

2021 [01/20] / **NLD** - Jaime-Acuna, O.E. - San-Juan Farfan, R.E. - Villavicencio, H. - Herrera, M. - Raymond, Herrera O. **Photoluminescence up-conversion and cathodoluminescence in quaternary Cdx Zny Ogamma Sdelta nanoparticles embedded on zeolite** [elektronický dokument] In: **Journal of Physics and Chemistry of Solids**: an International Journal. Amsterdam: Elsevier, 2021, Roč. 153, [tlačená forma]. ISSN (online) 0022-3697. - SCO, s. Art. No. 110004

2020 [01/12] / **USA** - Treps, L. - Gomez, A. - Bruin, T.D. - Chizallet, C. **Environment, Stability and Acidity of External Surface Sites of Silicalite-1 and ZSM-5 Micro and Nano Slabs, Sheets, and Crystals** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 5, [online]. ISSN (online) 2155-5435. - SCO, s. 3297 - 3312

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2019 [01/12] / Hernandez-Tamargo, C. - Roldan, A. - de Leeuw, N.H. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 13. - SCIE ; WOS CC, s. 7604 - 7614

2017 [01/12] / **NLD** - Hernandez-Tamargo, C.E. - Roldan, A. - de Leeuw, N.H. **In: Molecular Catalysis**. Amsterdam: Elsevier, 2017, Roč. 433, [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCIE ; WOS CC, s. 334 - 345

2017 [01/12] / **USA** - Lari, G.M. - Chen, Z.P. - Mondelli, C. - Perez-Ramirez, J. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2195 - 2202

2017 [01/12] / **USA** - Rey, J. - Raybaud, P. - Chizallet, C. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2176 - 2185

2017 [01/12] / **USA** - Zhai, D. - Liu, Y. - Zheng, H.M. - Zhao, L. - Gao, J.S. - Xu, C.M. - Shen, B.J. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 352, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 627 - 637

2016 [01/12] / **NLD** - Hernandez-Tamargo, C.E. - Roldan, A. - de Leeuw, N.H. **In: Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2016, Roč. 237, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCIE ; WOS CC, s. 192 - 203

2012 [01/12] / Skarlis, S.A. - Berthout, D. - Nicolle, A. - Dujardin, C. - Granger, P. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 15. - SCIE ; WOS CC, s. 8437 - 8448

2012 [01/12] / Zokaie, M. - Olsbye, U. - Lillerud, K.P. - Swang, O. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 13. - SCIE ; WOS CC, s. 7255 - 7259

2012 [01/12] / **NLD** - Gutierrez, L. - Boix, A. - Decolatti, H. - Solt, H. - Lonyi, F. - Miro, E. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2012, Roč. 163, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 307 - 320

2012 [01/12] / **GBR** - Nachtigall, P. - Delgado, M.R. - Nachtigallova, D. - Arean, C.O. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2012, Roč. 14, č. 5, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 1552 - 1569

2008 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kuznicki, S.M. - Kovalenko, A. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 17. - SCIE ; WOS CC, s. 6794 - 6810

2006 [01/12] / Sholl, D.S. **In: Chemical Modelling: Applications and Theory**, 2006, Roč. 4. - SCIE ; WOS CC, s. 108 - 160

2006 [01/12] / **USA** - Bromley, S.T. - Moreira, I.D.P.R. - Illas, F. - Wojdel, J.C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2006, Roč. 73, č. 13, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 134202

2004 - spolu : **3**

ADC_003: / Benco, Ľubomír (Autor) (25%) - Bučko, Tomáš (Autor) (25%) - Hafner, Jürgen (Autor) (25%) - Toulhoat, H. (Autor) (25%): **Ab initio simulation of Lewis sites in mordenite and comparative study of the strength of active sites via CO adsorption**. – text. – CCC ; SCO ; WOS CC ; SCIE.
In: *Journal of Physical Chemistry B* [textový dokument (print)] [elektronický dokument] : Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. – Washington (USA) : American Chemical Society. – ISSN 1520-6106. – ISSN (online) 1520-5207. – ISSN (zrušené) 1089-5647. – Roč. 108, č. 36 (2004), s. 13656-13666 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 69
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (46):
2025 [01/20] / **USA** - Zhao, Shengying - Geng, Hailun - Zhang, Tao - Tan, Minghui - Yao, Jie - Fan, Jiaqi - Zhou, Zhongbo - Shang, Tiecheng - Shen, Wenzhong - Yang, Guohui - Tsubaki, Noritatsu. **Molecular Regulator in Mordenite-Catalyzed DME Carbonylation: Eliminating Deactivation Sites, Modulating Microenvironments, and Enhancing Activity** [elektronický dokument]. DOI 10.1021/acscatal.5c00739 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, č. 11, s. 9150-9157 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 9150 - 9157

2025 [01/20] / **GBR** - Kolganov, Alexander A. - Pidko, Evgeny A. **Computational Chemistry in Zeolite Catalysis**. DOI 10.1039/9781837676859-00312 In: **Zeolites from Fundamentals to Emerging Applications**. London: The Royal Society of Chemistry, 2025, s. 312-369 [tlačená forma] [online]. ISBN [9781837675456, 9781837676859]. - SCO, s. 312 - 369

2025 [01/20] / **USA** - Bekele, Bereket Tassew - Gounder, Rajamani. **Extra-Framework Aluminum Moieties Occluded within Zeolite Micropores Strengthen Dispersive Stabilization of Confined Alkanes and Carbocationic Transition States** [elektronický dokument]. DOI 10.1021/acscatal.5c06537 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, s. 21100-21114 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE, s. 21100 - 21114

2024 [01/20] / **GBR** - Jiang, Yiming - Hao, Aijing - Zhan, Ensheng - Beato, Pablo - Chen, Siyu - Fan, Fengtao - Li, Can. **Boron-incorporated nanosized SUZ-4 zeolite for DME carbonylation** [elektronický dokument]. DOI 10.1039/d4cc00952e In: **Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 60, č. 44, s. 5727-5730 [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCO ; CCC ; WOS CC, s. 5727 - 5730

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2022 [01/20] / **CHN** - Zhao, S.-Y. - Geng, H.-L. - Xu, B. - Wu, X.-M. - Tan, M.-H. - Yang, G.-H. - Tan, Y.-S. **Research progress on mordenite catalyzed carbonylation of dimethyl ether** In: **Ranliao Huaxue Xuebao/Journal of Fuel Chemistry and Technology**, 2022, Roč. 50, č. 2. ISSN 02532409. - SCO, s. 166 - 179

2022 [01/20] / **NLD** - Lawrence, A.S. - Sivakumar, B. - Dhakshinamoorthy, A. **Detecting Lewis acid sites in metal-organic frameworks by density functional theory** [elektronický dokument] In: **Molecular Catalysis**. Amsterdam: Elsevier, 2022, Roč. 517, [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO, s. Art. No. 112042

2021 [01/20] / **USA** - Palagin, D. - Sushkevich, V.L. - Knorpp, A.J. - Ranocchiari, M. - van, Bokhoven J.A. **Mapping Vibrational Spectra to the Structures of Copper Species in Zeolites Based on Calculated Stretching Frequencies of Adsorbed Nitrogen and Carbon Monoxides** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 22. - SCO, s. 12094 - 12106

2021 [01/20] / **GBR** - Zhang, D. - Liu, H. - Ling, L. - Zhang, H. - Zhang, R. - Liu, P. - Wang, B. **The effect of introducing Ga on the ZSM-5-catalyzed methanol to aromatics reaction: Taking methylcyclopentane to benzene as an example** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 18, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 10988 - 11003

2021 [01/20] / **NLD** - Hessou, E.P. - Jabraoui, H. - Khalil, I. - Dziurla, M.-A. - Badawi, M. **Ab initio screening of zeolite Y formulations for efficient adsorption of thiophene in presence of benzene** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 541, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 148515

2020 [01/12] / **NLD** - Jung, H.S. - Ham, H. - Bae, J.W. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 339, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 79 - 85

2020 [01/12] / **GBR** - Newton, M.A. - Knorpp, A.J. - Sushkevich, V.L. - Palagin, D. - Van Bokhoven, J.A. **Active sites and mechanisms in the direct conversion of methane to methanol using Cu in zeolitic hosts: A critical examination** [elektronický dokument] In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 49, č. 5,

[tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO, s. 1449 - 1486

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2020 [01/12] / **CHE** - Chen, X. - Li, R. - Yan, H. - Liu, Y. - Yang, C. **A dft study for catalytic deoxygenation of methyl butyrate on a lewis acid site of zsm-5 zeolite** In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 10, č. 11, [online]. ISSN 2073-4344. - SCO, s. Art. No. 1233

2019 [01/12] / Rejmak, P. - Datka, J. - Broclawik, E. **In: : International journal of quantum chemistry,** 2019, Roč. 119, č. 9. - SCIE ; WOS CC, s. Art. No. 25873

2019 [01/12] / Jabraoui, H. - Khalil, I. - Lebegue, S. - Badawi, M. **In: Molecular Systems Design & Engineering**, 2019, Roč. 4, č. 4. - SCIE ; WOS CC, s. 882 - 892

2018 [01/12] / Kim, J. - Ham, H. - Jung, H.S. - Wang, Y. - He, Y.L. - Tsubaki, N. - Cho, S.J. - Han, G.Y. - Bae, J.W. **In: Catalysis Science & Technology**, 2018, Roč. 8, č. 12. - SCIE ; WOS CC, s. 3060 - 3072

2018 [01/12] / **NLD** - Ham, H. - Kim, J. - Lim, J.H. - Sung, W.C. - Lee, D.H. - Bae, J.W. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2018, Roč. 303, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 93 - 99

2018 [01/12] / Rejmak, P. - Datka, J. - Broclawik, E. **In: : International journal of quantum chemistry,** 2018, Roč. 118, č. 16. - SCIE ; WOS CC, s. Art. No. 25625

2017 [01/12] / **USA** - Reule, A.A.C. - Sawada, J.A. - Semagina, N. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 349, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 98 - 109

2017 [01/12] / **USA** - Lari, G.M. - Chen, Z.P. - Mondelli, C. - Perez-Ramirez, J. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2195 - 2202

2017 [01/12] / **USA** - Rey, J. - Raybaud, P. - Chizallet, C. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2176 - 2185

2017 [01/12] / **GBR** - Hu, Z.G. - Zhao, D. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 29, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 4066 - 4081

2017 [01/12] / **GBR** - Rybakov, A.A. - Larin, A.V. - Vercauteren, D.P. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 31, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 20930 - 20940

2016 [01/12] / **USA** - Cybulskis, V.J. - Harris, J.W. - Zvinevich, Y. - Ribeiro, F.H. - Gounder, R. **In: Review of scientific instruments**. Woodbury: American Institute of Physics. AIP Publishing, 2016, Roč. 87, č. 10, [tlačená forma] [online]. ISSN 0034-6748. ISSN (online) 1089-7623. - SCIE ; WOS CC, s. Art. No. 103101

2016 [01/12] / **NLD** - Cherkasov, N. - Vazhnova, T. - Lukyanov, D.B. **In: Vibrational Spectroscopy**. Amsterdam: Elsevier, 2016, Roč. 83, [tlačená forma] [online]. ISSN 0924-2031. ISSN (online) 1873-3697. - SCIE ; WOS CC, s. 170 - 179

2016 [01/12] / **USA** - Silaghi, M.C. - Chizallet, C. - Sauer, J. - Raybaud, P. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2016, Roč. 339, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 242 - 255

2015 [01/12] / **USA** - Odoh, S.O. - Cramer, C.J. - Truhlar, D.G. - Gagliardi, L. **In: Chemical Reviews**. Washington: American Chemical Society, 2015, Roč. 115, č. 12, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 6051 - 6111

2015 [01/12] / **DEU** - Wang, H.F. - Zhao, L.M. - Xu, W.B. - Wang, S.P. - Ding, Q.Y. - Lu, X.Q. - Guo, W.Y. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2015, Roč. 134, č. 3, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 31

2015 [01/12] / Wang, S.R. - Guo, W.W. - Zhu, L.J. - Wang, H.X. - Qiu, K.Z. - Cen, K.F. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 1. - SCIE ; WOS CC, s. 524 - 533

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2014 [01/12] / **USA** - Larin, A.V. - Zhidomirov, G.M. **In: Journal of Structural Chemistry**. New York: Pleiades Publishing, 2014, Roč. 55, č. 4, [tlačená forma] [online]. ISSN 0022-4766. ISSN (online) 1573-8779. - SCIE ; WOS CC, s. 583 - 594

2012 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kovalenko, A. **Industrial Applications of Molecular Simulations** [textový dokument (print)] . Boca Raton: CRC Press, 2012. 1 vyd. - BKCI-S ; WOS CC, s. 203 - 230

2010 [01/12] / Liu, D.H. - Zhong, C.L. **In: Journal of Physical Chemistry Letters**, 2010, Roč. 1, č. 1. - SCIE ; WOS CC, s. 97 - 101

2010 [01/12] / Fang, H.J. - Zheng, A.M. - Chu, Y.Y. - Deng, F. **In: Journal of Physical Chemistry C**, 2010, Roč. 114, č. 29. - SCIE ; WOS CC, s. 12711 - 12718

2009 [01/12] / **GBR** - Kumashiro, R. - Fujie, K. - Kondo, A. - Mori, T. - Nagao, M. - Kobayashi, H. - Kuroda, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2009, Roč. 11, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 5041 - 5051

2009 [01/12] / **USA** - Gounder, R. - Iglesia, E. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2009, Roč. 131, č. 5, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 1958 - 1971

2008 [01/12] / **USA** - Sun, K.J. - Su, W.G. - Fan, F.T. - Feng, Z.C. - Jansen, T.A.P.J. - van Santen, R.A. - Li, C. **In: Journal of Physical Chemistry A**, 2008, Roč. 112, č. 6. - SCIE ; WOS CC, s. 1352 - 1358

2008 [01/12] / **USA** - Bailey, C.L. - Wander, A. - Mukhopadhyay, S. - Searle, B.G. - Harrison, N.M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2008, Roč. 128, č. 22, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 224703

2008 [01/12] / Sun, K.J. - Fan, F.T. - Xia, H.A. - Feng, Z.C. - Li, W.X. - Li, C. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 41. - SCIE ; WOS CC, s. 16036 - 16041

2008 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kuznicki, S.M. - Kovalenko, A. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 17. - SCIE ; WOS CC, s. 943 - 951

2007 [01/12] / **GBR** - Arean, C.O. - Nachtigallova, D. - Nachtigall, P. - Garrone, E. - Delgado, M.R. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2007, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 1421 - 1436

2007 [01/12] / **USA** - Joshi, Y.V. - Thomson, K.T. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2007, Roč. 246, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 249 - 265

2007 [01/12] / **USA** - Cheung, P. - Bhan, A. - Sunley, G.J. - Law, D.J. - Iglesia, E. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2007, Roč. 245, č. 1, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 110 - 123

2006 [01/12] / Cheung, P. - Bhan, A. - Sunley, G.J. - Iglesia, E. **In: Angewandte Chemie-International Edition**, 2006, Roč. 45, č. 10. - SCIE ; WOS CC, s. 1617 - 1620

2005 [01/12] / **NLD** - Elanany, M. - Koyama, M. - Kubo, M. - Broclawik, E. - Miyamoto, A. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2005, Roč. 246, č. 1-3, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 96 - 101

ADC_004: / Bučko, Tomáš (Autor) (33.333%) - Hafner, Jürgen (Autor) (33.334%) - Benco, Ľubomír (Autor) (33.333%): **Active sites for the vapor phase Beckmann rearrangement over mordenite: An ab initio study**. – CCC ; SCO ; WOS CC.
In: *The Journal of Physical Chemistry A* [textový dokument (print)] [elektronický dokument] : Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. – Washington (USA) : American Chemical Society. – ISSN 1089-5639. – ISSN (online) 1520-5215. – Roč. 108, č. 51 (2004), s. 11388-11397 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (37):
2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Zhang, Peng - Wang, Xiaoxu - Yi, Xianfeng - Ou, Qi - Xia, Changjiu - Peng, Xinxin - Zhang, Xiaoxin - Zheng, Anmin - Luo, Yibin - Shu, Xingtian. **Modulating the Microenvironment of Silanols in Pure-Silicon Zeolites for**

Boosting Vapor-phase Beckmann Rearrangement of Cyclohexanone Oxime [elektronický dokument]. DOI 10.1021/acsami.3c07016 In: **ACS applied materials and interfaces**. Washington: American Chemical Society, 2023, Roč. 15, č. 34, s. 40478-40487 [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCO ; WOS CC, s. 40478 - 40487

2023 [01/20] / **CHE** - Zhang, Peng - Yi, Xianfeng - Xia, Changjiu - Peng, Xinxin - Zhang, Shuai - Li, Chengxiang - Zheng, Anmin - Zhang, Xiaoxin - Luo, Yibin - Cui, Lifeng - Yu, Fuhong - Shu, Xingtian. **Rational construction of multiple hollow silicalite-1 zeolite with enhanced quasi acidity for robust vapor-phase Beckmann rearrangement** [elektronický dokument]. DOI 10.1007/s12274-022-5305-3 In: **Nano research**. Peking: Tshinghua Press, 2023, Roč. 16, č. 5, s. 7958-7966 [tlačená forma] [online]. ISSN 1998-0124. ISSN (online) 1998-0000. - SCO ; WOS CC, s. 7958 - 7966

2023 [01/20] / **NLD** - Liu, Weiliao - Jiang, Zhaobin - Pei, Jiansong - Xu, Xinlian - Liu, Xiaolong - Tian, Zhen - Cheng, Youwei - Li, Xi - Wang, Lijun. **Deactivation kinetic study on vapor phase Beckmann rearrangement of cyclohexanone oxime and design of the multi-layer inclined channel bionic reactor** [elektronický dokument]. DOI 10.1016/j.cherd.2022.12.031 In: **Chemical Engineering Research and Design**: a Publication of the Institution of Chemical Engineers: an Official Journal of the European Federation of Chemical Engineering. Amsterdam: Elsevier, 2023, Roč. 190, s. 476-488 [tlačená forma]. ISSN 0263-8762. ISSN (online) 1744-3563. ISSN (zrušené) 0734-9769. - SCO ; CCC ; WOS CC, s. 476 - 488

2022 [01/20] / **NLD** - Jin, X. - Peng, R. - Tong, W. - Yin, J. - Xu, H. - Wu, P. **Investigation of the active centers and structural modifications for TS-1 in catalyzing the Beckmann rearrangement** [elektronický dokument] In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2022, Roč. 405-406, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO, s. 193 - 202

2021 [01/20] / **GBR** - Peng, R. - Wan, Z. - Lv, H. - Guan, Y. - Xu, H. - Wu, P. **Al-Modified Ti-MOR as a robust catalyst for cyclohexanone ammoximation with enhanced anti-corrosion performance** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 22, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 7287 - 7299

2020 [01/12] / **GBR** - Zhang, L. - Wang, S. - Shi, D. - Qin, Z. - Wang, P. - Wang, G. - Li, J. - Dong, M. - Fan, W. - Wang, J. **Methanol to olefins over H-RUB-13 zeolite: Regulation of framework aluminum siting and acid density and their relationship to the catalytic performance** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 10, č. 6, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 1835 - 1847

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2019 [01/12] / Chu, Y.Y. - Lo, A.Y. - Wang, C. - Deng, F. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 25. - SCIE ; WOS CC, s. 15503 - 15512

2019 [01/12] / Chapman, S. - O'Malley, A.J. - Miletto, I. - Carravetta, M. - Cox, P. - Gianotti, E. - Marchese, L. - Parker, S.F. - Raja, R. **In: Chemistry-A European Journal**, 2019, Roč. 25, č. 42. - SCIE ; WOS CC, s. 9938 - 9947

2018 [01/12] / **USA** - Wang, S. - Wang, P.F. - Qin, Z.F. - Chen, Y.Y. - Dong, M. - Li, J.F. - Zhang, K. - Liu, P. - Wang, J.G. - Fang, W.B. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 6, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 5485 - 5505

2017 [01/12] / **USA** - Puziy, A.M. - Kochkin, Y.N. - Poddubnaya, O.I. - Tsyba, M.M. **In: Adsorption science & technology**. Thousand Oaks: SAGE Publications, 2017, Roč. 35, č. 5-6, [tlačená forma] [online]. ISSN 0263-6174. ISSN

(online) 2048-4038. - SCIE ; WOS CC, s. 473 - 481

2017 [01/12] / **USA** - Potter, M.E. - Chapman, S. - O'Malley, A.J. - Levy, A. - Carravetta, M. - Mezza, T.M. - Parker, S.F. - Raja, R. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 11, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 1897 - 1900

2017 [01/12] / Chu, Y.Y. - Li, G.C. - Huang, L. - Yi, X.F. - Xia, H.Q. - Zheng, A.M. - Deng, F. **In: Catalysis Science & Technology**, 2017, Roč. 7, č. 12. - SCIE ; WOS CC, s. 2512 - 2523

2016 [01/12] / **GBR** - Maronna, M.M. - Kruissink, E.C. - Parton, R.F. - Soulimani, F. - Weckhuysen, B.M. - Hoelderich, W.F. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 32, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 22636 - 22646

2016 [01/12] / **USA** - Maronna, M.M. - Kruissink, E.C. - Tinge, J.T. - Agar, D.W. - Hoelderich, W.F. **In: Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2016, Roč. 55, č. 5, [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCIE ; WOS CC, s. 1202 - 1214

2015 [01/12] / **NLD** - Meng, X.J. - Yu, Q.J. - Gao, Y.N. - Zhang, Q. - Li, C.Y. - Cui, Q.K. **In: Catalysis Communications**. Amsterdam: Elsevier, 2015, Roč. 61, [tlačená forma]. ISSN 1566-7367. ISSN (online) 1873-3905. - SCIE ; WOS CC, s. 67 - 71

2014 [01/12] / Kumar, R. - Chowdhury, B. **In: Industrial and Engineering Chemistry Research**, 2014, Roč. 53, č. 43. - SCIE ; WOS CC, s. 16587 - 16599

2011 [01/12] / Ikeshoji, T. **In: Journal of the Japan Petroleum Institute**, 2011, Roč. 54, č. 3, [tlačená forma]. ISSN 1346-8804. ISSN (online) 1349-273X. - SCIE ; WOS CC, s. 159 - 167

2010 [01/12] / **GBR** - Lezcano-Gonzalez, I. - Vidal-Moya, A. - Boronat, M. - Blasco, T. - Corma, A. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 24, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 6396 - 6403

2010 [01/12] / **NLD** - Cesana, A. - Palmery, S. - Buzzoni, R. - Spano, G. - Rivetti, F. - Carnelli, L. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2010, Roč. 154, č. 3-4, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 264 - 270

2009 [01/12] / **GBR** - Fernandez, A.B. - Lezcano-Gonzalez, I. - Boronat, M. - Blasco, T. - Corma, A. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2009, Roč. 11, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 5134 - 5141

2009 [01/12] / **GBR** - Sirijaraensre, J. - Limtrakul, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2009, Roč. 11, č. 3, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 578 - 585

2008 [01/12] / **USA** - Marthala, V.R.R. - Rabl, S. - Huang, J. - Rezai, S.A.S. - Thomas, B. - Hunger, M. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2008, Roč. 257, č. 1, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 134 - 141

2007 [01/12] / Catlow, R. - Bell, R. - Cora, F. - Slater, B. **In: Introduction to Zeolite Science and Practice**, 2007, Roč. 168. - SCIE ; WOS CC, s. 659 - 700

2007 [01/12] / **USA** - Fernandez, A.B. - Lezcano-Gonzalez, I. - Boronat, M. - Blasco, T. - Corma, A. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2007, Roč. 249, č. 1, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 116 - 119

2007 [01/12] / **CHE** - Thomas, B. - Prathapan, S. - Sugunan, S. **In: Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2007, Roč. 133, č. 1-3, [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCIE ; WOS CC, s. 59 - 68

2007 [01/12] / Zhang, Z. - Xing, J.P. - Li, J. - Yang, X.G. **In: Journal of Molecular Catalysis A-Chemical**, 2007, Roč. 275, č. 1-2. - SCIE ; WOS CC, s. 36 - 46

2007 [01/12] / Hunger, M. **In: Chemie Ingenieur Technik**: Verfahrenstechnik, technische Chemie, Apparatewesen, Biotechnologie, 2007, Roč. 79, č. 6, [tlačená forma]. ISSN 0009-286X. ISSN (online) 1522-2640. - SCIE ; WOS CC, s. 781 - 793

2007 [01/12] / **NLD** - Thomas, B. - Prabhu, U.R. - Prathapan, S. - Sugunan, S. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2007, Roč. 102, č. 1-3, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 138 - 150

2006 [01/12] / **USA** - Jardillier, N. - Berthomieu, D. - Goursot, A. - Reveles, J.U. - Koster, A.M. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2006, Roč. 110, č. 37, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 18440 - 18446

2006 [01/12] / **USA** - Fernandez, A.B. - Marinas, A. - Blasco, T. - Fornes, V. - Corma, A. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2006, Roč. 243, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 270 - 277

2006 [01/12] / **USA** - Marthala, V.R.R. - Jiang, Y.J. - Huang, J. - Wang, W. - Glaser, R. - Hunger, M. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2006, Roč. 128, č. 46, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 14812 - 14813

2006 [01/12] / Sirijaraensre, J. - Limtrakul, J. **In: ChemPhysChem**, 2006, Roč. 7, č. 11. - SCIE ; WOS CC, s. 2424 - 2432

2006 [01/12] / Sholl, D.S. **In: Chemical Modelling: Applications and Theory**, 2006, Roč. 4. - SCIE ; WOS CC, s. 108 - 160

2005 [01/12] / **USA** - Yamabe, S. - Tsuchida, N. - Yamazaki, S. **In: Journal of Organic Chemistry**. Washington, D.C.: American Chemical Society. ACS Publications, 2005, Roč. 70, č. 26, [tlačená forma] [online]. ISSN 0022-3263. ISSN (online) 1520-6904. - SCIE ; WOS CC, s. 10638 - 10644

ADC_005: / Bučko, Tomáš (Autor) (33.333%) - Hafner, Jürgen (Autor) (33.334%) - Benco, Ľubomír (Autor) (33.333%): **Adsorption and vibrational spectroscopy of ammonia at mordenite: Ab initio study**. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 120, č. 21 (2004), s. 10263-10277 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]

Lit.: 54158
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
Nordic List: 2 - 2004

Ohlasy (34):

2024 [01/20] / **TUR** - Ergurhan, Orkun - Erdogan, Burcu. **Structural and Ammonia Adsorption Properties of the Gördes Clinoptilolite After HCl Acid Treatment** [elektronický dokument]. DOI 10.35378/gujs.1311206 In: **Gazi University Journal of Science**. Ankara: Gazi Üniversitesi, 2024, Roč. 37, č. 4, s. 1902-1916 [online]. ISSN (online) 2147-1762. - SCO, s. 1902 - 1916

2024 [01/20] / **NLD** - Luque-Álvarez, Ligia A. - Torres-Sempere, Guillermo - Romero-Sarria, Francisca - Bobadilla, Luis F. - Ramírez-Reina, Tomás - Odriozola, José A. **Controlling copper location on exchanged MOR-type aluminosilicate zeolites for methanol carbonylation: In situ/operando IR spectroscopic studies** [elektronický dokument]. DOI 10.1016/j.micromeso.2024.113258 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2024, Roč. 378, art. no. 113258 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO ; CCC ; WOS CC, s. art. no. 113258

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2022 [01/20] / **GBR** - Hahn, C. - Seidel, J. - Mertens, F. - Kureti, S. **Study on the kinetics of the adsorption and desorption of NH3 on Fe/HBEA zeolite** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 12, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 7493 - 7504

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2020 [01/12] / **USA** - Stolz, R.M. - Mahdavi-Shakib, A. - Frederick, B.G. - Mirica, K.A. **Host-Guest Interactions and Redox Activity in Layered Conductive Metal-Organic Frameworks** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2020, Roč. 32, č. 18, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 7639 - 7652

2020 [01/12] / **CHE** - Chen, X. - Li, R. - Yan, H. - Liu, Y. - Yang, C. **A dft study for catalytic deoxygenation of methyl butyrate on a lewis acid site of zsm-5 zeolite** In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 10, č. 11, [online]. ISSN 2073-4344. - SCO, s. Art. No. 1233

2019 [01/12] / **NLD** - Gadekar, S.P. - Lande, M.K. **In: Research on Chemical Intermediates**: An International Journal. Dordrecht: Springer Nature. Springer, 2019, Roč. 45, č. 2, [tlačená forma] [online]. ISSN 0922-6168. ISSN (online) 1568-5675. - SCIE ; WOS CC, s. 237 - 247

2019 [01/12] / Sushkevich, V.L. - Kots, P.A. - Kolyagin, Y.G. - Yakimov, A.V. - Marikutsa, A.V. - Ivanova, I.I. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 9. - SCIE ; WOS CC, s. 5540 - 5548

2019 [01/12] / **NLD** - Jabraoui, H. - Hessou, E.P. - Chibani, S. - Cantrel, L. - Lebegue, S. - Badawi, M. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 485, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 56 - 63

2018 [01/12] / Ardila-Suarez, C. - Perez-Beltran, S. - Ramirez-Caballero, G.E. - Balbuena, P.B. **In: Catalysis Science & Technology**, 2018, Roč. 8, č. 3. - SCIE ; WOS CC, s. 847 - 857

2017 [01/12] / **USA** - Rey, J. - Raybaud, P. - Chizallet, C. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2176 - 2185

2017 [01/12] / **USA** - Lari, G.M. - Chen, Z.P. - Mondelli, C. - Perez-Ramirez, J. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2195 - 2202

2017 [01/12] / **USA** - Zhai, D. - Liu, Y. - Zheng, H.M. - Zhao, L. - Gao, J.S. - Xu, C.M. - Shen, B.J. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 352, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 627 - 637

2016 [01/12] / Perez-Beltran, S. - Balbuena, P.B. - Ramirez-Caballero, G.E. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 32. - SCIE ; WOS CC, s. 18105 - 18114

2016 [01/12] / **GBR** - Xu, Y.Z. - Wang, L.L. - Liu, X. - Zhang, S.Q. - Liu, C.B. - Yan, D.F. - Zeng, Y.X. - Pei, Y. - Liu, Y.T. - Luo, S.L. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2016, Roč. 4, č. 42, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 16524 - 16530

2015 [01/12] / **USA** - Suganuma, S. - Murakami, Y. - Ohyama, J. - Torikai, T. - Okumura, K. - Katada, N. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2015, Roč. 145, č. 10, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 1904 - 1912

2015 [01/12] / Goclon, J. - Kozlowska, M. - Rodziewicz, P. **In: ChemPhysChem**, 2015, Roč. 16, č. 13. - SCIE ; WOS CC, s. 2775 - 2782

2014 [01/12] / **NLD** - Katada, N. - Tamagawa, H. - Niwa, M. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2014, Roč. 226, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 37 - 46

2012 [01/12] / **USA** - Lescouet, T. - Chizallet, C. - Farrusseng, D. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2012, Roč. 4, č. 11, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 1725 - 1728

2011 [01/12] / Zhu, J.F. - Huang, Y.N. **In: Canadian Journal of Chemistry-Revue Canadienne de Chimie**, 2011, Roč. 89, č. 7. - SCIE ; WOS CC, s. 803 - 813

2010 [01/12] / Chizallet, C. - Raybaud, P. **In: ChemPhysChem**, 2010, Roč. 11, č. 1. - SCIE ; WOS CC, s. 105 - 108

2010 [01/12] / Sastre, G. - Katada, N. - Niwa, M. **In: Journal of Physical Chemistry C**, 2010, Roč. 114, č. 36. - SCIE ; WOS CC, s. 15424 - 15431

2009 [01/12] / **USA** - Zhu, J.F. - Huang, Y.N. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2009, Roč. 48, č. 21, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 10186 - 10192

2009 [01/12] / Kassab, E. - Castella-Ventura, M. - Akacem, Y. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 47. - SCIE ; WOS CC, s. 20388 - 20395

2008 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kuznicki, S.M. - Kovalenko, A. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 17. - SCIE ; WOS CC, s. 6794 - 6810

2008 [01/12] / **USA** - Bailey, C.L. - Wander, A. - Mukhopadhyay, S. - Searle, B.G. - Harrison, N.M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2008, Roč. 128, č. 22, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 224703

2008 [01/12] / Castella-Ventura, M. - Akacem, Y. - Kassab, E. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 48. - SCIE ; WOS CC, s. 19045 - 19054

2007 [01/12] / **USA** - Zicovich-Wilson, C.M. - San-Roman, M.L. - Camblor, M.A. - Pascale, F. - Durand-Niconoff, J.S. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2007, Roč. 129, č. 37, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 11512 - 11523

2007 [01/12] / Regli, L. - Lamberti, C. - Busco, C. - Zecchina, A. - Prestipino, C. - Lillerud, K.P. - Zones, S.I. - Bordiga, S. **Structural incorporation of carbon and nitrogen into B-SSZ-13: a spectroscopic and computational studies** In: **From Zeolites to Porous mof Materials: the Anniversary of Materials. Book Series: Studies in Surface Science and Catalysis**, 2007, Roč. 170. - CPCI-S ; WOS CC, s. 585 - 593

2006 [01/12] / Sholl, D.S. **In: Chemical Modelling: Applications and Theory**, 2006, Roč. 4. - SCIE ; WOS CC, s. 108 - 160

2006 [01/12] / **DEU** - Gualtieri, A.F. - Passaglia, E. **In: European Journal of Mineralogy**: an international journal of mineralogy, petrology, geochemistry and related sciences. Stuttgart: E. Schweizerbart'sche Verlagsbuchhandlung, 2006, Roč. 18, č. 3, [tlačená forma]. ISSN 0935-1221. - SCIE ; WOS CC, s. 351 - 359

2006 [01/12] / Elanany, M. - Vercauteren, D.P. - Koyama, M. - Kubo, M. - Selvam, P. - Broclawik, E. - Miyamoto, A. **In: Journal of Molecular Catalysis A-Chemical**, 2006, Roč. 243, č. 1. - SCIE ; WOS CC, s. 1 - 7

2006 [01/12] / Viswanadham, N. - Dixit, L. - Gupta, J.K. - Garg, M.O. **In: Journal of Molecular Catalysis A-Chemical**, 2006, Roč. 258, č. 1-2. - SCIE ; WOS CC, s. 15 - 21

2005 - **spolu** : **5**

ADC_006: / Benco, Ľubomír (Autor) (25%) - Bučko, Tomáš (Autor) (25%) - Hafner, Jürgen (Autor) (25%) - Toulhoat, H. (Autor) (25%): **A density functional theory study of molecular and dissociative adsorption of H-2 on active sites in mordenite**. – text. – CCC ; SCO ; WOS CC.
In: *Journal of Physical Chemistry B* [textový dokument (print)] [elektronický dokument] : Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. – Washington (USA) : American Chemical Society. – ISSN 1520-6106. – ISSN (online) 1520-5207. – ISSN (zrušené) 1089-5647. – Roč. 109, č. 47 (2005), s. 22491-22501 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 43
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (40):

2023 [01/20] / **USA** - Singh, Omvir - Ramteke, Akshata Vijay - Joshi, Bhanu - Vempatapu, Bhanu Prasad - Pant, Kamal Kishore - Ray, Anjan - Sarkar, Bipul. **Sustainable Bioaromatics from Sapium Oil over Encaged AlPO4 Zeolite Material: A Feasibility Study** [elektronický dokument]. DOI 10.1021/acssuschemeng.3c05236 In: **ACS Sustainable Chemistry & Engineering**. Washington: American Chemical Society, 2023, Roč. 11, č. 48, s. 17061-17074 [online]. ISSN (online) 2168-0485. - SCO ; CCC ; WOS CC, s. 17061 - 17074

2022 [01/20] / **GBR** - Randrianandraina, J. - Badawi, M. - Ramseyer, C. - Cardey, B. - Groetz, J.-E. - Perreau, N. - Torrealba-Anzola, F. - Chambelland, C. - Ducret, D. - Grivet, M. **Effect of the water coverage on the interaction of O2 and H2 with the Na-LTA zeolite by first-principles simulations** [elektronický dokument] In: **Inorganic Chemistry Frontiers**. London: The Royal Society of Chemistry, 2022, Roč. 10, č. 2, [tlačená forma] [online]. ISSN 2052-1545. ISSN (online) 2052-1553. - SCO, s. 383 - 395

2022 [01/20] / **NLD** - Diaz Soto, L.J. - Nascimento, M.A.C. **The impact of the zeolite local environment on the stability and spectroscopy features of the (CO, NO, NO2)-Pd-(H-MOR, MOR) systems** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 344, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 112228

2022 [01/20] / **GBR** - Batalha, N. - Comparot, J.-D. - Le Valant, A. - Pinard, L. **In situ FTIR spectroscopy to unravel the bifunctional nature of aromatics hydrogenation synergy on zeolite/metal catalysts** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 12, č. 4, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 1117 - 1129

2019 [01/12] / Mir, M.A. - Bhat, M.A. - Majid, S.A. **In: Encyclopedia of Polymer Applications, Vols I-Iii**, 2019. - SCIE ; WOS CC, s. 2345 - 2366

2019 [01/12] / Jabraoui, H. - Khalil, I. - Lebegue, S. - Badawi, M. **In: Molecular Systems Design & Engineering**, 2019, Roč. 4, č. 4. - SCIE ; WOS CC, s. 882 - 892

2018 [01/12] / **NLD** - Garnica, M.M. - Torres, A.E. - Ramirez-Caballer, G.E. - Balbuena, P.B. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2018, Roč. 265, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 241 - 249

2017 [01/12] / **NLD** - Xu, M.J. - Liu, G.D. - Ao, B.Y. - Chen, P.H. - Hu, W.Y. - Deng, H.Q. **In: Journal of Nuclear Materials**. Amsterdam: Elsevier, 2017, Roč. 493, [tlačená forma] [online]. ISSN 0022-3115. ISSN (online) 1873-4820. - SCIE ; WOS CC, s. 124 - 131

2016 [01/12] / **GBR** - Wang, S.R. - Yin, S. - Guo, W.W. - Liu, Y.C. - Zhu, L.J. - Wang, X.L. **In: New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2016, Roč. 40, č. 7, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCIE ; WOS CC, s. 6460 - 6466

2016 [01/12] / **GBR** - Kozyra, P. - Piskorz, W. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 18, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 12592 - 12603

2016 [01/12] / **NLD** - Vilhena, F.D. - Serra, R.M. - Boix, A.V. - Ferreira, G.B. - Carneiro, J.W.D. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2016, Roč. 1091, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 115 - 121

2016 [01/12] / **USA** - Coperet, C. - Estes, D.P. - Larmier, K. - Searles, K. **In: Chemical Reviews**. Washington: American Chemical Society, 2016, Roč. 116, č. 15, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ;

WOS CC, s. 8463 - 8505

2016 [01/12] / **NLD** - Mir, M.A. - Bhat, M.A. - Naikoo, R.A. - Dipak, P. - Bhat, R.A. - Tomar, R. - Sharma, P.K. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2016, Roč. 233, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 53 - 61

2016 [01/12] / **GBR** - Chibani, S. - Chebbi, M. - Lebegue, S. - Cantrel, L. - Badawi, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 36, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 25574 - 25581

2012 [01/12] / Aleksandrov, H.A. - Shor, E.A.I. - Shor, A.M. - Nasluzov, V.A. - Vayssilov, G.N. - Rosch, N. **In: Soft Materials**, 2012, Roč. 10, č. 1-3. ISSN 1539445X. ISSN (online) 15394468. - SCIE ; WOS CC, s. 216 - 234

2012 [01/12] / Aleksandrov, H.A. - Zdravkova, V.R. - Mihaylov, M.Y. - St Petkov, P. - Vayssilov, G.N. - Hadjiivanov, K.I. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 43. - SCIE ; WOS CC, s. 22823 - 22831

2012 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kovalenko, A. **Industrial Applications of Molecular Simulations** [textový dokument (print)] . Boca Raton: CRC Press, 2012. 1 vyd. - BKCI-S ; WOS CC, s. 203 - 230

2011 [01/12] / **CHN** - Liang, J.M. - Zhang, R.G. - Zhao, Q. - Dong, J.X. - Wang, B.J. - Li, J.P. **In: Acta Physico-Chimica Sinica**. Peking: Peking University Press, 2011, Roč. 27, č. 7. ISSN 1000-6818. ISSN (online) 1872-1508. - SCIE ; WOS CC, s. 1647 - 1653

2011 [01/12] / Aleksandrov, H.A. - Petkov, P.S. - Vayssilov, G.N. **In: Energy & Environmental Science**, 2011, Roč. 4, č. 5. - SCIE ; WOS CC, s. 1879 - 1885

2010 [01/12] / **GBR** - Gabrienko, A.A. - Arzumanov, S.S. - Toktarev, A.V. - Danilova, I.G. - Freude, D. - Stepanov, A.G. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 19, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 5149 - 5155

2010 [01/12] / Solans-Monfort, X. - Sodupe, M. - Eckert, J. **In: Journal of Physical Chemistry C**, 2010, Roč. 114, č. 32. - SCIE ; WOS CC, s. 13926 - 13934

2009 [01/12] / **NLD** - Mikhailov, M.N. - Mishin, I.V. - Kustov, L.M. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2009, Roč. 117, č. 3, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 603 - 608

2009 [01/12] / **RUS** - Lapidus, A.L. - Mikhailov, M.N. - Mishin, I.V. - Dergachev, A.A. - Mordkovich, V.Z. **In: Kinetics and catalysis**. [Moscow]: Nauka Publishers. MAIK Nauka/Interperiodica, 2009, Roč. 50, č. 2, [tlačená forma] [online]. ISSN 0023-1584. ISSN (online) 1608-3210. - SCIE ; WOS CC, s. 247 - 254

2009 [01/12] / Lonyi, F. - Kovacs, A. - Szegedi, A. - Valyon, J. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 24. - SCIE ; WOS CC, s. 10527 - 10540

2009 [01/12] / Vayssilov, G.N. - Aleksandrov, H.A. - Petrova, G.P. - St Petkov, P. **Computational Modelling of Nanoporous Materials** In: **Ordered Porous Solids: Recent Advances and Prospects**. Amsterdam: Elsevier, 2009. - BKCI-S ; WOS CC, s. 211 - 238

2009 [01/12] / **USA** - Lapidus, A.L. - Mikhailov, M.N. - Kustov, L.M. **In: Russian Chemical Bulletin**. [s.l.]: Springer Nature, 2009, Roč. 58, č. 2, [tlačená forma] [online]. ISSN 1066-5285. ISSN (online) 1573-9171. - SCIE ; WOS CC, s. 273 - 279

2008 [01/12] / Anderson, P.A. **In: Solid-State Hydrogen Storage: Materials and Chemistry**, 2008. - SCIE ; WOS CC, s. 223 - 260

2008 [01/12] / **GBR** - Torres, F.J. - Ugliengo, P. - Civalleri, B. - Terentyev, A. - Pisani, C. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2008, Roč. 33, č. 2, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 746 - 754

2008 [01/12] / Civalleri, B. - Torres, F.J. - Demichelis, R. - Terentyev, A. - Ugliengo, P. **In: Ab Initio Simulation of Crystalline Solids: History and Prospects - Contributions in Honor of Cesare Pisani**, 2008, Roč. 117. - SCIE ; WOS CC, s. 12012

2008 [01/12] / Lapidus, A.L. - Mikhailov, M.N. - Dergachev, A.A. - Mishin, I.V. **In: Doklady Physical Chemistry**, 2008, Roč. 422. - SCIE ; WOS CC, s. 240 - 243

2008 [01/12] / Castella-Ventura, M. - Akacem, Y. - Kassab, E. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 48. - SCIE ; WOS CC, s. 19045 - 19054

2008 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kuznicki, S.M. - Kovalenko, A. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 17. - SCIE ; WOS CC, s. 943 - 951

2007 [01/12] / Dinca, M. - Han, W.S. - Liu, Y. - Dailly, A. - Brown, C.M. - Long, J.R. **In: Angewandte Chemie-International Edition**, 2007, Roč. 46, č. 9. - SCIE ; WOS CC, s. 1419 - 1422

2007 [01/12] / Torres, F.J. - Vitillo, J.G. - Civalleri, B. - Ricchiardi, G. - Zecchina, A. **In: Journal of Physical Chemistry C**, 2007, Roč. 111, č. 6. - SCIE ; WOS CC, s. 2505 - 2513

2007 [01/12] / Barbosa, L.A.M.M. - van Santen, R.A. **In: Journal of Physical Chemistry C**, 2007, Roč. 111, č. 23. - SCIE ; WOS CC, s. 8337 - 8348

2007 [01/12] / Thuwachaowsoan, K. - Chotpattananont, D. - Sirivat, A. - Rujiravanit, R. - Schwank, J.W. **In: Materials Science and Engineering B-Solid State Materials for Advanced**, 2007, Roč. 140, č. 1-2. - SCIE ; WOS CC, s. 23 - 30

2007 [01/12] / Nachtigall, P. - Sauer, J. **In: Introduction to Zeolite Science and Practice**, 2007, Roč. 168. - SCIE ; WOS CC, s. 701 - 736

2006 [01/12] / **GBR** - Nachtigall, P. - Garrone, E. - Palomino, G.T. - Delgado, M.R. - Nachtigallova, D. - Arean, C.O. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2006, Roč. 8, č. 19, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 2286 - 2292

2006 [01/12] / **USA** - Torres, F.J. - Civalleri, B. - Pisani, C. - Ugliengo, P. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2006, Roč. 110, č. 21, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 10467 - 10474

2006 [01/12] / Aleksandrov, H.A. - Vayssilov, G.N. - Rosch, N. **In: Journal of Molecular Catalysis A-Chemical**, 2006, Roč. 256, č. 1-2. - SCIE ; WOS CC, s. 149 - 155

ADC_007: / Bučko, Tomáš (Autor) (33.333%) - Hafner, Jürgen (Autor) (33.334%) - Benco, Ľubomír (Autor) (33.333%): **Adsorption and vibrational spectroscopy of CO on mordenite: Ab initio density-functional study**. – text. – CCC ; SCO ; WOS CC ; SCIE.
In: *Journal of Physical Chemistry B* [textový dokument (print)] [elektronický dokument] : Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. – Washington (USA) : American Chemical Society. – ISSN 1520-6106. – ISSN (online) 1520-5207. – ISSN (zrušené) 1089-5647. – Roč. 109, č. 15 (2005), s. 7345-7357 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 63
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (31):
2023 [01/20] / **DEU** - Cárdenas-Galindo, María Guadalupe - Handy, Brent E. **The correspondence of calorimetric studies with DFT simulations in heterogeneous catalysis**. DOI 10.1515/9783110590449-005 In: **Thermal Analysis and Calorimetry: Versatile Techniques**. Berlín: De Gruyter, 2023, s. 159-182. ISBN 9783110590449. ISBN 9783110590432. - SCO, s. 159 - 182

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2021 [01/20] / **USA** - Palagin, D. - Sushkevich, V.L. - Knorpp, A.J. - Ranocchiari, M. - van, Bokhoven J.A. **Mapping Vibrational Spectra to the Structures of Copper Species in Zeolites Based on Calculated Stretching Frequencies of Adsorbed Nitrogen and Carbon Monoxides** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 22. - SCO, s. 12094 - 12106

2021 [01/20] / **USA** - Lyu, S. - Wang, Y. - Qian, J. - Liu, S. - Li, Z. - Zhang, Y. - Wang, L. - Li, J. **Role of Residual CO Molecules in OX-ZEO Relay Catalysis for Syngas Direct Conversion** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2021, Roč. 11, č. 7, [online]. ISSN (online) 2155-5435. - SCO, s. 4278 - 4287

2020 [01/12] / **USA** - Yi, X. - Xiao, Y. - Li, G. - Liu, Z. - Chen, W. - Liu, S.-B. - Zheng, A. **From One to Two: Acidic Proton Spatial Networks in Porous Zeolite Materials** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2020, Roč. 32, č. 3, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 1332 - 1342

2020 [01/12] / **GBR** - Newton, M.A. - Knorpp, A.J. - Sushkevich, V.L. - Palagin, D. - Van Bokhoven, J.A. **Active sites and mechanisms in the direct conversion of methane to methanol using Cu in zeolitic hosts: A critical examination** [elektronický dokument] In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 49, č. 5, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO, s. 1449 - 1486

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2020 [01/12] / Arvidsson, A.A. - Plessow, P.N. - Studt, F. - Hellman, A. **Influence of Acidity on the Methanol-to-DME Reaction in Zeotypes: A First Principles-Based Microkinetic Study** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 27. - SCO, s. 14658 - 14663

2020 [01/12] / **CHE** - Chen, X. - Li, R. - Yan, H. - Liu, Y. - Yang, C. **A dft study for catalytic deoxygenation of methyl butyrate on a lewis acid site of zsm-5 zeolite** In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 10, č. 11, [online]. ISSN 2073-4344. - SCO, s. Art. No. 1233

2019 [01/12] / **NLD** - Jabraoui, H. - Hessou, E.P. - Chibani, S. - Cantrel, L. - Lebegue, S. - Badawi, M. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 485, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 56 - 63

2019 [01/12] / Rejmak, P. - Datka, J. - Broclawik, E. **In: : International journal of quantum chemistry,** 2019, Roč. 119, č. 9. - SCIE ; WOS CC, s. Art. No. 25873

2019 [01/12] / Hoffman, A. - DeLuca, M. - Hibbitts, D. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 11. - SCIE ; WOS CC, s. 6572 - 6585

2018 [01/12] / **NLD** - Gackowski, M. - Tarach, K. - Kuterasinski, L. - Podobinski, J. - Jarczewski, S. - Kustrowski, P. - Datka, J. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2018, Roč. 263, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 282 - 288

2018 [01/12] / Rejmak, P. - Datka, J. - Broclawik, E. **In: : International journal of quantum chemistry,** 2018, Roč. 118, č. 16. - SCIE ; WOS CC, s. Art. No. 25625

2017 [01/12] / **USA** - Lari, G.M. - Chen, Z.P. - Mondelli, C. - Perez-Ramirez, J. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2195 - 2202

2017 [01/12] / **USA** - Rey, J. - Raybaud, P. - Chizallet, C. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 2176 - 2185

2016 [01/12] / **NLD** - Decolatti, H.P. - Gioria, E.G. - Ibarlin, S.N. - Navascues, N. - Irusta, S. - Miro, E.E. - Gutierrez, L.B. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2016, Roč. 222, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 9 - 22

2015 [01/12] / Zhang, Y.W. - Yu, J.Y. - Yeh, Y.H. - Gorte, R.J. - Rangarajan, S. - Mavrikakis, M. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 52. - SCIE ; WOS CC, s. 28970 - 28978

2012 [01/12] / Fang, H.J. - Kamakoti, P. - Zang, J. - Cundy, S. - Paur, C. - Ravikovitch, P.I. - Sholl, D.S. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 19. - SCIE ; WOS CC, s. 10692 - 10701

2012 [01/12] / **DEU** - Morpurgo, S. - Moretti, G. - Bossa, M. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2012, Roč. 131, č. 3, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 1180

2011 [01/12] / Nguyen, N.H. - Le, M.C. **In: : International journal of quantum chemistry,** 2011, Roč. 111, č. 12. - SCIE ; WOS CC, s. 3151 - 3166

2011 [01/12] / Dominguez-Soria, V.D. - Calaminici, P. - Goursot, A. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 14. - SCIE ; WOS CC, s. 6508 - 6512

2010 [01/12] / **GBR** - Corno, M. - Rimola, A. - Bolis, V. - Ugliengo, P. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 24, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online)

1463-9084. - SCIE ; WOS CC, s. 6309 - 6329

2010 [01/12] / Bleken, F. - Svelle, S. - Lillerud, K.P. - Olsbye, U. - Arstad, B. - Swang, O. **In: Journal of Physical Chemistry A**, 2010, Roč. 114, č. 27. - SCIE ; WOS CC, s. 7391 - 7397

2010 [01/12] / **USA** - Chizallet, C. - Lazare, S. - Bazer-Bachi, D. - Bonnier, F. - Lecocq, V. - Soyer, E. - Quoineaud, A.A. - Bats, N. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2010, Roč. 132, č. 35, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 12365 - 12377

2009 [01/12] / **GBR** - Nachtigall, P. - Bludsky, O. - Grajciar, L. - Nachtigallova, D. - Delgado, M.R. - Arean, C.O. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2009, Roč. 11, č. 5, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 791 - 802

2008 [01/12] / Sun, K.J. - Su, W.G. - Fan, F.T. - Feng, Z.C. - Jansen, T.A.P.J. - van Santen, R.A. - Li, C. **In: Journal of Physical Chemistry A**, 2008, Roč. 112, č. 6. - SCIE ; WOS CC, s. 1352 - 1358

2007 [01/12] / Llewellyn, P.L. - Maurin, G. **In: Introduction to Zeolite Science and Practice**, 2007, Roč. 168. - SCIE ; WOS CC, s. 555 - 610

2007 [03/12] / Sauer, J. **Turning Points in Solid-State, Materials and Surface Science** [textový dokument (print)] . [s.n.]: [s.n.], 2007. 1 vyd., s. 441 - 456

2006 [01/12] / Sholl, D.S. **In: Chemical Modelling: Applications and Theory**, 2006, Roč. 4. - SCIE ; WOS CC, s. 108 - 160

2006 [01/12] / **USA** - Rimola, A. - Sodupe, M. - Tosoni, S. - Civalleri, B. - Ugliengo, P. **In: Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2006, Roč. 22, č. 15, [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCIE ; WOS CC, s. 6593 - 6604

ADC_008: / Bučko, Tomáš (Autor) (33.333%) - Hafner, Jürgen (Autor) (33.334%) - Ángyán, János G. (Autor) (33.333%): **Geometry optimization of periodic systems using internal coordinates**. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 122, č. 12 (2005), art. no. 124508, s. [1-1] [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 4635
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
Nordic List: 2 - 2005

Ohlasy (110):
2025 [01/20] / **CHE** - Hirle, Anna - Dörflinger, Philipp - Fuger, Christoph - Gutschka, Christian - Wojcik, Tomasz - Podsednik, Maximilian - Limbeck, Andreas - Kolozsvári, Szilárd - Polcik, Peter - Jerg, Carmen - Riedl, Helmut - Hahn, Rainer. **Mechanical properties of DCMS and HiPIMS deposited Ti1-xMoxB2±z coatings** [elektronický dokument]. DOI 10.1016/j.surfcoat.2025.131750 In: **Surface and Coatings Technology**: an international journal devoted to the science and application of advanced surface treatments for improvement of material properties. Amsterdam: Elsevier, 2025, č. 497, art.

no. 131750 [tlačená forma] [online]. ISSN 0257-8972. ISSN (online) 1879-3347. - SCO ; SCIE ; CCC ; WOS CC, s.

2025 [01/20] / **USA** - Wu, Hanlin - Song, Yuxuan - Gong, Jingjing - Cao, Ziyao - Ouyang, Yawen - Zhang, Jianbing - Zhou, Hao - Ma, Wei Ying - Liu, Jingjing. **A Periodic Bayesian Flow for Material Generation** [elektronický dokument] In: **13th International Conference on Learning Representations (ICLR 2025)**. [s.l.]: International Conference on Learning Representations, 2025, s. 56780-56809 [USB kľúč]. ISBN (online) 9798331320850. - SCO, s. 56780 - 56809

2025 [01/20] / **NLD** - Gutschka, C. - Zauner, L. - Glechner, T. - Holec, D. - Riedl, H. **Metastable AlB2 structured TM-Si-B2±z (TM = Ti, Zr, Hf) solid solutions from first-principles** [elektronický dokument]. DOI 10.1016/j.actamat.2025.120857 In: **Acta Materialia**. Amsterdam: Acta Materialia, 2025, Roč. 289, art. no. 120857 [tlačená forma] [online]. ISSN 1359-6454. ISSN (online) 1873-2453. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 120857

2025 [01/20] / **USA** - Wei, Wei - Gebhardt, Julian - Urban, Daniel F. - Elsässer, Christian. **Influence of interstitial Li on the electronic properties of Lix CsPbI3 for photovoltaic and battery applications** [elektronický dokument]. DOI 10.1103/nvxh-kwzt In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 112, č. 24, art. no. 245103 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; WOS CC ; SCIE ; OA, s. art. no. 245103

2025 [01/20] / **CHE** - Shang, Shun Li - Gao, Michael C. - Liu, Zi Kui. **Temperature-Dependent Mechanical Properties of Ni-Based Concentrated Alloys: Insights from First-Principles Calculations** [elektronický dokument]. DOI 10.1007/s44210-025-00068-0 In: **High Entropy Alloys and Materials**. Cham: Springer Nature, 2025, Roč. 3, č. 2, s. 307-321 [tlačená forma] [online]. ISSN 27315819. ISSN (online) 27315827. - SCO ; OA, s. 307 - 321

2025 [01/20] / **GBR** - de Moura, Geanso M. - de Azevedo, Sérgio Alves - Sambrano, Julio Ricardo - Lage, Mateus R. - dos Santos, Adenilson O. - Stoyanov, Stanislav R. - Andrade-Filho, T. **Optical properties of sarcosine crystal under hydrostatic pressure: a DFT-based computational study** [elektronický dokument]. DOI 10.1039/d5cp01046b In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 26, s. 14042-14053 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 14042 - 14053

2025 [01/20] / **USA** - Bracht, Jean M. - Querne, Mateus B.P. - Da Silva, Juarez L.F. - Lima, Matheus P. **Theoretical Investigation of Stacked Two-Dimensional Transition-Metal Dichalcogenide Materials: The Role of Chemical Species and Number of Monolayers** [elektronický dokument]. DOI 10.1021/acsomega.4c05423 In: **ACS Omega**. Washington: American Chemical Society, 2025, Roč. 10, č. 9, s. 8922-8934 [online]. ISSN (online) 2470-1343. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 8922 - 8934

2025 [01/20] / **GBR** - Lin, Shuang - Shang, Shun Li - Shimanek, John D. - Wang, Yi - Beese, Allison M. - Liu, Zi Kui. **Investigation of ideal shear strength of dilute binary and ternary Ni-based alloys using first-principles calculations, CALPHAD modeling and correlation analysis** [elektronický dokument]. DOI 10.1016/j.mtcomm.2024.111271 In: **Materials today. Communications.**. Oxford: Elsevier, 2025, Roč. 42, art. no. 111271 [online]. ISSN (online) 2352-4928. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 111271

2024 [01/20] / **USA** - Rezende, Armando de - Pantoya, Michelle L. - Tunega, Daniel - Aquino, Adelia J.A. **Prediction of Phase Transition and Ignition Sensitivity of Ammonium Periodate** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c07439 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 5, s. 2205-2214 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 2205 - 2214

2024 [01/20] / **USA** - Franzke, Yannick J. - Schosser, Werner M. - Pauly, Fabian. **Efficient treatment of relativistic effects with periodic density functional methods: Energies, gradients, and stress tensors** [elektronický dokument]. DOI 10.1103/PhysRevB.109.165144 In: **Physical Review B**. College Park: American Institute of Physics. American Physical

Society, 2024, Roč. 109, č. 16, art. no. 165144 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **CHE** - Shang, Shun Li - Gao, Michael C. - Wang, Yi - Li, Jingjing - Beese, Allison M. - Liu, Zi Kui. **Mechanical properties of pure elements from a comprehensive first-principles study to data-driven insights** [elektronický dokument]. DOI 10.1016/j.msea.2024.147446 In: **Materials Science and Engineering A. Structural Materials. Properties, Microstructure and Processing**. Lausanne: Elsevier. Elsevier Science, 2024, Roč. 918, art. no. 147446 [tlačená forma] [online]. ISSN 0921-5093. ISSN (online) 1873-4936. - SCO ; CCC ; WOS CC, s. art. no. 147446

2024 [01/20] / **DEU** - Heczko, Martin - Šesták, Petr - Seiner, Hanuš - Zelený, Martin. **Shear Deformation of Non-modulated Ni2MnGa Martensite: An Ab Initio Study** [elektronický dokument]. DOI 10.1007/s40830-024-00510-z In: **Shape Memory and Superelasticity**. Berlín: Springer Nature, 2024, Roč. 10, č. 4, s. 474-486. ISSN 2199-384X. ISSN (online) 2199-3858. - SCO ; WOS CC, s. 474 - 486

2024 [01/20] / **GBR** - Hunnisett, Lily M. - Francia, Nicholas - Nyman, Jonas - Abraham, Nathan S. - Aitipamula, Srinivasulu - Alkhidir, Tamador - Almehairbi, Mubarak - Anelli, Andrea - Anstine, Dylan M. - Anthony, John E. - Arnold, Joseph E. - Bahrami, Faezeh - Bellucci, Michael A. - Beran, Gregory J.O. - Bhardwaj, Rajni M. - Bianco, Raffaello - Bis, Joanna A. - Boese, A. Daniel - Bramley, James - Braun, Doris E. - Butler, Patrick W.V. - Cadden, Joseph - Carino, Stephen - Červinka, Ctirad - Chan, Eric J. **The seventh blind test of crystal structure prediction: structure ranking methods**. DOI 10.1107/S2052520624008679 In: **Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials**. Chester: International Union of Crystallography, 2024, Roč. 80, č. Pt 6, s. 548-574. ISSN 2052-5206. - SCO ; CCC ; WOS CC, s. 548 - 574

2024 [01/20] / **NLD** - Kızılcan, Dilek Şeyma - Güzel, Yahya - Türkmenoğlu, Burçin. **Clustering of atoms relative to vector space in the Z-matrix coordinate system and 'graphical fingerprint' analysis of 3D pharmacophore structure** [elektronický dokument]. DOI 10.1007/s11030-023-10798-1 In: **Molecular Diversity**. Dordrecht: Springer Nature. Springer, 2024, Roč. 28, č. 6, s. 4087-4104 [tlačená forma] [online]. ISSN 1381-1991. ISSN (online) 1573-501X. - SCO ; CCC ; WOS CC, s. 4087 - 4104

2024 [01/20] / **GBR** - Giunchi, Andrea - Pandolfi, Lorenzo - Della Valle, Raffaele G. - Salzillo, Tommaso - Venuti, Elisabetta - Demitri, Nicola - Riegler, Hans - Petschacher, Christina - Liu, Jie - Werzer, Oliver. **Structural properties and lattice phonons evolution in phenothiazine/iminostilbene solid solutions**. DOI 10.1039/d4ce00605d In: **CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2024, Roč. 26, č. 46, s. 6573-6584 [tlačená forma] [online]. ISSN 1466-8033. - SCO ; CCC ; WOS CC, s. 6573 - 6584

2024 [01/20] / **NLD** - Weiser, Adam - Todt, Juraj - Holcova, Jitka - Zalezak, Tomas - Paulik, Anna M. - Holec, David - Jary, Milan - Zobac, Ondrej - Mrazek, Jan - Frenzel, Jan - Keckes, Jozef - Dlouhy, Antonin. **Hydrogen penetration into the NiTi superelastic alloy investigated in-situ by synchrotron diffraction experiments** [elektronický dokument]. DOI 10.1016/j.actamat.2024.120217 In: **Acta Materialia**. Amsterdam: Acta Materialia, 2024, Roč. 277, art. no. 120217 [tlačená forma] [online]. ISSN 1359-6454. ISSN (online) 1873-2453. - SCO ; CCC ; WOS CC, s. art. no. 120217

2024 [01/20] / **USA** - Wei, Wei - Gebhardt, Julian - Urban, Daniel F. - Elsässer, Christian. **Location and migration of interstitial Li ions in CsPbI3 crystals** [elektronický dokument]. DOI 10.1103/PhysRevB.109.144104 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2024, Roč. 109, č. 14, art. no. 144104 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 144104

2024 [01/20] / **USA** - Brumovský, Miroslav - Tunega, Daniel. **Reductive Dechlorination of Chlorinated Ethenes at the Sulfidated Zero-Valent Iron Surface: A Mechanistic DFT Study** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c00865 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128,

č. 10, s. 4180-4191 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 4180 - 4191

2023 [01/20] / **GBR** - Leiner, Thomas - Koutná, Nikola - Janovec, Jozef - Zelený, Martin - Mayrhofer, Paul H. - Holec, David. **On energetics of allotrope transformations in transition-metal diborides via plane-by-plane shearing** [elektronický dokument]. DOI 10.1016/j.vacuum.2023.112329 In: **Vacuum**. Oxford: Elsevier. Pergamon Press, 2023, Roč. 215, art. no. 112329 [tlačená forma] [online]. ISSN 0042-207X. ISSN (online) 1879-2715. - SCO ; CCC ; WOS CC ; SCIE, s.

2023 [01/20] / **NLD** - Bac, Selin - Lan, Zhenzhuo - Mallikarjun Sharada, Shaama. **Transition Structures, Reaction Paths, and Kinetics: Methods and Applications in Catalysis** [elektronický dokument]. DOI 10.1016/B978-0-12-821978-2.00006-4 In: **Comprehensive Computational Chemistry**. Amsterdam: Elsevier, 2023, s. 496-518 [tlačená forma]. ISBN 978-0-12-821978-2. ISBN (online) 978-0-12-823256-9. ISBN (chybné) 978-0-12-823256-9. - SCO, s. 496 - 518

2023 [01/20] / **DEU** - Papež, P. - Zelený, M. - Friák, M. - Dlouhý, I. **The effect of spin-polarization, atomic ordering and charge transfer on the stability of CoCrNi medium entropy alloy** [elektronický dokument]. DOI 10.1016/j.matchemphys.2023.127783 In: **Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2023, Roč. 304, art. no. 127783 [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCO ; CCC ; WOS CC, s. art. no. 127783

2023 [01/20] / **NLD** - Hu, Lianjie - Liu, Ziran - He, Xinfu. **Wrinkled strong quasi-atomic planes caused by partial covalent bonds in α-uranium** [elektronický dokument]. DOI 10.1016/j.jnucmat.2023.154242 In: **Journal of Nuclear Materials**. Amsterdam: Elsevier, 2023, Roč. 576, art. no. 154242 [tlačená forma] [online]. ISSN 0022-3115. ISSN (online) 1873-4820. - SCO ; CCC ; WOS CC, s. art. no. 154242

2023 [01/20] / **CHE** - Grančič, Peter - Böhm, Leonard - Gerzabek, Martin H. - Tunega, Daniel. **On the Nature of Hydrophobic Organic Compound Adsorption to Smectite Minerals Using the Example of Hexachlorobenzene-Montmorillonite Interactions** [elektronický dokument]. DOI 10.3390/min13020280 In: **Minerals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 2, art. no. 280 [online]. ISSN (online) 2075-163X. - SCO ; CCC ; WOS CC, s. art. no. 280

2023 [01/20] / **NLD** - Brumovský, Miroslav - Micić, Vesna - Oborná, Jana - Filip, Jan - Hofmann, Thilo - Tunega, Daniel. **Iron nitride nanoparticles for rapid dechlorination of mixed chlorinated ethene contamination** [elektronický dokument]. DOI 10.1016/j.jhazmat.2022.129988 In: **Journal of Hazardous Materials**: Environmental Control, Risk Assessment, Impact and Management. Amsterdam: Elsevier, 2023, Roč. 442, art. no. 129988 [tlačená forma] [online]. ISSN 0304-3894. ISSN (online) 1873-3336. - SCO ; CCC ; WOS CC, s. art. no. 129988

2023 [01/20] / **USA** - Brumovský, Miroslav - Tunega, Daniel. **Intrinsic Effects of Sulfidation on the Reactivity of Zero-Valent Iron With Trichloroethene: A DFT Study** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c04459 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 43, s. 21063-21074 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 21063 - 21074

2023 [01/20] / **USA** - Giunchi, Andrea - Pandolfi, Lorenzo - Della Valle, Raffaele G. - Salzillo, Tommaso - Venuti, Elisabetta - Girlando, Alberto. **Lattice Dynamics of Quinacridone Polymorphs: A Combined Raman and Computational Approach** [elektronický dokument]. DOI 10.1021/acs.cgd.3c00634 In: **Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2023, Roč. 23, č. 9, s. 6765-6773 [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCO ; CCC ; WOS CC, s. 6765 - 6773

2023 [01/20] / **USA** - Pracht, Philipp - Morgan, John W.R. - Wales, David J. **Exploring energy landscapes for solid-state systems with variable cells at the extended tight-binding level** [elektronický dokument]. DOI 10.1063/5.0159367 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 6, art. no. 064801 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 064801

2023 [01/20] / **USA** - Kendrick, John - Burnett, Andrew David. **Exploring the Stability and Disorder in the Polymorphs of L-Cysteine through Density Functional Theory and Vibrational Spectroscopy** [elektronický dokument]. DOI 10.1021/acs.cgd.3c00375 In: **Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2023, Roč. 23, č. 8, s. 5734-5747 [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCO ; CCC ; WOS CC, s. 5734 - 5747

2022 [01/20] / **CHE** - Adekoya, O.C. - Adekoya, G.J. - Sadiku, E.R. - Hamam, Y. - Ray, S.S. **Application of DFT Calculations in Designing Polymer-Based Drug Delivery Systems: An Overview** [elektronický dokument] In: **Pharmaceutics**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 14, č. 9, [online]. ISSN (online) 1999-4923. - SCO, s. Art. No. 1972

2022 [01/20] / **NLD** - Shimanek, J.D. - Shang, S.-L. - Beese, A.M. - Liu, Z.-K. **Insight into ideal shear strength of Ni-based dilute alloys using first-principles calculations and correlational analysis** [elektronický dokument] In: **Computational Materials Science**. Amsterdam: Elsevier, 2022, Roč. 212, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO, s. Art. No. 111564

2022 [01/20] / **USA** - Gebhardt, J. - Elsasser, C. **The Electronic Structure of Cs2AgBiBr6 at Room Temperature** In: **Physica Status Solidi (B) Basic Research**, 2022, Roč. 259, č. 8. - SCO, s. Art. No. 2200124

2022 [01/20] / **USA** - Brenner, T.M. - Grumet, M. - Till, P. - Asher, M. - Zeier, W.G. - Egger, D.A. - Yaffe, O. **Anharmonic Lattice Dynamics in Sodium Ion Conductors** In: **Journal of Physical Chemistry Letters**, 2022, Roč. 13, č. 25. - SCO, s. 5938 - 5945

2022 [01/20] / **DEU** - Giunchi, A. - Pandolfi, L. - Salzillo, T. - Brillante, A. - Della Valle, R.G. - d'Agostino, S. - Venuti, E. **Visualizing a Single-Crystal-to-Single-Crystal [2+2] Photodimerization through its Lattice Dynamics: An Experimental and Theoretical Investigation** In: **ChemPhysChem**, 2022, Roč. 23, č. 12. - SCO, s. Art. No. e202200168

2022 [01/20] / **GBR** - Moravcik, I. - Zeleny, M. - Dlouhy, A. - Hadraba, H. - Moravcikova-Gouvea, L. - Papez, P. - Fikar, O. - Dlouhy, I. - Raabe, D. - Li, Z. **Impact of interstitial elements on the stacking fault energy of an equiatomic CoCrNi medium entropy alloy: theory and experiments** [elektronický dokument] In: **Science and Technology of Advanced Materials**. Abingdon: Taylor & Francis Group, 2022, Roč. 23, č. 1, [tlačená forma] [online]. ISSN 1468-6996. ISSN (online) 1878-5514. - SCO, s. 376 - 392

2021 [01/20] / **USA** - Galimberti, D.R. - Sauer, J. **Chemically Accurate Vibrational Free Energies of Adsorption from Density Functional Theory Molecular Dynamics: Alkanes in Zeolites** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 9, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 5849 - 5862

2021 [01/20] / **USA** - Gebhardt, J. - Wei, W. - Elsasser, C. **Efficient Modeling Workflow for Accurate Electronic Structures of Hybrid Perovskites** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 34. - SCO, s. 18597 - 18603

2021 [01/20] / **GBR** - Chong, X. - Shang, S.-L. - Krajewski, A.M. - Shimanek, J.D. - Du, W. - Wang, Y. - Feng, J. - Shin, D. - Beese, A.M. - Liu, Z.-K. **Correlation analysis of materials properties by machine learning: Illustrated with stacking fault energy from first-principles calculations in dilute fcc-based alloys** In: **Journal of Physics Condensed Matter**, 2021, Roč. 33, č. 29. - SCO, s. Art. No. 295702

2021 [01/20] / **GBR** - Xu, J. - Cao, X.-M. - Hu, P. **Perspective on computational reaction prediction using machine learning methods in heterogeneous catalysis** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 19, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 11155 - 11179

2021 [01/20] / **NLD** - Ge, L. - Qiu, H. - Li, H. - Bo, M. - Huang, Z. - Li, L. - Yao, C. **Electronic and magnetic properties of twisted silver and palladium nanorods using density functional theory** [elektronický dokument] In: **Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2021, Roč. 771, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCO, s. Art. No. 138549

2021 [01/20] / **GBR** - Hofmann, O.T. - Zojer, E. - Hormann, L. - Jeindl, A. - Maurer, R.J. **First-principles calculations of hybrid inorganic-organic interfaces: From state-of-the-art to best practice** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 8132 - 8180

2021 [01/20] / **GBR** - Ozturk, Z. **Lithium decoration characteristics for hydrogen storage enhancement in novel periodic porous graphene frameworks** [elektronický dokument] In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2021, Roč. 46, č. 21, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO, s. 11804 - 11814

2021 [01/20] / **NLD** - Gonzalez Fa, A.J. - Faccio, R. - Lopez-Corral, I. **Detection of SOF2 and SO2F2 through aluminium nitride nanosheets: A DFT study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 538, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 147899

2021 [01/20] / **NLD** - Tang, H. - Xing, W. - Li, X. - Chen, B. - Zhao, P. - Shu, L. - Zhang, M. - Ma, Y. - Liu, K. **Insights into the gradient-characteristic precipitation behaviors of laves phase induced by Fe/W/Mo addition in Ti42Al5Mn alloy** [elektronický dokument] In: **Intermetallics**: including complex structural and functional alloys. Amsterdam: Elsevier, 2021, Roč. 128, [tlačená forma] [online]. ISSN 0966-9795. ISSN (online) 1879-0216. - SCO, s. Art. No. 107022

2020 [01/12] / **GBR** - Rivalta, A. - Giunchi, A. - Pandolfi, L. - Salzillo, T. - d'Agostino, S. - Werzer, O. - Schrode, B. - Demitri, N. - Mas-Torrent, M. - Brillante, A. - Della Valle, R.G. - Venuti, E. **In: Dyes and Pigments**: an international journal. Oxford: Elsevier, 2020, Roč. 172, [tlačená forma] [online]. ISSN 0143-7208. ISSN (online) 1873-3743. - SCIE ; WOS CC, s. Art. No. UNSP

2020 [01/12] / Zeleny, M. - Heczko, M. - Janovec, J. - Holec, D. - Straka, L. - Heczko, O. **In: Shape Memory and Superelasticity**, 2020, Roč. 6, č. 1. - SCIE ; WOS CC, s. 35 - 44

2020 [01/12] / **NLD** - Gonzalez Fa, A.J. - Orazi, V. - Jasen, P. - Marchetti, J.M. - Lopez-Corral, I. **Adsorption of carbonyl sulfide on Pt-doped vacancy-defected SWCNT: A DFT study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 525, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 146331

2020 [01/12] / **GBR** - Xing, W. - Chen, X.-Q. - Li, X. - Ma, Y. - Chen, B. - Liu, K. **First-principles study of hydrogen trapping behavior in face centered cubic metals (M=Ni, Cu and Al) with monovacancy** [elektronický dokument] In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2020, Roč. 45, č. 46, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO, s. 25555 - 25566

2020 [01/12] / Pandolfi, L. - Rivalta, A. - Salzillo, T. - Giunchi, A. - D'Agostino, S. - Della Valle, R.G. - Brillante, A. - Venuti, E. **In Search of Surface-Induced Crystal Structures: The Case of Tyrian Purple** In: **Journal of Physical**

Chemistry C, 2020, Roč. 124, č. 32. - SCO, s. 17702 - 17710

2020 [01/12] / **DEU** - Georgieva, I. - Kersten, M. - Tunega, D. **Molecular modeling of MCPA herbicide adsorption by goethite (110) surface in dependence of pH** [elektronický dokument] In: **Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2020, Roč. 139, č. 8, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCO, s. Art. No. 132

2020 [01/12] / **NLD** - Zeleny, M. - Straka, L. - Rames, M. - Sozinov, A. - Heczko, O. **Origin of magnetocrystalline anisotropy in Ni-Mn-Ga-Co-Cu tetragonal martensite** [elektronický dokument] In: **Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2020, Roč. 503, [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCO, s. Art. No. 166522

2020 [01/12] / **USA** - Shang, S.-L. - Shimanek, J. - Qin, S. - Wang, Y. - Beese, A.M. - Liu, Z.-K. **Unveiling dislocation characteristics in N i3Al from stacking fault energy and ideal strength: A first-principles study via pure alias shear deformation** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 101, č. 2, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 024102

2020 [01/12] / Bodnarova, L. - Zeleny, M. - Sedlak, P. - Straka, L. - Heczko, O. - Sozinov, A. - Seiner, H. **Switching the soft shearing mode orientation in Ni-Mn-Ga non-modulated martensite by Co and Cu doping** In: **Smart Materials and Structures**, 2020, Roč. 29, č. 4. - SCO, s. Art. No. 045022

2019 [01/12] / **USA** - Beck, H. - Gehrmann, C. - Egger, D.A. **In: APL materials**. Melville: ACA and AIP Publishing, 2019, Roč. 7, č. 2, [online]. ISSN (online) 2166-532X. - SCIE ; WOS CC, s. Art. No. 021108

2019 [01/12] / **GBR** - Nyman, J. - Yu, L. - Reutzel-Edens, S.M. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 13, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 2080 - 2088

2019 [01/12] / **USA** - Zahradnik, M. - Maroutian, T. - Zeleny, M. - Horak, L. - Kurij, G. - Malecek, T. - Beran, L. - Visnovsky, S. - Agnus, G. - Lecoeur, P. - Veis, M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 99, č. 19, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 195138

2019 [01/12] / **USA** - Nishimura, Y. - Nakai, H. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2019, Roč. 40, č. 15, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 1538 - 1549

2019 [01/12] / **USA** - Giunchi, A. - Rivalta, A. - Bedoya-Martinez, N. - Schrode, B. - Braun, D.E. - Werzer, O. - Venuti, E. - Della Valle, R.G. **In: Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2019, Roč. 19, č. 11, [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCIE ; WOS CC, s. 6067 - 6073

2019 [01/12] / Caicedo-Davila, S. - Funk, H. - Lovrincic, R. - Muller, C. - Sendner, M. - Cojocaru-Miredin, O. - Lehmann, F. - Gunder, R. - Franz, A. - Levcenco, S. - Cohen, A.V. - Kronik, L. - Haas, B. - Koch, C.T. - Abou-Ras, D. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 29. - SCIE ; WOS CC, s. 17666 - 17677

2019 [01/12] / Reocreux, R. - Michel, C. - Fleurat-Lessard, P. - Sautet, P. - Steinmann, S.N. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 47. - SCIE ; WOS CC, s. 28828 - 28835

2019 [01/12] / **USA** - Zhang, G. - Hirsch, A. - Shmul, G. - Avram, L. - Elad, N. - Brumfeld, V. - Pinkas, I. - Feldman, Y. - Ben Asher, R. - Palmer, B.A. - Kronik, L. - Leiserowitz, L. - Weiner, S. - Addadi, L. **In: Journal of the American**

Chemical Society. Washington: American Chemical Society, 2019, Roč. 141, č. 50, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 19736 - 19745

2018 [01/12] / **GBR** - Kabakova, I.V. - Azuri, I. - Chen, Z.Y. - Nayak, P.K. - Snaith, H.J. - Kronik, L. - Paterson, C. - Bakulin, A.A. - Egger, D.A. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2018, Roč. 6, č. 15, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 3861 - 3868

2018 [01/12] / **USA** - Bedoya-Martinez, N. - Giunchi, A. - Salzillo, T. - Venuti, E. - Della Valle, R.G. - Zojer, E. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4380 - 4390

2018 [01/12] / **USA** - Loboda, O.A. - Dolgonos, G.A. - Boese, A.D. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124104

2018 [01/12] / **GBR** - Ozturk, Z. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2018, Roč. 43, č. 49, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 22365 - 22376

2018 [01/12] / **GBR** - Le, M.H. - Tieu, A.K. - Zhu, H. - Ta, D.T. - Yu, H. - Ta, T.T.H. - Tran, V.N. - Wan, S. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 11, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 7819 - 7835

2018 [01/12] / **USA** - Lahnsteiner, J. - Kresse, G. - Heinen, J. - Bokdam, M. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 2, č. 7, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 073604

2018 [01/12] / **USA** - Son, W. - Duong, T. - Talapatra, A. - Prehn, E. - Tan, Z.Y. - Radovic, M. - Arroyave, R. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2018, Roč. 123, č. 22, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 225102

2018 [01/12] / **USA** - Plessow, P.N. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 2, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 981 - 990

2017 [01/12] / **NLD** - Fa, A.J.G. - Orazi, V. - Gonzalez, E.A. - Juan, A. - Lopez-Corral, I. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2017, Roč. 423, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 542 - 548

2017 [01/12] / **NLD** - Freysoldt, C. **In: Computational Materials Science**. Amsterdam: Elsevier, 2017, Roč. 133, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 71 - 81

2017 [01/12] / **USA** - Son, W. - Gao, H.L. - Duong, T. - Talapatra, A. - Radovic, M. - Arroyave, R. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235131

2017 [01/12] / **USA** - Verwuster, E. - Wruss, E. - Zojer, E. - Hofmann, O.T. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 147, č. 2, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 024706

2017 [01/12] / Cabarcos, O.M. - Schuster, S. - Hehn, I. - Zhang, P.P. - Maitani, M.M. - Sullivan, N. - Giguere, J.B. - Morin, J.F. - Weiss, P.S. - Zojer, E. - Zhamikov, M. - Allara, D.L. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 29. - SCIE ; WOS CC, s. 15815 - 15830

2017 [01/12] / **USA** - Baby, A. - Gruenewald, M. - Zwick, C. - Otto, F. - Forker, R. - van Straaten, G. - Franke, M. - Stadtmuller, B. - Kumpf, C. - Brivio, G.P. - Fratesi, G. - Fritz, T. - Zojer, E. **In: ACS Nano**. Washington: American Chemical Society, 2017, Roč. 11, č. 10, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 10495 - 10508

2016 [01/12] / Wruss, E. - Hofmann, O.T. - Egger, D.A. - Verwuster, E. - Gerlach, A. - Schreiber, F. - Zojer, E. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 12. - SCIE ; WOS CC, s. 6869 - 6875

2016 [01/12] / Taucher, T.C. - Hehn, I. - Hofmann, O.T. - Zharnikov, M. - Zojer, E. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 6. - SCIE ; WOS CC, s. 3428 - 3437

2016 [01/12] / Endres, J. - Egger, D.A. - Kulbak, M. - Kerner, R.A. - Zhao, L.F. - Silver, S.H. - Hodes, G. - Rand, B.P. - Cahen, D. - Kronik, L. - Kahn, A. **In: Journal of Physical Chemistry Letters**, 2016, Roč. 7, č. 14. - SCIE ; WOS CC, s. 2722 - 2729

2016 [01/12] / **USA** - Dastidar, S. - Egger, D.A. - Tan, L.Z. - Cromer, S.B. - Dillon, A.D. - Liu, S. - Kronik, L. - Rappe, A.M. - Fafarman, A.T. **In: Nano letters**. Washington: American Chemical Society, 2016, Roč. 16, č. 6, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 3563 - 3570

2016 [01/12] / Hehn, I. - Schuster, S. - Wachter, T. - Abu-Husein, T. - Terfort, A. - Zharnikov, M. - Zojer, E. **In: Journal of Physical Chemistry Letters**, 2016, Roč. 7, č. 15. - SCIE ; WOS CC, s. 2994 - 3000

2016 [01/12] / **USA** - Krautgasser, K. - Panosetti, C. - Palagin, D. - Reuter, K. - Maurer, R.J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 8, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 084117

2016 [01/12] / **USA** - Zwick, C. - Baby, A. - Gruenewald, M. - Verwuster, E. - Hofmann, O.T. - Forker, R. - Fratesi, G. - Brivio, G.P. - Zojer, E. - Fritz, T. **In: ACS Nano**. Washington: American Chemical Society, 2016, Roč. 10, č. 2, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 2365 - 2374

2015 [01/12] / **USA** - Hirsch, A. - Gur, D. - Polishchuk, I. - Levy, D. - Pokroy, B. - Cruz-Cabeza, A.J. - Addadi, L. - Kronik, L. - Leiserowitz, L. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2015, Roč. 27, č. 24, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 8289 - 8297

2015 [01/12] / Verwuster, E. - Hofmann, O.T. - Egger, D.A. - Zojer, E. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 14. - SCIE ; WOS CC, s. 7817 - 7825

2015 [01/12] / **DEU** - Abu-Husein, T. - Schuster, S. - Egger, D.A. - Kind, M. - Santowski, T. - Wiesner, A. - Chiechi, R. - Zojer, E. - Terfort, A. - Zharnikov, M. **In: Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2015, Roč. 25, č. 25, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCIE ; WOS CC, s. 3943 - 3957

2015 [01/12] / Toledano, T. - Garrick, R. - Sinai, O. - Bendikov, T. - Haj-Yahia, A.E. - Lerman, K. - Alon, H. - Sukenik, C.N. - Vilan, A. - Kronik, L. - Cahen, D. **In: Journal of Electron Spectroscopy and Related Phenomena**, 2015, Roč. 204. ISSN 03682048. - SCIE ; WOS CC, s. 149 - 158

2015 [01/12] / **DEU** - Kraberger, G.J. - Egger, D.A. - Zojer, E. **In: Advanced Materials Interfaces**. Weinheim: John Wiley & Sons. Wiley-VCH, 2015, Roč. 2, č. 17, [online]. ISSN 2196-7350. - SCIE ; WOS CC, s. Art. No. 1500323

2015 [01/12] / Zeleny, M. - Straka, L. - Sozinov, A. **In: Esomat - European Symposium on Martensitic Transformations**, 2015, Roč. 33. - SCIE ; WOS CC, s. Art. No. 05006

2014 [01/12] / Egger, D.A. - Kronik, L. **In: Journal of Physical Chemistry Letters**, 2014, Roč. 5, č. 15. - SCIE ; WOS CC, s. 2728 - 2733

2014 [01/12] / **USA** - Piccini, G. - Sauer, J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2479 - 2487

2014 [01/12] / **USA** - Chen, Z.H. - Li, J.B. - Li, S.S. - Wang, L.W. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 14, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 144110

2014 [01/12] / **NLD** - Shang, S.L. - Wang, W.Y. - Zhou, B.C. - Wang, Y. - Darling, K.A. - Kecskes, L.J. - Mathaudhu, S.N. - Liu, Z.K. **In: Acta Materialia**. Amsterdam: Acta Materialia, 2014, Roč. 67, [tlačená forma] [online]. ISSN 1359-6454. ISSN (online) 1873-2453. - SCIE ; WOS CC, s. 168 - 180

2014 [01/12] / **GBR** - Watts, H.D. - Mohamed, M.N.A. - Kubicki, J.D. **In: Cellulose**. London: Blackie Academic & Professional, 2014, Roč. 21, č. 1, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 53 - 70

2014 [01/12] / **GBR** - Xing, W.W. - Chen, X.Q. - Liu, P.T. - Wang, X. - Zhang, P.C. - Li, D.Z. - Li, Y.Y. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2014, Roč. 39, č. 32, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 18506 - 18519

2013 [01/12] / Egger, D.A. - Zojer, E. **In: Journal of Physical Chemistry Letters**, 2013, Roč. 4, č. 20. - SCIE ; WOS CC, s. 3521 - 3526

2012 [01/12] / Shang, S.L. - Wang, W.Y. - Wang, Y. - Du, Y. - Zhang, J.X. - Patel, A.D. - Liu, Z.K. **In: Journal of Physics-Condensed Matter**, 2012, Roč. 24, č. 15. - SCIE ; WOS CC, s. Art. No. 155402

2011 [01/12] / **GBR** - Ma, Z.Y. - Rissner, F. - Wang, L.J. - Heimel, G. - Li, Q.K. - Shuai, Z.G. - Zojer, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2011, Roč. 13, č. 20, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 9747 - 9760

2011 [01/12] / Schlegel, H.B. **In: Wiley Interdisciplinary Reviews-Computational Molecular Science**, 2011, Roč. 1, č. 5. - SCIE ; WOS CC, s. 790 - 809

2011 [01/12] / Demichelis, R. - Noel, Y. - Ugiengo, P. - Zicovich-Wilson, C.M. - Dovesi, R. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 27. - SCIE ; WOS CC, s. 13107 - 13134

2010 [01/12] / **GBR** - Doll, K. **In: Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2010, Roč. 108, č. 3, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCIE ; WOS CC, s. 223 - 227

2010 [01/12] / **GBR** - Egger, D.A. - Rissner, F. - Rangger, G.M. - Hofmann, O.T. - Wittwer, L. - Heimel, G. - Zojer, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 17, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 4291 - 4294

2010 [01/12] / **GBR** - Wang, L.J. - Rangger, G.M. - Ma, Z.Y. - Li, Q.K. - Shuai, Z.G. - Zojer, E. - Heimel, G. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 17, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 4287 - 4290

2010 [01/12] / **USA** - Nemeth, K. - Challacombe, M. - Van Veenendaal, M. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2010, Roč. 31, č. 10, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 2078 - 2086

2010 [01/12] / **USA** - Dubbeldam, D. - Oxford, G.A.E. - Krishna, R. - Broadbelt, L.J. - Snurr, R.Q. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2010, Roč. 133, č. 3, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 034114

2010 [01/12] / **USA** - Rissner, F. - Egger, D.A. - Romaner, L. - Heimel, G. - Zojer, E. **In: ACS Nano**. Washington: American Chemical Society, 2010, Roč. 4, č. 11, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 6735 - 6746

2010 [01/12] / **USA** - Amsler, M. - Goedecker, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2010, Roč. 133, č. 22, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 224104

2009 [01/12] / Dubbeldam, D. - Krishna, R. - Snurr, R.Q. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 44. - SCIE ; WOS CC, s. 19317 - 19327

2007 [01/12] / **USA** - Civalleri, B. - Doll, K. - Zicovich-Wilson, C.M. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2007, Roč. 111, č. 1, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 26 - 33

2006 [01/12] / **USA** - Weber, V. - Tymczak, C.J. - Challacombe, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2006, Roč. 124, č. 22, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 224107

2006 [01/12] / **USA** - Weber, V. - Daul, C. - Challacombe, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2006, Roč. 124, č. 21, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 214105

2005 [01/12] / **USA** - Nemeth, K. - Challacombe, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2005, Roč. 123, č. 19, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 194112

ADC_009: / Benco, Ľubomír (Autor) (25%) - Bučko, Tomáš (Autor) (25%) - Hafner, Jürgen (Autor) (25%) - Toulhoat, H. (Autor) (25%): **Periodic DFT calculations of the stability of Al/Si substitutions and extraframework Zn2+ cations in mordenite and reaction pathway for the dissociation of H-2 and CH4**. – text. – CCC ; SCO ; WOS CC.
In: *Journal of Physical Chemistry B* [textový dokument (print)] [elektronický dokument] : Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. – Washington (USA) : American Chemical Society. – ISSN 1520-6106. – ISSN

(online) 1520-5207. – ISSN (zrušené) 1089-5647. – Roč. 109, č. 43 (2005), s. 20361-20369 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 51
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (44):

2025 [01/20] / **USA** - Sun, Yuting - Liang, Lixin - Yang, Min - Ji, Yi - Hou, Guangjin - Chen, Kuizhi. **Identification and Quantification of Al Pairs and Their Impact on Dealumination in Zeolites** [elektronický dokument]. DOI 10.1021/jacs.4c14741 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2025, Roč. 147, č. 12, s. 10160-10171 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC, s. 10160 - 10171

2025 [01/20] / **CHE** - Wang, Chao - Hu, Min - Xu, Jun - Deng, Feng. **Mechanistic studies of zeolite catalysis via in situ solid-state nuclear magnetic resonance spectroscopy: progress and prospects** [elektronický dokument]. DOI 10.1007/s11705-024-2505-2 In: **Frontiers of Chemical Science and Engineering**. Cham: Springer Nature. Springer-VDI-Verlag, 2025, Roč. 19, č. 1, art. no. 1 [tlačená forma] [online]. ISSN 2095-0179. ISSN (online) 2095-0187. - SCO ; CCC ; WOS CC, s. art. no. 1

2024 [01/20] / **USA** - Aigner, Martina - Van Daele, Stijn - Minoux, Delphine - Nesterenko, Nikolai - Zhao, Ruixue - Baumgärtl, Martin - Khare, Rachit - Jentys, Andreas - Schroeder, Christian - Sanchez-Sanchez, Maricruz - Lercher, Johannes A. **Direct methane utilization through benzene dehydroalkylation catalyzed by Co2+ sites in ZSM-5 intersections** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115686 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 438, art. no. 115686 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. art. no. 115686

2024 [01/20] / **NLD** - Campa, Maria Cristina - Pietrogiacomi, Daniela - Catracchia, Carlotta - Morpurgo, Simone - Olszowka, Joanna - Mlekodaj, Kinga - Lemishka, Mariia - Dedecek, Jiri - Kornas, Agnieszka - Tabor, Edyta. **Fe-MOR and Fe-FER as catalysts for abatement of N2O with CH4: in situ UV–vis DRS and operando FTIR study**. DOI 10.1016/j.apcatb.2023.123360 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2024, Roč. 342, art. no. 123360 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s. art. no. 123360

2023 [01/20] / **USA** - Daouli, Ayoub - Rey, Jérôme - Lahrar, El Hassane - Valtchev, Valentin - Badawi, Michael - Guillet-Nicolas, Rémy. **Ab Initio Screening of Divalent Cations for CH4, CO2, H2, and N2 Separations in Chabazite Zeolite** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c01882 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 45, s. 15962-15973 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 15962 - 15973

2022 [01/20] / **NLD** - Antunez-Garcia, J. - Galvan, D.H. - Petranovskii, V. - Murrieta-Rico, F.N. - Yocupicio-Gaxiola, R.I. - Shelyapina, M.G. - Fuentes-Moyado, S. **Aluminum distribution in mordenite-zeolite framework: A new outlook based on density functional theory calculations** [elektronický dokument] In: **Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2022, Roč. 306, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCO, s. Art. No. 122725

2021 [01/20] / **USA** - Nozik, D. - Tinga, F.M.P. - Bell, A.T. **Propane Dehydrogenation and Cracking over Zn/H-MFI Prepared by Solid-State Ion Exchange of ZnCl2** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2021, Roč. 11, č. 23, [online]. ISSN (online) 2155-5435. - SCO, s. 14489 - 14506

2021 [01/20] / **NLD** - Xie, L. - Wang, R. - Chai, Y. - Weng, X. - Guan, N. - Li, L. **Propane dehydrogenation catalyzed by in-situ partially reduced zinc cations confined in zeolites** In: **Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2021, Roč. 63, [tlačená forma] [online]. ISSN 2095-4956. - SCO, s. 262 - 269

2021 [01/20] / **CHE** - Jajko, G. - Kozyra, P. - Strzempek, M. - Indyka, P. - Zajac, M. - Witkowski, S. - Piskorz, W. **Structural studies of aluminated form of zeolites-exafs and xrd experiment, stem micrography, and dft modelling** [elektronický dokument] In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 26, č. 12, [online]. ISSN (online) 1420-3049. - SCO, s. Art. No. 3566

2021 [01/20] / **USA** - Zhao, P. - Qian, W. - Ma, H. - Sheng, H. - Zhang, H. - Ying, W. **Effect of Zr Incorporation on Mordenite Catalyzed Dimethyl Ether Carbonylation** [elektronický dokument] In: **Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2021, Roč. 151, č. 4, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCO, s. 940 - 954

2021 [01/20] / **GBR** - Strzempek, M. - Tarach, K. - Gora-Marek, K. - Rey, F. - Palomino, M. - Valencia, S. - Piskorz, W. **Multiscale exploration of hydrocarbon adsorption and hopping through ZSM-5 channels - From Monte Carlo modelling to experiment** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 4, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 2981 - 2990

2020 [01/12] / **CHE** - Zhao, X. - Xu, J. - Deng, F. **Solid-state NMR for metal-containing zeolites: From active sites to reaction mechanism** [elektronický dokument] In: **Frontiers of Chemical Science and Engineering**. Cham: Springer Nature. Springer-VDI-Verlag, 2020, Roč. 14, č. 2, [tlačená forma] [online]. ISSN 2095-0179. ISSN (online) 2095-0187. - SCO, s. 159 - 187

2019 [01/12] / Sanchez-Lopez, P. - Antunez-Garcia, J. - Fuentes-Moyado, S. - Galvan, D.H. - Petranovskii, V. - Chavez-Rivas, F. **In: Journal of Materials Science**, 2019, Roč. 54, č. 10. ISSN 0022-2461, 1573-4803. - SCIE ; WOS CC, s. 7745 - 7757

2019 [01/12] / **DEU** - Dedecek, J. - Tabor, E. - Sklenak, S. **In: ChemSusChem**. Weinheim: John Wiley & Sons. Wiley-VCH, 2019, Roč. 12, č. 3, [tlačená forma] [online]. ISSN 1864-5631. ISSN (online) 1864-564X. - SCIE ; WOS CC, s. 556 - 576

2019 [01/12] / **USA** - Oda, A. - Ohkubo, T. - Yumura, T. - Kobayashi, H. - Kuroda, Y. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2019, Roč. 58, č. 1, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 327 - 338

2019 [01/12] / **NLD** - Vorontsov, A.V. - Valdes, H. - Smirniotis, P.G. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2019, Roč. 1166, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / Li, Y. - Huang, S.Y. - Cheng, Z.Z. - Cai, K. - Li, L.D. - Milan, E. - Lv, J. - Wang, Y. - Sun, Q. - Ma, X.B. **In: Applied Catalysis B-environmental**, 2019, Roč. 256. - SCIE ; WOS CC, s. Art. No. UNSP

2018 [01/12] / Reule, A.A.C. - Shen, J. - Semagina, N. **In: ChemPhysChem**, 2018, Roč. 19, č. 12. - SCIE ; WOS CC, s. 1500 - 1506

2018 [01/12] / **NLD** - Reule, A.A.C. - Prasad, V. - Semagina, N. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2018, Roč. 263, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 220 - 230

2018 [01/12] / **USA** - Snyder, B.E.R. - Bols, M.L. - Schoonheydt, R.A. - Sels, B.F. - Solomon, E.I. **In: Chemical Reviews**. Washington: American Chemical Society, 2018, Roč. 118, č. 5, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 2718 - 2768

2017 [01/12] / **USA** - Wang, X.M. - Xu, J. - Qi, G.D. - Wang, C. - Wang, W.Y. - Gao, P. - Wang, Q. - Liu, X.L. - Feng, N.D. - Deng, F. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 345, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 228 - 235

2017 [01/12] / Chibani, S. - Medlej, I. - Lebegue, S. - Angyan, J.G. - Cantrel, L. - Badawi, M. **In: ChemPhysChem**, 2017, Roč. 18, č. 12. - SCIE ; WOS CC, s. 1642 - 1652

2016 [01/12] / **USA** - Ghashghaee, M. - Ghambarian, M. - Azizi, Z. **In: Structural Chemistry**: an international journal concerned with energy, structure, and their relationships to chemical, physical, and biological properties: Computational and Experimental Studies of Chemical and Biological Systems. New York: Springer Nature, 2016, Roč. 27, č. 2, [tlačená forma]. ISSN 1040-0400. ISSN (online) 1572-9001. - SCIE ; WOS CC, s. 467 - 475

2016 [01/12] / **GBR** - Stepniewski, A. - Radon, M. - Gora-Marek, K. - Broclawik, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 5, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 3716 - 3729

2016 [01/12] / **USA** - Sazama, P. - Tabor, E. - Klein, P. - Wichterlova, B. - Sklenak, S. - Mokrzycki, L. - Pashkkova, V. - Ogura, M. - Dedecek, J. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2016, Roč. 333, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 102 - 114

2014 [01/12] / Sobalik, Z. - Sazama, P. - Dedecek, J. - Wichterlova, B. **In: Applied Catalysis A-General**, 2014, Roč. 474. - SCIE ; WOS CC, s. 178 - 185

2013 [01/12] / **GBR** - Shen, Y.L. - Meng, Q.S. - Huang, S.Y. - Gong, J.L. - Ma, X.B. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 31, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 13116 - 13127

2012 [01/12] / Aleksandrov, H.A. - Shor, E.A.I. - Shor, A.M. - Nasluzov, V.A. - Vayssilov, G.N. - Rosch, N. **In: Soft Materials**, 2012, Roč. 10, č. 1-3. ISSN 1539445X. ISSN (online) 15394468. - SCIE ; WOS CC, s. 216 - 234

2012 [01/12] / **GBR** - Shen, Y.L. - Meng, Q.S. - Huang, S.Y. - Wang, S.P. - Gong, J.L. - Ma, X.B. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2012, Roč. 2, č. 18, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 7109 - 7119

2012 [01/12] / **GBR** - Xu, J. - Zheng, A.M. - Wang, X.M. - Qi, G.D. - Su, J.H. - Du, J.F. - Gan, Z.H. - Wu, J.F. - Wang, W. - Deng, F. **In: Chemical Science**. Cambridge: The Royal Society of Chemistry, 2012, Roč. 3, č. 10, [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCIE ; WOS CC, s. 2932 - 2940

2012 [01/12] / **USA** - Wischert, R. - Laurent, P. - Coperet, C. - Delbecq, F. - Sautet, P. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2012, Roč. 134, č. 35, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 14430 - 14449

2012 [01/12] / Dedecek, J. - Sobalik, Z. - Wichterlova, B. **In: Catalysis Reviews-Science and Engineering**, 2012, Roč. 54, č. 2. - SCIE ; WOS CC, s. 135 - 223

2011 [01/12] / **USA** - Li, G.N. - Pidko, E.A. - van Santen, R.A. - Feng, Z.C. - Li, C. - Hensen, E.J.M. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2011, Roč. 284, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 194 - 206

2010 [01/12] / Ratnasamy, P. **In: Structure Property Correlations for Nanoporous Materials**, 2010. - SCIE ; WOS CC,

s. 263 - 330

2010 [01/12] / **NLD** - Aleksandrov, H.A. - Vayssilov, G.N. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2010, Roč. 152, č. 1-4, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 78 - 87

2009 [01/12] / Pidko, E.A. - van Santen, R.A. **In: Zeolite Characterization and Catalysis: a Tutorial**, 2009. - SCIE ; WOS CC, s. 223 - 250

2009 [01/12] / Vayssilov, G.N. - Aleksandrov, H.A. - Petrova, G.P. - St Petkov, P. **Computational Modelling of Nanoporous Materials** In: **Ordered Porous Solids: Recent Advances and Prospects**. Amsterdam: Elsevier, 2009. - BKCI-S ; WOS CC, s. 211 - 238

2008 [01/12] / Anderson, P.A. **In: Solid-State Hydrogen Storage: Materials and Chemistry**, 2008. - SCIE ; WOS CC, s. 223 - 260

2008 [01/12] / **GBR** - Kang, L.H. - Deng, W.Q. - Han, K.L. - Zhang, T. - Liu, Z.M. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2008, Roč. 33, č. 1, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 105 - 110

2008 [01/12] / Bortnovsky, O. - Dedecek, J. - Tvaruzkova, Z. - Sobalik, Z. - Subrt, J. **In: Journal of the American Ceramic Society**, 2008, Roč. 91, č. 9. ISSN 0002-7220. - SCIE ; WOS CC, s. 3052 - 3057

2007 [01/12] / Pidko, E.A. - van Santen, R.A. **In: Journal of Physical Chemistry C**, 2007, Roč. 111, č. 6. - SCIE ; WOS CC, s. 2643 - 2655

2007 [01/12] / **USA** - Joshi, Y.V. - Thomson, K.T. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2007, Roč. 246, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 249 - 265

2007 [01/12] / Barbosa, L.A.M.M. - van Santen, R.A. **In: Journal of Physical Chemistry C**, 2007, Roč. 111, č. 23. - SCIE ; WOS CC, s. 8337 - 8348

2007 [01/12] / Torninaga, H. - Nagai, M. **In: Applied Catalysis A-General**, 2007, Roč. 328, č. 1. - SCIE ; WOS CC, s. 35 - 42

ADC_010: / Bludský, Ota (Autor) (16.667%) - Šilhan, Martin (Autor) (16.667%) - Nachtigall, Petr (Autor) (16.666%) - Bučko, Tomáš (Autor) (16.667%) - Benco, Ľubomír (Autor) (16.666%) - Hafner, Jürgen (Autor) (16.667%): **Theoretical investigation of CO interaction with copper sites in zeolites: Periodic DFT and hybrid quantum mechanical/interatomic potential function study**. – text. – CCC ; SCO ; WOS CC.
In: *Journal of Physical Chemistry B* [textový dokument (print)] [elektronický dokument] : Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. – Washington (USA) : American Chemical Society. – ISSN 1520-6106. – ISSN (online) 1520-5207. – ISSN (zrušené) 1089-5647. – Roč. 109, č. 19 (2005), s. 9631-9638 [tlačená forma] [online]
Počet všetkých autorov: 6
[článok]
Lit.: 66
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (39):

2024 [01/20] / **GBR** - Rafiq, Qaiser - Khan, Muhammad Tahir - Hayat, Sardar Sikandar - Azam, Sikander - Rahman, Amin Ur - Elansary, Hosam O. - Shan, Muhammad. **Adsorption and solar light activity of noble metal adatoms (Au and Zn) on Fe(111) surface: a first-principles study** [elektronický dokument]. DOI 10.1039/d3cp04504h In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2024, Roč. 26, č. 24, s. 17118-17131 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 17118 - 17131

2023 [01/20] / **GBR** - Dai, Chengna - Zhang, Yuchan - Liu, Ning - Yu, Gangqiang - Wang, Ning - Xu, Ruinian - Chen, Biaohua. **Mechanistic insight into the effect of active site motif structures on direct oxidation of methane to methanol over Cu-ZSM-5** [elektronický dokument]. DOI 10.1039/d3cp01906c In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 36, s. 24894-24903 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 24894 - 24903

2023 [01/20] / **DEU** - Sambare, Amogh A. - Pawar, Ramkisan - Shirsat, Mahendra. **A DFT investigation on transition metal (Co, Cr, Cu, Mn, Mo and Nb)-doped bismuth ferrite oxide (BiFeO3) for CO gas adsorption** [elektronický dokument]. DOI 10.1007/s00214-023-03000-0 In: **Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2023, Roč. 142, č. 7, art. no. 61 [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCO ; CCC ; WOS CC, s. art. no. 61

2022 [01/20] / **USA** - Sambare, A.A. - Datta, K.P. - Shirsat, M.D. - Pawar, R.S. **Adsorption of gas molecules (CO, CO 2 , NO, NO 2 , and CH 4) on undoped and Ag-doped bismuth ferrite oxide (BFO) by DFT investigation** [elektronický dokument] In: **Journal of Materials Research**. Warrendale: Materials Research Society, 2022, Roč. 37, č. 23, [tlačená forma] [online]. ISSN 0884-2914. ISSN (online) 2044-5326. - SCO, s. 4296 - 4311

2019 [01/12] / Rejmak, P. - Datka, J. - Broclawik, E. **In: : International journal of quantum chemistry,** 2019, Roč. 119, č. 9. - SCIE ; WOS CC, s. Art. No. e25873

2018 [01/12] / **DEU** - Gatta, G.D. - Lotti, P. - Tabacchi, G. **In: Physics and Chemistry of Minerals**. Berlín: Springer Nature, 2018, Roč. 45, č. 2, [tlačená forma]. ISSN 0342-1791. ISSN (online) 1432-2021. - SCIE ; WOS CC, s. 115 - 138

2018 [01/12] / **USA** - Beheshtian, J. - Ravaei, I. **In: Structural Chemistry**: an international journal concerned with energy, structure, and their relationships to chemical, physical, and biological properties: Computational and Experimental Studies of Chemical and Biological Systems. New York: Springer Nature, 2018, Roč. 29, č. 1, [tlačená forma]. ISSN 1040-0400. ISSN (online) 1572-9001. - SCIE ; WOS CC, s. 231 - 241

2017 [01/12] / **NLD** - Feng, P. - Chen, X.F. - Li, X.J. - Zhao, D. - Xie, S.J. - Xu, L.Y. - He, G.Z. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2017, Roč. 239, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 354 - 362

2016 [01/12] / Anggara, T. - Paolucci, C. - Schneider, W.F. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 49. - SCIE ; WOS CC, s. 27934 - 27943

2015 [01/12] / **NLD** - Tarach, K.A. - Walas, S. - Datka, J. - Gora-Marek, K. **In: Vibrational Spectroscopy**. Amsterdam: Elsevier, 2015, Roč. 79, [tlačená forma] [online]. ISSN 0924-2031. ISSN (online) 1873-3697. - SCIE ; WOS CC, s. 31 - 35

2015 [01/12] / **USA** - Morpurgo, S. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2015, Roč. 36, č. 9, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 660 - 669

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2014 [01/12] / **NLD** - Frolich, K. - Bulanek, R. - Frydova, E. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2014, Roč. 186, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 37 - 45

2013 [01/12] / **GBR** - Hofmann, O.T. - Atalla, V. - Moll, N. - Rinke, P. - Scheffler, M. **In: New Journal of Physics**. Bristol: Institute of Physics. IOP Publishing, 2013, Roč. 15, [online]. ISSN (online) 1367-2630. - SCIE ; WOS CC, s. Art. No. 123028

2012 [01/12] / Aleksandrov, H.A. - Zdravkova, V.R. - Mihaylov, M.Y. - St Petkov, P. - Vayssilov, G.N. - Hadjiivanov, K.I. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 43. - SCIE ; WOS CC, s. 22823 - 22831

2012 [01/12] / **DEU** - Morpurgo, S. - Moretti, G. - Bossa, M. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2012, Roč. 131, č. 3, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. 134 - 144

2010 [01/12] / **GBR** - Yumura, T. - Yamashita, H. - Torigoe, H. - Kobayashi, H. - Kuroda, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 10, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 2392 - 2400

2010 [01/12] / **GBR** - Rejmak, P. - Mitoraj, M. - Broclawik, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 10, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 2321 - 2330

2010 [01/12] / Torigoe, H. - Mori, T. - Fujie, K. - Ohkubo, T. - Itadani, A. - Gotoh, K. - Ishida, H. - Yamashita, H. - Yumura, T. - Kobayashi, H. - Kuroda, Y. **In: Journal of Physical Chemistry Letters**, 2010, Roč. 1, č. 18. - SCIE ; WOS CC, s. 2642 - 2650

2010 [01/12] / Yumura, T. - Hasegawa, S. - Itadani, A. - Kobayashi, H. - Kuroda, Y. **In: Materials**, 2010, Roč. 3, č. 4. - SCIE ; WOS CC, s. 2516 - 2535

2009 [01/12] / **GBR** - Sirijaraensre, J. - Limtrakul, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2009, Roč. 11, č. 3, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 578 - 585

2009 [01/12] / **USA** - Yumura, T. - Takeuchi, M. - Kobayashi, H. - Kuroda, Y. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2009, Roč. 48, č. 2, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 508 - 517

2009 [01/12] / **NLD** - Jiang, S.J. - Huang, S.P. - Tu, W.X. - Zhu, J.Q. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2009, Roč. 255, č. 11, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 5764 - 5769

2009 [01/12] / Archipov, T. - Santra, S. - Ene, A.B. - Stoll, H. - Rauhut, G. - Roduner, E. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 10. - SCIE ; WOS CC, s. 4107 - 4116

2009 [01/12] / **GBR** - Santra, S. - Archipov, T. - Ene, A.B. - Komnik, H. - Stoll, H. - Roduner, E. - Rauhut, G. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2009, Roč. 11, č. 39, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 8855 - 8866

2009 [01/12] / de Farias, R.F. **Chemistry on Modified Oxide and Phosphate Surfaces: Fundamentals and Applications** In: **Book Series: Interface Science and Technology**. San Diego: Elsevier, 2009. - BKCI-S ; WOS CC, s.

2009 [01/12] / Vayssilov, G.N. - Aleksandrov, H.A. - Petrova, G.P. - St Petkov, P. **Computational Modelling of Nanoporous Materials** In: **Ordered Porous Solids: Recent Advances and Prospects**. Amsterdam: Elsevier, 2009. - BKCI-S ; WOS CC, s. 211 - 238

2008 [01/12] / Rejmak, P. - Broclawik, E. - Gora-Marek, K. - Radon, M. - Datka, J. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 46. - SCIE ; WOS CC, s. 17998 - 18010

2008 [01/12] / Milanesio, M. - Croce, G. - Viterbo, D. - Pastore, H.O. - Mascarenhas, A.J.D. - Munsignatti, E.C.D.O. - Meda, L. **In: Journal of Physical Chemistry A**, 2008, Roč. 112, č. 36. - SCIE ; WOS CC, s. 8403 - 8410

2008 [01/12] / **CZE** - Bulanek, R. - Cicmanec, P. **In: Collection of Czechoslovak Chemical Communications**. Praha: Akademie věd České republiky. Ústav organické chemie a biochemie AV ČR, 2008, Roč. 73, č. 8, [tlačená forma] [online]. ISSN 0010-0765. ISSN (online) 1212-6950. - SCIE ; WOS CC, s. 1132 - 1148

2007 [01/12] / **GBR** - Morpurgo, S. - Moretti, G. - Bossa, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2007, Roč. 9, č. 3, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 417 - 424

2007 [01/12] / Barbosa, L.A.M.M. - van Santen, R.A. **In: Journal of Physical Chemistry C**, 2007, Roč. 111, č. 23. - SCIE ; WOS CC, s. 8337 - 8348

2007 [01/12] / **USA** - Zhang, Y. - Lin, H. - Truhlar, D.G. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2007, Roč. 3, č. 4, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 1378 - 1398

2007 [01/12] / Ivanova, E. - Mihaylov, M. - Aleksandrov, H.A. - Daturi, M. - Thibault-Starzyk, F. - Vayssilov, G.N. - Rosch, N. - Hadjiivanov, K.I. **In: Journal of Physical Chemistry C**, 2007, Roč. 111, č. 28. - SCIE ; WOS CC, s. 10412 - 10418

2007 [01/12] / Zheng, X.B. - Zhang, Y.H. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2007, Roč. 111, č. 36. - SCIE ; WOS CC, s. 13442 - 13451

2007 [01/12] / **GBR** - Rejmak, P. - Sierka, M. - Sauer, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2007, Roč. 9, č. 40, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 5446 - 5456

2006 [01/12] / **NLD** - Plant, D.F. - Maurin, G. - Deroche, I. - Gaberova, L. - Llewellyn, P.L. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2006, Roč. 426, č. 4-6, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 387 - 392

2006 [01/12] / **USA** - Jardillier, N. - Villagomez, E.A. - Delahay, G. - Coq, B. - Berthomieu, D. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2006, Roč. 110, č. 33, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 16413 - 16421

2006 [01/12] / Sirijaraensre, J. - Limtrakul, J. **In: ChemPhysChem**, 2006, Roč. 7, č. 11. - SCIE ; WOS CC, s. 2424 - 2432

2006 - spolu : **1**

ADC_011: / Hafner, Jürgen (Autor) (33.333%) - Benco, Ľubomír (Autor) (33.334%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (33.333%): **Acid-based catalysis in zeolites investigated by density-functional methods**. – WOS CC ; CCC.
In: *Topics in Catalysis* [textový dokument (print)] . – New York (USA) : Springer Nature. Springer International Publishing AG. – ISSN 1022-5528. – ISSN (online) 1572-9028. – Roč. 37, č. 1 (2006), s. 41-54 [tlačená forma]
Počet všetkých autorov: 3
[článok]
Lit.: 95132

Ohlasy (26):
2018 [01/12] / **NLD** - Garnica, M.M. - Torres, A.E. - Ramirez-Caballer, G.E. - Balbuena, P.B. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2018, Roč. 265, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 241 - 249

2018 [01/12] / **GBR** - Maestri, M. - Iglesia, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 23, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 15725 - 15735

2018 [01/12] / van Santen, R.A. - Liu, C. **In: Modelling and Simulation in the Science of Micro- and Meso-Porous Materials**, 2018. - SCIE ; WOS CC, s. 151 - 188

2016 [01/12] / Perez-Beltran, S. - Balbuena, P.B. - Ramirez-Caballero, G.E. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 32. - SCIE ; WOS CC, s. 18105 - 18114

2015 [01/12] / **USA** - Tuma, C. - Sauer, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 143, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 102810

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2014 [01/12] / **NLD** - Ghorbanpour, A. - Rimer, J.D. - Grabow, L.C. **In: Catalysis Communications**. Amsterdam: Elsevier, 2014, Roč. 52, [tlačená forma]. ISSN 1566-7367. ISSN (online) 1873-3905. - SCIE ; WOS CC, s. 98 - 102

2014 [01/12] / **GBR** - Chizallet, C. - Raybaud, P. **In: Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 4, č. 9, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCIE ; WOS CC, s. 2797 - 2813

2012 [01/12] / Gomes, J. - Zimmerman, P.M. - Head-Gordon, M. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 29. - SCIE ; WOS CC, s. 15406 - 15414

2011 [01/12] / **USA** - Leydier, F. - Chizallet, C. - Chaumonnot, A. - Digne, M. - Soyer, E. - Quoineaud, A.A. - Costa, D. - Raybaud, P. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2011, Roč. 284, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 215 - 229

2011 [01/12] / Heine, V. **In: Journal of Physics-Condensed Matter**, 2011, Roč. 23, č. 40. - SCIE ; WOS CC, s. Art. No. 400301

2011 [01/12] / **USA** - Gies, H. - Muller, U. - Yilmaz, B. - Tatsumi, T. - Xie, B. - Xiao, F.S. - Bao, X.H. - Zhang, W.P. - De Vos, D. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical

Society, 2011, Roč. 23, č. 10, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 2545 - 2554

2011 [01/12] / Zacher, D. - Schmid, R. - Woll, C. - Fischer, R.A. **In: Angewandte Chemie-International Edition**, 2011, Roč. 50, č. 1. - SCIE ; WOS CC, s. 176 - 199

2010 [01/12] / **NLD** - Tafipolsky, M. - Amirjalayer, S. - Schmid, R. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2010, Roč. 129, č. 3, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 304 - 318

2010 [01/12] / **GBR** - Pirngruber, G.D. - Raybaud, P. - Belmabkhout, Y. - Cejka, J. - Zukal, A. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 41, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 13534 - 13546

2009 [01/12] / Suzuki, K. - Noda, T. - Sastre, G. - Katada, N. - Niwa, M. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 14. - SCIE ; WOS CC, s. 5672 - 5680

2009 [01/12] / Chizallet, C. - Raybaud, P. **In: Angewandte Chemie-International Edition**, 2009, Roč. 48, č. 16. - SCIE ; WOS CC, s. 2891 - 2893

2009 [01/12] / **USA** - Navrotsky, A. - Trofymluk, O. - Levchenko, A.A. **In: Chemical Reviews**. Washington: American Chemical Society, 2009, Roč. 109, č. 9, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 3885 - 3902

2008 [01/12] / **USA** - Praprotnik, M. - Hocevar, S. - Hodoscek, M. - Penca, M. - Janezic, D. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2008, Roč. 29, č. 1, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 122 - 129

2008 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kuznicki, S.M. - Kovalenko, A. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 17. - SCIE ; WOS CC, s. 6794 - 6810

2007 [01/12] / Raybaud, P. **In: Applied Catalysis A-General**, 2007, Roč. 322. - SCIE ; WOS CC, s. 76 - 91

2007 [01/12] / **USA** - Mikhailov, M.N. - Kazansky, V.B. - Kustov, L.M. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2007, Roč. 116, č. 1-2, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 81 - 86

2007 [01/12] / Nachtigall, P. - Sauer, J. **In: Introduction to Zeolite Science and Practice**, 2007, Roč. 168. - SCIE ; WOS CC, s. 701 - 736

2007 [03/12] / **GBR** - Rejmak, P. - Sierka, M. - Sauer, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2007, Roč. 9, č. 40, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 441 - 456

2006 [01/12] / **USA** - Pichon, B. - Kahl, O. - Hammer, B. - Gray, J.S. **In: Vector-Borne and Zoonotic Diseases**. New Rochelle: Mary Ann Liebert, 2006, Roč. 6, č. 4, [tlačená forma] [online]. ISSN 1530-3667. ISSN (online) 1557-7759. - SCIE ; WOS CC, s. 3 - 16

2006 [01/12] / **GBR** - Tuma, C. - Sauer, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2006, Roč. 8, č. 34, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s.

3955 - 3965

2007 - **spolu** : **4**

ADC_012: / Benco, Ľubomír (Autor) (14.286%) - Bučko, Tomáš (Autor) (14.286%) - Grybos, Robert (Autor) (14.286%) - Hafner, Jürgen (Autor) (14.286%) - Sobalik, Z. (Autor) (14.285%) - Dedecek, J. (Autor) (14.285%) - Hrusak, J. (Autor) (14.286%): **Adsorption of NO in Fe2+-exchanged ferrierite. A density functional theory study**. – text. – CCC ; SCO ; WOS CC.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 111, č. 2 (2007), s. 586-595 [tlačená forma] [online]
Počet všetkých autorov: 7
[článok]
Lit.: 45
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (16):
2024 [01/20] / **USA** - Liu, Chunli - Liu, Yonghua - Xu, Gaomou - Wang, Tao. **Associative-Distal Mechanism of the Haber-Bosch Process on a Ferrierite Catalyst with Spatially Isolated Dual Molybdenum Sites** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c01107 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 16, s. 6711-6718 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 6711 - 6718

2023 [01/20] / **USA** - Liu, Chunli - Xu, Gaomou - Wang, Tao. **Theoretical Approach toward a Mild Condition Haber-Bosch Process on the Zeolite Catalyst with Confined Dual Active Sites** [elektronický dokument]. DOI 10.1021/jacsau.3c00546 In: **JACS Au**. Washington: American Chemical Society, 2023, Roč. 3, č. 12, s. 3374-3380 [online]. ISSN (online) 2691-3704. - SCO ; WOS CC, s. 3374 - 3380

2022 [01/20] / **USA** - Yasumura, S. - Qian, Y. - Kato, T. - Mine, S. - Toyao, T. - Maeno, Z. - Shimizu, K.-I. **In Situ/ Operando Spectroscopic Studies on the NH3-SCR Mechanism over Fe-Zeolites** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 16, [online]. ISSN (online) 2155-5435. - SCO, s. 9983 - 9993

2020 [01/12] / **USA** - Zhao, G. - Adesina, A. - Kennedy, E. - Stockenhuber, M. **Formation of Surface Oxygen Species and the Conversion of Methane to Value-Added Products with N2O as Oxidant over Fe-Ferrierite Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 2, [online]. ISSN (online) 2155-5435. - SCO, s. 1406 - 1416

2017 [01/12] / **CHE** - He, M. - Zhang, J. - Liu, R. - Sun, X.L. - Chen, B.H. **In: Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2017, Roč. 7, č. 1, [online]. ISSN 2073-4344. - SCIE ; WOS CC, s. Art. No. 11

2015 [01/12] / **NLD** - Boron, P. - Chmielarz, L. - Gurgul, J. - Latka, K. - Gil, B. - Marszalek, B. - Dzwigaj, S. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2015, Roč. 203, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 73 - 85

2015 [01/12] / Mao, Y. - Wang, H.F. - Hu, P. **In: : International journal of quantum chemistry,** 2015, Roč. 115, č. 10. -

SCIE ; WOS CC, s. 618 - 630

2011 [01/12] / **USA** - Li, G.N. - Pidko, E.A. - van Santen, R.A. - Feng, Z.C. - Li, C. - Hensen, E.J.M. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2011, Roč. 284, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 194 - 206

2011 [01/12] / Basiuk, V.A. **In: : International journal of quantum chemistry,** 2011, Roč. 111, č. 15. - SCIE ; WOS CC, s. 4197 - 4205

2011 [01/12] / **NLD** - Kim, S.H. - Komarneni, S. - Heo, N.H. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2011, Roč. 143, č. 1, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 243 - 248

2010 [01/12] / **NLD** - Danilczuk, M. - Lund, A. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2010, Roč. 490, č. 4-6, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 205 - 209

2009 [01/12] / Guan, J. - Yang, G. - Zhou, D.H. - Zhang, W.P. - Liu, X.C. - Han, X.W. - Bao, X.H. **In: Journal of Molecular Catalysis A-Chemical**, 2009, Roč. 300, č. 1-2. - SCIE ; WOS CC, s. 41 - 47

2009 [01/12] / Fan, F.T. - Sun, K.J. - Feng, Z.C. - Xia, H.A. - Han, B. - Lian, Y.X. - Ying, P.L. - Li, C. **In: Chemistry-A European Journal**, 2009, Roč. 15, č. 13. - SCIE ; WOS CC, s. 3268 - 3276

2009 [01/12] / Blasin-Aube, V. - Marie, O. - Saussey, J. - Plesniar, A. - Daturi, M. - Nguyen, N. - Hamon, C. - Mihaylov, M. - Ivanova, E. - Hadjiivanov, K. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 19. - SCIE ; WOS CC, s. 8387 - 8393

2008 [01/12] / **USA** - Kozyra, P. - Zalucka, J. - Mitoraj, M. - Broclawik, E. - Datka, J. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2008, Roč. 126, č. 3-4, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 241 - 246

2008 [01/12] / Moore, E.A. **In: Chemical Modelling: Applications and Theory**, 2008, Roč. 5. - SCIE ; WOS CC, s. 119 - 149

ADC_013: / East, A.L.L. (Autor) (33.333%) - Bučko, Tomáš (Autor) (33.334%) - Hafner, Jürgen (Autor) (33.333%): **Carbocation branching observed in a simulation**. – text. – CCC ; SCO ; WOS CC.
In: *The Journal of Physical Chemistry A* [textový dokument (print)] [elektronický dokument] : Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. – Washington (USA) : American Chemical Society. – ISSN 1089-5639. – ISSN (online) 1520-5215. – Roč. 111, č. 27 (2007), s. 5945-5947 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 26
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (7):
2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on**

Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2016 [01/12] / **DEU** - Hare, S.R. - Tantillo, D.J. **In: Beilstein Journal of Organic Chemistry**. Frankfurt nad Mohanom: Beilstein-Institut zur Förderung der Chemischen Wissenschaften, 2016, Roč. 12, [tlačená forma]. ISSN 2195-951X. ISSN (online) 1860-5397. - SCIE ; WOS CC, s. 377 - 390

2014 [01/12] / **USA** - Knaeble, W. - Carr, R.T. - Iglesia, E. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2014, Roč. 319, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 283 - 296

2011 [01/12] / **USA** - Chiang, H. - Bhan, A. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2011, Roč. 283, č. 1, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 98 - 107

2011 [01/12] / Aue, D.H. **In: Wiley Interdisciplinary Reviews-Computational Molecular Science**, 2011, Roč. 1, č. 4. - SCIE ; WOS CC, s. 487 - 508

2009 [01/12] / **USA** - Macht, J. - Carr, R.T. - Iglesia, E. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2009, Roč. 131, č. 18, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 6554 - 6565

2008 [01/12] / **GBR** - Macht, J. - Iglesia, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2008, Roč. 10, č. 35, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 5331 - 5343

ADC_014: / Benco, Ľubomír (Autor) (12.5%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (12.5%) - Grybos, Robert (Autor) (12.5%) - Hafner, Jürgen (Autor) (12.5%) - Sobalik, Z. (Autor) (12.5%) - Dedecek, J. (Autor) (12.5%) - Sklenak, S. (Autor) (12.5%) - Hrusak, J. (Autor) (12.5%): **Multiple adsorption of NO on Fe2+ cations in the alpha- and beta-positions of ferrierite: An experimental and density functional study**.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 111, č. 26 (2007), s. 9393-9402 [tlačená forma] [online]
Počet všetkých autorov: 8
[článok]
Lit.: 38144
Indikátor časopisu:
Nordic List: 1 - 2007

Ohlasy (24):
2020 [01/12] / **USA** - Zhao, G. - Adesina, A. - Kennedy, E. - Stockenhuber, M. **Formation of Surface Oxygen Species and the Conversion of Methane to Value-Added Products with N2O as Oxidant over Fe-Ferrierite Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 2, [online]. ISSN (online) 2155-5435. - SCO, s. 1406 - 1416

2020 [01/12] / **USA** - Zhang, T. - Qiu, Y. - Liu, G. - Chen, J. - Peng, Y. - Liu, B. - Li, J. **Nature of active Fe species and reaction mechanism over high-efficiency Fe/CHA catalysts in catalytic decomposition of N2O** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2020, Roč. 392, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 322 - 335

2018 [01/12] / **NLD** - Avdeev, V.I. - Bedilo, A.F. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2018, Roč. 695, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 222 - 227

2016 [01/12] / **GBR** - Szanyi, J. - Gao, F. - Kwak, J.H. - Kollar, M. - Wang, Y.L. - Peden, C.H.F. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 15, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 10473 - 10485

2015 [01/12] / **NLD** - Kawakami, K. - Ogura, M. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2015, Roč. 242, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 343 - 350

2015 [01/12] / Gao, F. - Kollar, M. - Kukkadapu, R.K. - Washton, N.M. - Wang, Y.L. - Szanyi, J. - Peden, C.H.F. **In: Applied Catalysis B-environmental**, 2015, Roč. 164. - SCIE ; WOS CC, s. 407 - 419

2015 [01/12] / Mao, Y. - Wang, H.F. - Hu, P. **In: : International journal of quantum chemistry,** 2015, Roč. 115, č. 10. - SCIE ; WOS CC, s. 618 - 630

2015 [01/12] / **GBR** - Beale, A.M. - Gao, F. - Lezcano-Gonzalez, I. - Peden, C.H.F. - Szanyi, J. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7371 - 7405

2014 [01/12] / **NLD** - Pietrogiacomi, D. - Campa, M.C. - Occhiuzzi, M. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2014, Roč. 227, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 116 - 122

2013 [01/12] / **USA** - Wang, J.Y. - Xia, H.A. - Ju, X.H. - Feng, Z.C. - Fan, F.T. - Li, C. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2013, Roč. 300, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 251 - 259

2013 [01/12] / Li, G.N. - Pidko, E.A. - van Santen, R.A. - Li, C. - Hensen, E.J.M. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 1. - SCIE ; WOS CC, s. 413 - 426

2012 [01/12] / **NLD** - Yang, G. - Zhou, L.J. - Liu, X.C. - Han, X.W. - Bao, X.H. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2012, Roč. 161, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 168 - 178

2011 [01/12] / **NLD** - Chu, Z.K. - Fu, G. - Xu, X. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2011, Roč. 165, č. 1, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 112 - 119

2010 [01/12] / **GBR** - Berlier, G. - Lamberti, C. - Rivallan, M. - Mul, G. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 2, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 358 - 364

2010 [01/12] / Mihaylov, M. - Ivanova, E. - Drenchev, N. - Hadjiivanov, K. **In: Journal of Physical Chemistry C**, 2010, Roč. 114, č. 2. - SCIE ; WOS CC, s. 1004 - 1014

2010 [01/12] / Ivanova, E. - Mihaylov, M. - Hadjiivanov, K. - Blasin-Aube, V. - Marie, O. - Plesniar, A. - Daturi, M. **In: Applied Catalysis B-environmental**, 2010, Roč. 93, č. 3-4. - SCIE ; WOS CC, s. 325 - 338

2010 [01/12] / **NLD** - Danilczuk, M. - Lund, A. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences,

Materials and Biological Systems. Amsterdam: Elsevier, 2010, Roč. 490, č. 4-6, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 205 - 209

2010 [01/12] / **NLD** - Hadjiivanov, K. - Ivanova, E. - Kefirov, R. - Janas, J. - Plesniar, A. - Dzwigaj, S. - Che, M. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2010, Roč. 131, č. 1-3, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 1 - 12

2010 [01/12] / **GBR** - Lamberti, C. - Zecchina, A. - Groppo, E. - Bordiga, S. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2010, Roč. 39, č. 12, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 4951 - 5001

2010 [01/12] / Chu, Z.K. - Fu, G. - Guo, W.P. - Xu, X. **In: Journal of Theoretical & Computational Chemistry**, 2010, Roč. 9. - SCIE ; WOS CC, s. 39 - 47

2009 [01/12] / Vayssilov, G.N. - Aleksandrov, H.A. - Petrova, G.P. - St Petkov, P. **Computational Modelling of Nanoporous Materials** In: **Ordered Porous Solids: Recent Advances and Prospects**. Amsterdam: Elsevier, 2009. - BKCI-S ; WOS CC, s. 211 - 238

2009 [01/12] / Guan, J. - Yang, G. - Zhou, D.H. - Zhang, W.P. - Liu, X.C. - Han, X.W. - Bao, X.H. **In: Journal of Molecular Catalysis A-Chemical**, 2009, Roč. 300, č. 1-2. - SCIE ; WOS CC, s. 41 - 47

2009 [01/12] / Blasin-Aube, V. - Marie, O. - Saussey, J. - Plesniar, A. - Daturi, M. - Nguyen, N. - Hamon, C. - Mihaylov, M. - Ivanova, E. - Hadjiivanov, K. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 19. - SCIE ; WOS CC, s. 8387 - 8393

2009 [01/12] / Li, X. - Guan, J. - Zhou, D.H. - Li, G.H. - Han, X.W. - Zhang, W.P. - Bao, X.H. **In: Journal of Molecular Structure-Theochem**, 2009, Roč. 913, č. 1-3. - SCIE ; WOS CC, s. 167 - 172

ADC_015: / Bučko, Tomáš (Autor) (25%) - Benco, Ľubomír (Autor) (25%) - Hafner, Jürgen (Autor) (25%) - Ángyán, János G. (Autor) (25%): **Proton exchange of small hydrocarbons over acidic chabazite: Ab initio study of entropic effects**. – text. – CCC ; SCO ; WOS CC ; SCIE.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – Roč. 250, č. 1 (2007), s. 171-183 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 4995
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (41):
2024 [01/20] / **NLD** - Fo, Yumeng - Song, Shaojia - Yang, Kun - Ji, Xiangyang - Yang, Luyuan - Huang, Liusai - Chen, Xinyu - Wu, Xueqiu - Liu, Jian - Zhao, Zhen - Song, Weiyu. **Ab initio molecular dynamics simulation reveals the influence of entropy effect on Co@BEA zeolite-catalyzed dehydrogenation of ethane** [elektronický dokument]. DOI 10.1016/S1872-2067(24)60116-6 In: **Chinese Journal of Catalysis**: the Journal of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and the Chinese Chemical Society. Amsterdam: Elsevier, 2024, Roč. 65, s. 195-205 [tlačená forma]. ISSN 1872-2067. ISSN (online) 0253-9837. - SCO ; CCC, s. 195 - 205

2023 [01/20] / **DEU** - Arzumanov, Sergei S. - Gabrienko, Anton A. - Freude, Dieter - Haase, Jürgen - Stepanov, Alexander

G. **Tuning the Mechanism of H/D Exchange for Isobutane on H-BEA by Loading Zn Species in Zeolite** [elektronický dokument]. DOI 10.1002/chem.202202962 In: **Chemistry - A European Journal**. Weinheim: John Wiley & Sons. Wiley-VCH, 2023, Roč. 29, č. 5, art. no. e202202962 [tlačená forma] [online]. ISSN 0947-6539. ISSN (online) 1521-3765. - SCO ; CCC ; WOS CC, s.

2022 [01/20] / **USA** - Rybicki, Marcin - Sillar, Kaido - Sauer, Joachim. **Dual-Site Model for Ab Initio Calculations of Gibbs Free Energies and Enthalpies of Adsorption: Methane in Zeolite Mobile Five (H-MFI)** [elektronický dokument]. DOI 10.1021/acs.jpclett.2c03302 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2022, Roč. 13, č. 50, s. 11595-11600 [online]. ISSN (online) 1948-7185. - SCO, s. 11595 - 11600

2021 [01/20] / **USA** - Galimberti, D.R. - Sauer, J. **Chemically Accurate Vibrational Free Energies of Adsorption from Density Functional Theory Molecular Dynamics: Alkanes in Zeolites** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 9, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 5849 - 5862

2020 [01/12] / **USA** - Maliekkal, V. - Dauenhauer, P.J. - Neurock, M. **Glycosidic C-O Bond Activation in Cellulose Pyrolysis: Alpha Versus Beta and Condensed Phase Hydroxyl-Catalytic Scission** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 15, [online]. ISSN (online) 2155-5435. - SCO, s. 8454 - 8464

2019 [01/12] / **USA** - Li, G.N. - Pidko, E.A. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano-Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 134 - 156

2019 [01/12] / Reocreux, R. - Michel, C. - Fleurat-Lessard, P. - Sautet, P. - Steinmann, S.N. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 47. - SCIE ; WOS CC, s. 28828 - 28835

2018 [01/12] / **CHE** - Sahoo, S.K. - Nair, N.N. **In: Frontiers in Chemistry**. Lausanne: Frontiers Media, 2018, Roč. 6, [online]. ISSN (online) 2296-2646. - SCIE ; WOS CC, s. Art. No. 275

2018 [01/12] / Li, G.N. - Liu, C. - Rohling, R. - Hensen, E.J.M. - Pidko, E.A. **In: Modelling and Simulation in the Science of Micro- and Meso-Porous Materials**, 2018. - SCIE ; WOS CC, s. 229 - 263

2018 [01/12] / **USA** - Li, H. - Paolucci, C. - Schneider, W.F. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 2, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 929 - 938

2018 [01/12] / **GBR** - Grajciar, L. - Heard, C.J. - Bondarenko, A.A. - Polynski, M.V. - Meeprasert, J. - Pidko, E.A. - Nachtigall, P. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 47, č. 22, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 8307 - 8348

2018 [01/12] / Khalil, I. - Jabraoui, H. - Maurin, G. - Lebegue, S. - Badawi, M. - Thomas, K. - Mauge, F. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 46. - SCIE ; WOS CC, s. 26419 - 26429

2018 [01/12] / **USA** - Rybicki, M. - Sauer, J. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2018, Roč. 140, č. 51, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 18151 - 18161

2016 [01/12] / **USA** - Kundu, A. - Piccini, G. - Sillar, K. - Sauer, J. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 42, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 14047 - 14056

2016 [01/12] / Arzumanov, S.S. - Gabrienko, A.A. - Freude, D. - Stepanov, A.G. **In: Catalysis Science & Technology**, 2016, Roč. 6, č. 16. - SCIE ; WOS CC, s. 6381 - 6388

2015 [01/12] / De Wispelaere, K. - Ensing, B. - Ghysels, A. - Meijer, E.J. - Van Speybroeck, V. **In: Chemistry-A European Journal**, 2015, Roč. 21, č. 26. - SCIE ; WOS CC, s. 9385 - 9396

2015 [01/12] / Piccini, G. - Alessio, M. - Sauer, J. - Zhi, Y.C. - Liu, Y. - Kolvenbach, R. - Jentys, A. - Lercher, J.A. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 11. - SCIE ; WOS CC, s. 6128 - 6137

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2014 [01/12] / Arzumanov, S.S. - Moroz, I.B. - Freude, D. - Haase, J. - Stepanov, A.G. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 26. - SCIE ; WOS CC, s. 14427 - 14432

2014 [01/12] / **GBR** - Van Speybroeck, V. - De Wispelaere, K. - Van der Mynsbrugge, J. - Vandichel, M. - Hemelsoet, K. - Waroquier, M. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 43, č. 21, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7326 - 7357

2014 [01/12] / **USA** - Piccini, G. - Sauer, J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2479 - 2487

2013 [01/12] / **USA** - Piccini, G. - Sauer, J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2013, Roč. 9, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 5038 - 5045

2013 [01/12] / **USA** - Moors, S.L.C. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 11, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2556 - 2567

2013 [01/12] / **USA** - Reger, D.L. - Pascui, A.E. - Pellechia, P.J. - Smith, M.D. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2013, Roč. 52, č. 19, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 11638 - 11649

2013 [01/12] / **USA** - Borghese, S. - Haouas, M. - Sommer, J. - Taulelle, F. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2013, Roč. 305, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 130 - 134

2013 [01/12] / Patrylak, K.I. - Patrylak, L.K. - Repetskyi, I.A. **In: Theoretical and Experimental Chemistry**, 2013, Roč. 49, č. 3. - SCIE ; WOS CC, s. 143 - 157

2013 [01/12] / Hemelsoet, K. - Van der Mynsbrugge, J. - De Wispelaere, K. - Waroquier, M. - Van Speybroeck, V. **In: ChemPhysChem**, 2013, Roč. 14, č. 8. - SCIE ; WOS CC, s. 1526 - 1545

2013 [01/12] / **NLD** - Ghashghaee, M. - Karimzadeh, R. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2013, Roč. 170, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 318 - 330

2013 [01/12] / **GBR** - Kling, D.P. - Machado, E.S.A. - Chagas, H.C. - dos Santos, A.P.A. - Rosenbach, N. - Carneiro, J.W. - Mota, C.J.A. **In: Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 49, č. 40, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCIE ; WOS CC, s. 4480 - 4482

2013 [01/12] / Popeneciu, H. - Calborean, A. - Tudoran, C. - Buimaga-Iarinca, L. **In: Processes in Isotopes and Molecules**, 2013, Roč. 1565. - SCIE ; WOS CC, s. 67 - 70

2012 [01/12] / **DEU** - Sukrat, K. - Tunega, D. - Aquino, A.J.A. - Lischka, H. - Parasuk, V. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2012, Roč. 131, č. 6, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 1232

2011 [01/12] / **USA** - Mullen, G.M. - Janik, M.J. **In: ACS Catalysis**. Washington: American Chemical Society, 2011, Roč. 1, č. 2, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 105 - 115

2011 [01/12] / **USA** - Liu, D.X. - Bhan, A. - Tsapatsis, M. - Al Hashimi, S. **In: ACS Catalysis**. Washington: American Chemical Society, 2011, Roč. 1, č. 1, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 7 - 17

2010 [01/12] / Haouas, M. - Fink, G. - Taulelle, F. - Sommer, J. **In: Chemistry-A European Journal**, 2010, Roč. 16, č. 30. - SCIE ; WOS CC, s. 9034 - 9039

2010 [01/12] / Sastre, G. - Katada, N. - Niwa, M. **In: Journal of Physical Chemistry C**, 2010, Roč. 114, č. 36. - SCIE ; WOS CC, s. 15424 - 15431

2010 [01/12] / **USA** - Ghorai, P.K. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2010, Roč. 114, č. 19, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 6492 - 6499

2009 [01/12] / Berner, G.M. - East, A.L.L. **In: Canadian Journal of Chemistry-Revue Canadienne de Chimie**, 2009, Roč. 87, č. 10. - SCIE ; WOS CC, s. 1512 - 1520

2008 [01/12] / Stoyanov, S.R. - Gusarov, S. - Kuznicki, S.M. - Kovalenko, A. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 17. - SCIE ; WOS CC, s. 6794 - 6810

2008 [01/12] / Huang, J. - Jiang, Y.J. - Marthala, V.R.R. - Ooi, Y.S. - Hunger, M. **In: ChemPhysChem**, 2008, Roč. 9, č. 8. - SCIE ; WOS CC, s. 1107 - 1109

2008 [01/12] / Arzumanov, S.S. - Stepanov, A.C. - Freude, D. **In: Journal of Physical Chemistry C**, 2008, Roč. 112, č. 31. - SCIE ; WOS CC, s. 11869 - 11874

2008 [01/12] / Stepanov, A.G. - Arzumanov, S.S. - Gabrienko, A.A. - Parmon, V.N. - Ivanova, I.I. - Freude, D. **In: ChemPhysChem**, 2008, Roč. 9, č. 17. - SCIE ; WOS CC, s. 2559 - 2563

2008 - spolu : **1**

ADC_016: / Bučko, Tomáš (Autor) (100%): **Ab initio calculations of free-energy reaction barriers**. – CCC ; SCO ; WOS CC.
In: *Journal of Physics* [textový dokument (print)] [elektronický dokument] : Condensed Matter. – Bristol (Veľká Británia) : Institute of Physics. IOP Publishing. – ISSN 0953-8984. – ISSN (online) 1361-648X. – Roč. 20, č. 6 (2008), Art. No. 064211,

s. [1-1] [tlačená forma] [online]
Počet všetkých autorov: 1
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (79):

2025 [01/20] / **USA** - Chaudhary, Payal - Alexandrov, Vitaly. **Mechanism of Bicarbonate-Enhanced Solar Oxidation of Water to Hydrogen Peroxide over BiVO4** [elektronický dokument]. DOI 10.1021/acscatal.5c00478 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, č. 11, s. 9006-9012 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 9006 - 9012

2025 [01/20] / **USA** - Prajapati, Aditya - Zagalskaya, Alexandra - Hwee, Natalie - Davis, Jonathan T. - Jeong, Hui Yun - Moreno, Jennifer - Ynzunza, Jenna - Akhade, Sneha A. - Feaster, Jeremy T. **Decarbonizing nitrogen fertilizer production via the electrochemical nitrogen oxidation reaction** [elektronický dokument]. DOI 10.1016/j.checat.2024.101220 In: **Chem Catalysis**. Philadelphia: Elsevier, 2025, Roč. 5, č. 2, art. no. 101220 [tlačená forma] [online]. ISSN 2667-1107. ISSN (online) 2667-1093. - SCO ; WOS CC, s. art. no. 101220

2025 [01/20] / **USA** - Ospina-Acevedo, Francisco A. - Godínez-Salomón, José Fernando - Naymik, Zachary G. - Matthews, Kevin C. - Warner, Jamie H. - Rhodes, Christopher P. - Balbuena, Perla B. **Impacts of Surface Reconstruction and Metal Dissolution on Ru1-xTixO2 Acidic Oxygen Evolution Electrocatalysts** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c08119 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 7, s. 3595-3613 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO, s. 3595 - 3613

2025 [01/20] / **USA** - Carrillo, J. Luis - Ezazi, Andrew A. - Perez-Beltran, Saul - Larriuz, Carlos A. - Kohl, Harris - Ayala, Jaime A. - Maji, Arnab - Verkhoturov, Stanislav - Al-Hashimi, Mohammed - Bazzi, Hassan - Weiland, Conan - Jaye, Cherno - Fischer, Daniel A. - Zuin, Lucia - Wang, Jian - Banerjee, Sarbajit. **Electrochemical 6Li isotope enrichment based on selective insertion in 1D tunnel-structured V2O5** [elektronický dokument]. DOI 10.1016/j.chempr.2025.102486 In: **Chem**. Cambridge, MA: Elsevier. Cell Press, 2025, Roč. 11, č. 8, art. no. 102486 [tlačená forma] [online]. ISSN 2451-9308. ISSN (online) 2451-9294. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 102486

2025 [01/20] / **USA** - Stratulat, Ana Maria - Nesterova, Valentina - Korostelev, Vladislav - Beidaghi, Majid - Mochalin, Vadym - Klyukin, Konstantin. **Defect-Driven Degradation of MXenes in Aqueous Environments and Mitigation Strategies: Insights from First-Principles** [elektronický dokument]. DOI 10.1021/acsnano.5c09946 In: **ACS Nano**. Washington: American Chemical Society, 2025, Roč. 19, č. 42, s. 36994-37003 [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO ; CCC ; WOS CC ; SCIE, s. 36994 - 37003

2025 [01/20] / **GBR** - Ruffman, Charlie - Packwood, Daniel. **Cross-correlation for detecting and understanding patterns in ab initio molecular dynamics simulations of liquid metals** [elektronický dokument]. DOI 10.1088/1361-648X/adf932 In: **Journal of Physics**: Condensed Matter. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 37, č. 34, art. no. 345401 [tlačená forma] [online]. ISSN 0953-8984. ISSN (online) 1361-648X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 345401

2025 [01/20] / **USA** - Zutter, Brian T. - Oh, Sangheon - Brown, Timothy D. - Anderson, Jillian - Perez Beltran, Saul - Bishop, Sean - Finnegan, Patrick - Ievlev, Anton - Li, Yiyang - Sugar, Joshua - Lai, Hao En - Blanco, Brayan A.Arenas - Lopez-Meza, Andres - Kumar, Suhas - Fuller, Elliot J. - Williams, R. Stanley - Balbuena, Perla B. - Talin, A. Alec. **Mechanisms enabling reconfigurability and long-term retention in vanadium oxide electrochemical memory** [elektronický dokument]. DOI 10.1103/k616-d2q5 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 9, č. 8, art. no.085001 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC ; SCIE, s. art. no.085001

2025 [01/20] / **USA** - Zhang, Zhichao - Qin, Xueping - Kang, Feiyu - Hansen, Heine Anton - Li, Jia. **Surface-Hydrogen Modulated Hydrogen Bond Network Steering Two-Electron Pathways in CO2Electroreduction on Cu Surface** [elektronický dokument]. DOI 10.1021/acscatal.5c06490 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, s. 20332-20341 [online]. ISSN (online) 2155-5435. - SCO ; WOS CC ; SCIE, s. 20332 - 20341

2025 [01/20] / **GBR** - Xu, Chentao - Li, Ji - Shen, Zhizhang. **Questioning the role of adsorbed H in H2O2 decomposition on Pt(111) for the electrocatalytic green Fenton process** [elektronický dokument]. DOI 10.1039/d5cp03100a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 41, s. 22093-22102 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 22093 - 22102

2024 [01/20] / **USA** - Li, Yuke - Liu, Bing Yu - Chen, Yanxia - Liu, Zhi Feng. **From 2e− to 4e− pathway in the alkaline oxygen reduction reaction on Au(100): Kinetic circumvention of the volcano curve** [elektronický dokument]. DOI 10.1063/5.0211477 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2024, Roč. 160, č. 24, art. no. 244705 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 244705

2024 [01/20] / **USA** - Ospina-Acevedo, Francisco - Albiter, Luis A. - Bailey, Kathleen O. - Godínez-Salomón, José Fernando - Rhodes, Christopher P. - Balbuena, Perla B. **Catalytic Activity and Electrochemical Stability of Ru1-xMxO2 (M = Zr, Nb, Ta): Computational and Experimental Study of the Oxygen Evolution Reaction** [elektronický dokument]. DOI 10.1021/acsami.4c01408 In: **ACS applied materials and interfaces**. Washington: American Chemical Society, 2024, Roč. 16, č. 13, s. 16373-16398 [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCO ; WOS CC, s. 16373 - 16398

2024 [01/20] / **USA** - Wang, Jie - Wang, Gui Chang. **Mechanisms of CH4 activation over oxygen-preadsorbed transition metals by ReaxFF and AIMD simulations** [elektronický dokument]. DOI 10.1002/jcc.27233 In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2024, Roč. 45, č. 5, s. 238-246 [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO ; CCC ; WOS CC, s. 238 - 246

2024 [01/20] / **DEU** - Chaudhary, Payal - Zagalskaya, Alexandra - Over, Herbert - Alexandrov, Vitaly. **Strain-Dependent Activity-Stability Relations in RuO2 and IrO2 Oxygen Evolution Catalysts** [elektronický dokument]. DOI 10.1002/celc.202300659 In: **ChemElectroChem**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 11, č. 1, art. no. e202300659 [online] [tlačená forma]. ISSN (online) 2196-0216. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Xie, Yun - Xia, Guang Jie - Gong, Wei Ping - Zhu, Fang Long - Zhao, Zhen Ting - Wang, Yang Gang. **Mechanistic Insight into the Superior Catalytic Activity of Au/Co<inf>3</inf>O<inf>4</inf> Interface in Glucose Sensors** [elektronický dokument]. DOI 10.1021/acscatal.4c03419 In: **ACS Catalysis**. Washington: American Chemical Society, 2024, Roč. 14, č. 17, s. 12956-12969 [online]. ISSN (online) 2155-5435. - SCO ; WOS CC, s. 12956 - 12969

2023 [01/20] / **NLD** - Sun, Zeyang - Perez-Beltran, Saul - Zaheer, Wasif - Defliese, William F. - Banerjee, Sarbajit - Grossman, Ethan L. **Clumped isotope reordering kinetics in strontianite and witherite: Experiments and first-principles simulations** [elektronický dokument]. DOI 10.1016/j.epsl.2023.118467 In: **Earth and Planetary Science Letters**: a letter journal devoted to the development in time of the earth and planetary system. Amsterdam: Elsevier, 2023, Roč. 624, art. no. 118467 [tlačená forma] [online]. ISSN 0012-821X. ISSN (online) 1385-013X. - SCO ; CCC ; WOS CC, s. art. no. 118467

2023 [01/20] / **USA** - Intan, Nadia N. - Pfaendtner, Jim. **Role of Surface Features on the Initial Dissolution of CH3NH3PbI3 Perovskite in Liquid Water: An Ab Initio Molecular Dynamics Study** [elektronický dokument]. DOI 10.1021/acsnano.3c04601 In: **ACS Nano**. Washington: American Chemical Society, 2023, Roč. 17, č. 22, s. 22371-22387 [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO ; CCC ; WOS CC, s. 22371 - 22387

2023 [01/20] / **USA** - Singsen, Sirisak - Hirunsit, Pussana - Suthirakun, Suwit - Balbuena, Perla B. **Polysulfide cluster formation, surface reaction, and role of fluorinated additive on solid electrolyte interphase formation at sodium-metal anode for sodium-sulfur batteries** [elektronický dokument]. DOI 10.1063/5.0136005 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 12, art. no. 124706 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 124706

2023 [01/20] / **USA** - Cao, Wei - Xia, Guang Jie - Yao, Zhen - Zeng, Ke Han - Qiao, Ying - Wang, Yang Gang. **Aldehyde Hydrogenation by Pt/TiO2 Catalyst in Aqueous Phase: Synergistic Effect of Oxygen Vacancy and Solvent Water** [elektronický dokument]. DOI 10.1021/jacsau.2c00560 In: **JACS Au**. Washington: American Chemical Society, 2023, Roč. 3, č. 1, s. 143-153 [online]. ISSN (online) 2691-3704. - SCO ; WOS CC, s. 143 - 153

2023 [01/20] / **USA** - Perez-Beltran, Saul - Zaheer, Wasif - Sun, Zeyang - Defliese, William F. - Banerjee, Sarbajit - Grossman, Ethan L. **Density functional theory and ab initio molecular dynamics reveal atomistic mechanisms for carbonate clumped isotope reordering** [elektronický dokument]. DOI 10.1126/sciadv.adf1701 In: **Science advances**. Washington: American Association for the Advancement of Science, 2023, Roč. 9, č. 26, art. no. eadf1701 [online]. ISSN (online) 2375-2548. - SCO ; CCC ; WOS CC, s. art. no. eadf1701

2022 [01/20] / **USA** - Jiang, Z. - Rappe, A.M. **Uncovering the Electrolyte-Dependent Transport Mechanism of LiO2in Lithium-Oxygen Batteries** [elektronický dokument] In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2022, Roč. 144, č. 48, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 22150 - 22158

2022 [01/20] / **NLD** - Didar, B.R. - Gros, A. **Solvation structure and dynamics of Li and LiO2 and their transformation in non-aqueous organic electrolyte solvents from first-principles simulations** [elektronický dokument] In: **Chinese Journal of Catalysis**: the Journal of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and the Chinese Chemical Society. Amsterdam: Elsevier, 2022, Roč. 43, č. 11, [tlačená forma]. ISSN 1872-2067. ISSN (online) 0253-9837. - SCO, s. 2850 - 2857

2022 [01/20] / **USA** - Li, Y. - Chen, Y.-X. - Liu, Z.-F. **OH-… Au Hydrogen Bond and Its Effect on the Oxygen Reduction Reaction on Au(100) in Alkaline Media** In: **Journal of Physical Chemistry Letters**, 2022, Roč. 13, č. 39. - SCO, s. 9035 - 9043

2022 [01/20] / **USA** - Angarita-Gomez, S. - Balbuena, P.B. **Ion motion and charge transfer through a solid-electrolyte interphase: an atomistic view** [elektronický dokument] In: **Journal of Solid State Electrochemistry**: Current Research and Development in Science and Technology. New York, NY: Springer Nature, 2022, Roč. 26, č. 9, [tlačená forma]. ISSN 1432-8488. ISSN (online) 1433-0768. - SCO, s. 1931 - 1939

2022 [01/20] / **USA** - Godinez-Salomon, J.F. - Ospina-Acevedo, F. - Albiter, L.A. - Bailey, K.O. - Naymik, Z.G. - Mendoza-Cruz, R. - Balbuena, P.B. - Rhodes, C.P. **Titanium Substitution Effects on the Structure, Activity, and Stability of Nanoscale Ruthenium Oxide Oxygen Evolution Electrocatalysts: Experimental and Computational Study** [elektronický dokument] In: **ACS applied nano materials**. Washington: American Chemical Society, 2022, Roč. 5, č. 8, [online]. ISSN (online) 2574-0970. - SCO, s. 11752 - 11775

2022 [01/20] / **GBR** - Angarita-Gomez, S. - Balbuena, P.B. **Ion mobility and solvation complexes at liquid-solid interfaces in dilute, high concentration, and localized high concentration electrolytes** [elektronický dokument] In: **Materials advances**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 3, č. 15, [online]. ISSN (online) 2633-5409. - SCO, s. 6352 - 6363

2022 [01/20] / **USA** - Jiang, Z. - Rappe, A.M. **Structure, Diffusion, and Stability of Lithium Salts in Aprotic Dimethyl Sulfoxide and Acetonitrile Electrolytes** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 25. - SCO, s. 10266 - 10272

2022 [01/20] / **NLD** - Abidi, N. - Steinmann, S.N. **How are transition states modeled in heterogeneous electrocatalysis?** [elektronický dokument] In: **Current Opinion in Electrochemistry**. Amsterdam: Elsevier, 2022, Roč. 33, [tlačená forma] [online]. ISSN 2451-9103. ISSN (online) 2451-9111. - SCO, s. Art. No. 100940

2022 [01/20] / **USA** - Li, Q.-K. - Kutana, A. - Penev, E.S. - Yakobson, B.I. **Iron corrosion in the ´inert´ supercritical CO2, ab initio dynamics insights: How impurities matter** [elektronický dokument] In: **Matter**. Cambridge: Elsevier. Cell Press, 2022, Roč. 5, č. 2, [tlačená forma] [online]. ISSN 2590-2393. ISSN (online) 2590-2385. - SCO, s. 751 - 762

2022 [01/20] / **USA** - Raman, A.S. - Vojvodic, A. **Providing Atomistic Insights into the Dissolution of Rutile Oxides in Electrocatalytic Water Splitting** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 2. - SCO, s. 922 - 932

2022 [01/20] / **NLD** - Wirth, L.J. - Woodward, C. - Farajian, A.A. **Ab initio molecular dynamics of pipe diffusion in fcc Ni beyond transition state theory** [elektronický dokument] In: **Acta Materialia**. Amsterdam: Acta Materialia, 2022, Roč. 222, [tlačená forma] [online]. ISSN 1359-6454. ISSN (online) 1873-2453. - SCO, s. Art. No. 117357

2021 [01/20] / **GBR** - Qi, F. - Yang, Z. - Wang, Y. - Qiu, Q. - Li, H. **Defects in black zirconia responsible for solar energy harvesting** [elektronický dokument] In: **Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2021, Roč. 9, č. 46, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO, s. 16732 - 16740

2021 [01/20] / **NLD** - Hankins, K. - Kamphaus, E.P. - Balbuena, P.B. **Combined density functional theory/kinetic Monte Carlo investigation of surface morphology during cycling of Li-Cu electrodes** [elektronický dokument] In: **Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2021, Roč. 397, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCO, s. Art. No. 139272

2021 [01/20] / **USA** - Jin, M. - Vesely, O. - Heard, C.J. - Kubu, M. - Nachtigall, P. - Cejka, J. - Grajciar, L. **The role of water loading and germanium content in germanosilicate hydrolysis** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 43. - SCO, s. 23744 - 23757

2021 [01/20] / **GBR** - Xie, W. - Hu, P. **Influence of surface defects on activity and selectivity: A quantitative study of structure sensitivity of Pd catalysts for acetylene hydrogenation** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 15, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 5212 - 5222

2021 [01/20] / **USA** - Li, Y. - Liu, Z.-F. **Cross-Sphere Electrode Reaction: The Case of Hydroxyl Desorption during the Oxygen Reduction Reaction on Pt(111) in Alkaline Media** In: **Journal of Physical Chemistry Letters**, 2021, Roč. 12, č. 28. - SCO, s. 6448 - 6456

2021 [01/20] / **GBR** - Angarita-Gomez, S. - Balbuena, P.B. **Solvationvs.surface charge transfer: an interfacial chemistry game drives cation motion** [elektronický dokument] In: **Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 57, č. 50, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCO, s. 6189 - 6192

2021 [01/20] / **GBR** - Li, K. - Deng, L. - Yi, S. - Wu, Y. - Xia, G. - Zhao, J. - LU, D. - Min, Y. **Boosting the performance by the water solvation shell with hydrogen bonds on protonic ionic liquids: insights into the acid catalysis of the glycosidic bond** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 10, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 3527 - 3538

2021 [01/20] / **USA** - Xie, W. - Xu, J. - Ding, Y. - Hu, P. **Quantitative Studies of the Key Aspects in Selective Acetylene Hydrogenation on Pd(111) by Microkinetic Modeling with Coverage Effects and Molecular Dynamics** [elektronický

dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2021, Roč. 11, č. 7, [online]. ISSN (online) 2155-5435. - SCO, s. 4094 - 4106

2021 [01/20] / **USA** - Kristoffersen, H.H. - Chan, K. **Towards constant potential modeling of CO-CO coupling at liquid water-Cu(1 0 0) interfaces** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 396, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 251 - 260

2020 [01/12] / **NLD** - Ta, H.T.T. - Tieu, A.K. - Zhu, H. - Yu, H. - Tran, N.V. - Tran, B.H. - Wan, S. - Ta, T.D. **Ab initio study on physical and chemical interactions at borates and iron oxide interface at high temperature** [elektronický dokument] In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2020, Roč. 529, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO, s. Art. No. 110548

2020 [01/12] / **GBR** - Momeni, K. - Ji, Y. - Wang, Y. - Paul, S. - Neshani, S. - Yilmaz, D.E. - Shin, Y.K. - Zhang, D. - Jiang, J.-W. - Park, H.S. - Sinnott, S. - van Duin, A. - Crespi, V. - Chen, L.-Q. **Multiscale computational understanding and growth of 2D materials: a review** [elektronický dokument] In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2020, Roč. 6, č. 1, [online]. ISSN (online) 2057-3960. - SCO, s. Art. No. 22

2020 [01/12] / **GBR** - Nolte, T.M. - Nauser, T. - Gubler, L. - Hendriks, A.J. - Peijnenburg, W.J.G.M. **Thermochemical unification of molecular descriptors to predict radical hydrogen abstraction with low computational cost** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 40, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 23215 - 23225

2020 [01/12] / **GBR** - Li, Y. - Liu, Z.-F. **Solvated proton and the origin of the high onset overpotential in the oxygen reduction reaction on Pt(111)** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 39, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 22226 - 22235

2020 [01/12] / **GBR** - Xu, J. - Huang, H. - Hu, P. **An approach to calculate the free energy changes of surface reactions using free energy decomposition on: Ab initio brute-force molecular dynamics trajectories** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 21340 - 21349

2020 [01/12] / **GBR** - Angarita-Gomez, S. - Balbuena, P.B. **Insights into lithium ion deposition on lithium metal surfaces** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 21369 - 21382

2020 [01/12] / Zagalskaya, A. - Alexandrov, V. **Mechanistic Study of IrO2 Dissolution during the Electrocatalytic Oxygen Evolution Reaction** In: **Journal of Physical Chemistry Letters**, 2020, Roč. 11, č. 7. - SCO, s. 2695 - 2700

2020 [01/12] / **DEU** - Anjum, U. - Agarwal, M. - Khan, T.S. - Haider, M.A. **Mechanistic Elucidation of Surface Cation Segregation in Double Perovskite PrBaCo2O5+delta Material using MD and DFT Simulations for Solid Oxide Fuel Cells** [elektronický dokument] In: **Ionics**: International Journal of Ionics The Science and Technology of Ionic Motion. Berlín: Springer Nature. Springer International Publishing AG, 2020, Roč. 26, č. 3, [tlačená forma] [online]. ISSN 0947-7047. ISSN (online) 1862-0760. - SCO, s. 1307 - 1314

2020 [01/12] / **NLD** - Liu, W. - Wang, D. - Ren, J. **Methanol synthesis from CO2/H2 on Cu (1 0 0): Two-tier ab initio molecular dynamics study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 505, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 144528

2020 [01/12] / **GBR** - Kristoffersen, H.H. - Chan, K. - Vegge, T. - Hansen, H.A. **Energy-entropy competition in cation-hydroxyl interactions at the liquid water-Pt(111) interface** [elektronický dokument] In: **Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 56, č. 3, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCO, s. 427 - 430

2019 [01/12] / **USA** - Ke, H.B. - Taylor, C.D. **In: Corrosion**: journal of science and engineering. Houston: NACE International, 2019, Roč. 75, č. 7, [tlačená forma]. ISSN 0010-9312. ISSN (online) 1938-159X. - SCIE ; WOS CC, s. 708 - 726

2019 [01/12] / **USA** - Intan, N.N. - Klyukin, K. - Alexandrov, V. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2019, Roč. 11, č. 22, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 20110 - 20116

2019 [01/12] / Zheng, C. - Rubel, O. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 32. - SCIE ; WOS CC, s. 19385 - 19394

2019 [01/12] / **USA** - Bailleul, S. - Rogge, S.M.J. - Vanduyfhuys, L. - Van Speybroeck, V. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 16, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 3993 - 4010

2019 [01/12] / Reocreux, R. - Michel, C. - Fleurat-Lessard, P. - Sautet, P. - Steinmann, S.N. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 47. - SCIE ; WOS CC, s. 28828 - 28835

2019 [01/12] / Klyukin, K. - Zagalskaya, A. - Alexandrov, V. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 36. - SCIE ; WOS CC, s. 22151 - 22157

2019 [01/12] / **NLD** - Li, Y.K. - Liu, Z.F. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2019, Roč. 736, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / **GBR** - Anjum, U. - Agarwal, M. - Khan, T.S. - - Gupta, R.K. - Haider, M.A. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 11, č. 44, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 21404 - 21418

2018 [01/12] / Lowe, J.S. - Siegel, D.J. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 20. - SCIE ; WOS CC, s. 10714 - 10724

2018 [01/12] / **DEU** - Wang, D. - Sheng, T. - Chen, J.F. - Wang, H.F. - Hu, P. **In: Nature Catalysis**. Berlín: Springer Nature, 2018, Roč. 1, č. 4. ISSN (online) 2520-1158. - SCIE ; WOS CC, s. 291 - 299

2018 [01/12] / Tran, N.V. - Tieu, A.K. - Zhu, H.T. - Ta, H.T.T. - Ta, T.D. - Le, H.M. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 36. - SCIE ; WOS CC, s. 20827 - 20840

2018 [01/12] / **USA** - Chen, L. - Falsig, H. - Janssens, T.V.W. - Gronbeck, H. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2018, Roč. 358, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 179 - 186

2017 [01/12] / Sheng, T. - Sun, S.G. **In: Journal of Electroanalytical Chemistry**, 2017, Roč. 793. ISSN 0022-0728. - SCIE ; WOS CC, s. 184 - 187

2017 [01/12] / **USA** - Van der Mynsbrugge, J. - Janda, A. - Sharada, S.M. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ACS Catalysis**. Washington: American Chemical Society, 2017, Roč. 7, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2685 - 2697

2017 [01/12] / Benedek, R. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 40. - SCIE ; WOS CC, s. 22049 - 22053

2017 [01/12] / **USA** - Ming, Y. - Kumar, N. - Siegel, D.J. **In: ACS Omega**. Washington: American Chemical Society, 2017, Roč. 2, č. 8, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 4921 - 4928

2016 [01/12] / **GBR** - Sheng, T. - Lin, W.F. - Sun, S.G. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 22, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 15304 - 15311

2016 [01/12] / **NLD** - Sheng, T. - Wang, D. - Lin, W.F. - Hu, P. - Sun, S.G. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2016, Roč. 190, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 446 - 454

2016 [01/12] / **NLD** - Muir, J.M.R. - Brodholt, J.P. **In: Physics of the Earth and Planetary Interiors**: a journal devoted to observational and experimental studies of the earth and planetary interiors and their theoretical interpretation by the physical sciences. Amsterdam: Elsevier, 2016, Roč. 257, [tlačená forma] [online]. ISSN 0031-9201. ISSN (online) 1872-7395. - SCIE ; WOS CC, s. 12 - 17

2016 [01/12] / De Wispelaere, K. - Bailleul, S. - Van Speybroeck, V. **In: Catalysis Science & Technology**, 2016, Roč. 6, č. 8. - SCIE ; WOS CC, s. 2686 - 2705

2015 [01/12] / Kumar, N. - Radin, M.D. - Wood, B.C. - Ogitsu, T. - Siegel, D.J. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 17. - SCIE ; WOS CC, s. 9050 - 9060

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2015 [01/12] / **NLD** - Muir, J.M.R. - Brodholt, J.P. **In: Earth and Planetary Science Letters**: a letter journal devoted to the development in time of the earth and planetary system. Amsterdam: Elsevier, 2015, Roč. 417, [tlačená forma] [online]. ISSN 0012-821X. ISSN (online) 1385-013X. - SCIE ; WOS CC, s. 40 - 48

2014 [01/12] / Lanzillo, N.A. - Watson, E.B. - Thomas, J.B. - Nayak, S.K. - Curioni, A. **In: Geochimica et cosmochimica Acta**. [s.l.]: Published by Elsevier Ltd., 2014, Roč. 131. - SCIE ; WOS CC, s. 33 - 46

2014 [01/12] / Zheng, S.H. - Pfaendtner, J. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 20. - SCIE ; WOS CC, s. 10764 - 10770

2013 [01/12] / **USA** - Benco, L. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2013, Roč. 298, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 122 - 129

2012 [01/12] / **USA** - Nakano, H. - Yamamoto, T. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2012, Roč. 136, č. 13, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s.

2012 [01/12] / Hansen, N. - Keil, F.J. **In: Soft Materials**, 2012, Roč. 10, č. 1-3. ISSN 1539445X. ISSN (online) 15394468. -

SCIE ; WOS CC, s. 179 - 201

2010 [01/12] / **USA** - Walker, B. - Michaelides, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2010, Roč. 133, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 174306

2010 [01/12] / Wimmer, E. - Najafabadi, R. - Young, G.A. - Ballard, J.D. - Angeliu, T.M. - Vollmer, J. - Chambers, J.J. - Niimi, H. - Shaw, J.B. - Freeman, C. - Christensen, M. - Wolf, W. - Saxe, P. **In: Journal of Physics-Condensed Matter**, 2010, Roč. 22, č. 38. - SCIE ; WOS CC, s. Art. No. 384215

2009 - spolu : **7**

ADC_017: / Benco, Ľubomír (Autor) (33.333%) - Bučko, Tomáš (Autor) (33.334%) - Hafner, Jürgen (Autor) (33.333%): **Activity and Reactivity of Fe2+ Cations in the Zeolite. Ab Initio Free-Energy MD Calculation of the N2O Dissociation over Iron-Exchanged Ferrierite**. – [recenzované]. – DOI 10.1021/jp906901t. – CCC ; WOS CC ; SCO.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 113, č. 43 (2009), s. 18807-18816 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 4.224 - 2009
Kvartil Q:
2009, AIS - Nanoscience & nanotechnology - Q1; **2009, JIF** - Chemistry, physical - Q1; **2009, JIF** - Materials science, multidisciplinary - Q1; **2009, JIF** - Nanoscience & nanotechnology - Q1

Ohlasy (7):
2020 [01/12] / **GBR** - Bols, M.L. - Rhoda, H.M. - Snyder, B.E.R. - Solomon, E.I. - Pierloot, K. - Schoonheydt, R.A. - Sels, B.F. **Advances in the synthesis, characterisation, and mechanistic understanding of active sites in Fe-zeolites for redox catalysts** [elektronický dokument] In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2020, Roč. 49, č. 42, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO, s. 14749 - 14757

2018 [01/12] / **NLD** - Avdeev, V.I. - Bedilo, A.F. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2018, Roč. 695, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 222 - 227

2017 [01/12] / **CHE** - He, M. - Zhang, J. - Liu, R. - Sun, X.L. - Chen, B.H. **In: Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2017, Roč. 7, č. 1, [online]. ISSN 2073-4344. - SCIE ; WOS CC, s. Art. No. 11

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2013 [01/12] / **USA** - Moors, S.L.C. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 11, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2556 - 2567

2012 [01/12] / Tranca, D.C. - Hansen, N. - Swisher, J.A. - Smit, B. - Keil, F.J. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 44. - SCIE ; WOS CC, s. 23408 - 23417

2011 [01/12] / **USA** - Li, G.N. - Pidko, E.A. - van Santen, R.A. - Feng, Z.C. - Li, C. - Hensen, E.J.M. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2011, Roč. 284, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 194 - 206

ADC_018: / Africh, Cristina (Autor) (12.5%) - Köhler, Lukáš (Autor) (12.5%) - Esch, Friedrich (Autor) (12.5%) - Corso, Martina (Autor) (12.5%) - Dri, Carlo (Autor) (12.5%) - Bučko, Tomáš (Autor) (12.5%) - Kresse, Georg (Autor) (12.5%) - Comelli, Giovanni (Autor) (12.5%): **Effects of Lattice Expansion on the Reactivity of a One-Dimensional Oxide**. – text, ilustr., graf., tab. – [recenzované]. – DOI 10.1021/ja808100f. – SCO ; WOS CC ; SCIE.
In: *Journal of the American Chemical Society* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 0002-7863. – ISSN 1943-2984. – ISSN (online) 1520-5126. – Roč. 131, č. 9 (2009), s. 3253-3259 [tlačená forma] [CD-ROM] [online]
Počet všetkých autorov: 8
[článok]
Lit.: 22
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]

Ohlasy (11):
2024 [01/20] / **NLD** - Yang, Zechao - Freund, Hans Joachim. **High-speed scanning tunneling microscope technique and its application in studying structural dynamics on surfaces** [elektronický dokument]. DOI 10.1016/j.progsurf.2024.100744 In: **Progress in Surface Science**. Amsterdam: Elsevier, 2024, Roč. 99, č. 2, art. no. 100744. ISSN 0079-6816. ISSN (online) 1878-4240. - SCO ; CCC ; WOS CC, s. art. no. 100744

2021 [01/20] / **GBR** - Winkler, P. - Zeininger, J. - Suchorski, Y. - Stoger-Pollach, M. - Zeller, P. - Amati, M. - Gregoratti, L. - Rupprechter, G. **How the anisotropy of surface oxide formation influences the transient activity of a surface reaction** [elektronický dokument] In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2021, Roč. 12, č. 1, [online]. ISSN (online) 2041-1723. - SCO, s. Art. No. 69

2018 [01/12] / **USA** - Hiebel, F. - Karakalos, S. - Xu, Y.F. - Friend, C.M. - Madix, R.J. **In: Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2018, Roč. 61, č. 5-6, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCIE ; WOS CC, s. 299 - 307

2017 [01/12] / von Boehn, B. - Mentes, T.O. - Locatelli, A. - Sala, A. - Imbihl, R. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 36. - SCIE ; WOS CC, s. 19774 - 19785

2012 [01/12] / **USA** - Over, H. **In: Chemical Reviews**. Washington: American Chemical Society, 2012, Roč. 112, č. 6, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 3356 - 3426

2012 [01/12] / Gustafson, J. - Lundgren, E. - Mikkelsen, A. - Borg, M. - Klikovits, J. - Schmid, M. - Varga, P. - Andersen, J.N. **In: Journal of Physics-Condensed Matter**, 2012, Roč. 24, č. 22. - SCIE ; WOS CC, s. Art. No. 225006

2011 [01/12] / **USA** - Cai, Z.H. - Kuru, Y. - Han, J.W. - Chen, Y. - Yildiz, B. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2011, Roč. 133, č. 44, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 17696 - 17704

2010 [01/12] / **NLD** - McEwen, J.S. - Gaspard, P. - de Bocarme, T.V. - Kruse, N. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2010, Roč. 604, č. 17-18, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 1353 - 1368

2010 [01/12] / Mittendorfer, F. **In: Journal of Physics-Condensed Matter**, 2010, Roč. 22, č. 39. - SCIE ; WOS CC, s. Art. No. 393001

2010 [01/12] / **USA** - Li, F.H. - Allegretti, F. - Surnev, S. - Netzer, F.P. **In: Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2010, Roč. 26, č. 21, [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCIE ; WOS CC, s. 16474 - 16480

2009 [01/12] / Nilius, N. **In: Surface Science Reports**: a Review Journal, 2009, Roč. 64, č. 12, [tlačená forma]. ISSN 0167-5729. ISSN (online) 1879-274X. - SCIE ; WOS CC, s. 595 - 659

ADC_019: / Wang, LinJun (Autor) (11.111%) - Rangger, Gerold M. (Autor) (11.111%) - Romaner, Lorenz (Autor) (11.111%) - Heimel, Georg (Autor) (11.111%) - Bučko, Tomáš (Autor) (11.111%) - Ma, ZhongYun (Autor) (11.111%) - Li, QiKai (Autor) (11.111%) - Shuai, Zhigang (Autor) (11.111%) - Zojer, Egbert (Autor) (11.112%): **Electronic Structure of Self-Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability**. – CCC ; SCO ; WOS CC.
In: *Advanced Functional Materials* [textový dokument (print)] [elektronický dokument] . – Weinheim (Nemecko) : John Wiley & Sons. Wiley-VCH. – ISSN 1616-301X. – ISSN (online) 1616-3028. – Roč. 19, č. 23 (2009), s. 3766-3775 [tlačená forma] [online]
Počet všetkých autorov: 9
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (17):
2024 [01/20] / **DEU** - Chen, Lei - Merino, Juan Pedro - Torrent-Sucarrat, Miquel - Hou, Hui Lei - Prato, Maurizio. **Charge Transfer-Induced SERS Enhancement of MoS2/Dopants Dependent on their Interaction Difference**. DOI 10.1002/admi.202400272 In: **Advanced Materials Interfaces**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 11, č. 28, art. no. 2400272 [online]. ISSN 2196-7350. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Guo, Xuefeng - Chen, Hongqiang. **Interface Engineering in Organic Field-Effect Transistors** [textový dokument (print)] [elektronický dokument] . Hoboken: John Wiley & Sons, 2023. 1. vyd. ISBN 9783527840489. ISBN 9783527351459. ISBN 978-3-527-84047-2. - SCO, s. 1 - 272

2022 [01/20] / **CHE** - Xu, M. - Chen, D. - Lin, J. - Lu, X. - Deng, Y. - He, S. - Zhu, X. - Jin, W. - Jin, Y. **Quantum-dot light-emitting diodes with Fermi-level pinning at the hole-injection/hole-transporting interfaces** [elektronický dokument] In: **Nano research**. Peking: Tshinghua Press, 2022, Roč. 15, č. 8, [tlačená forma] [online]. ISSN 1998-0124. ISSN (online) 1998-0000. - SCO, s. 7453 - 7459

2021 [01/20] / **NLD** - Kang, H. - Seong, S. - Ito, E. - Isoshima, T. - Hara, M. - Yoon, H.J. - Noh, J. **Comparative study of structural order, thermal desorption behavior, and work function change of self-assembled monolayers of pentafluorobenzenethiols and tetrafluorobenzenethiols on Au(1 1 1)** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 555, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 149671

2021 [01/20] / **USA** - Diez Cabanes, V. - Van Dyck, C. - Osella, S. - Cornil, D. - Cornil, J. **Challenges for Incorporating Optical Switchability in Organic-Based Electronic Devices** In: **ACS Applied Materials and Interfaces**, 2021, Roč. 13, č. 24. - SCO, s. 27737 - 27748

2021 [01/20] / **USA** - Boucher, D.G. - Kearney, K. - Ertekin, E. - Rose, M.J. **Tuning p-Si(111) Photovoltage via MoleculeœSemiconductor Electronic Coupling** [elektronický dokument] In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2021, Roč. 143, č. 6, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 2567 - 2580

2020 [01/12] / Osella, S. - Kargul, J. - Izzo, M. - Trzaskowski, B. **Architecture and Function of Biohybrid Solar Cell and Solar-to-Fuel Nanodevices** In: **Springer Series in Materials Science**. Cham: Springer, 2020. - SCO, s. 227 - 274

2020 [01/12] / **USA** - Chen, H. - Zhang, W. - Li, M. - He, G. - Guo, X. **Interface Engineering in Organic Field-Effect Transistors: Principles, Applications, and Perspectives** [elektronický dokument] In: **Chemical Reviews**. Washington: American Chemical Society, 2020, Roč. 120, č. 5, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO, s. 2879 - 2949

2018 [01/12] / Abreu, D.S. - Temperini, M.L.A. - Abruna, H.D. - Diogenes, I.C.N. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 11. - SCIE ; WOS CC, s. 6083 - 6092

2017 [01/12] / **GBR** - Yokota, Y. - Akiyama, S. - Kaneda, Y. - Imanishi, A. - Inagaki, K. - Morikawa, Y. - Fukui, K. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 32715 - 32722

2017 [01/12] / Staffa, J.K. - Lorenz, L. - Stolarski, M. - Murgida, D.H. - Zebger, I. - Utesch, T. - Kozuch, J. - Hildebrandt, P. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 40. - SCIE ; WOS CC, s. 22274 - 22285

2016 [01/12] / Yokota, Y. - Akiyama, S. - Kaneda, Y. - Imanishi, A. - Inagaki, K. - Morikawa, Y. - Fukui, K. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 16. - SCIE ; WOS CC, s. 8684 - 8692

2014 [01/12] / **USA** - Tung, R.T. **In: Applied Physics Reviews**. Melville: American Institute of Physics, 2014, Roč. 1, č. 1, [online]. ISSN (online) 1931-9401. - SCIE ; WOS CC, s. Art. No. 011304

2012 [01/12] / Brete, D. - Przyrembel, D. - Eickhoff, C. - Carley, R. - Freyer, W. - Reuter, K. - Gahl, C. - Weinelt, M. **In: Journal of Physics-Condensed Matter**, 2012, Roč. 24, č. 39. - SCIE ; WOS CC, s. Art. No. 394015

2012 [01/12] / **CHE** - Schkolnik, G. - Salewski, J. - Millo, D. - Zebger, I. - Franzen, S. - Hildebrandt, P. **In: International journal of molecular sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2012, Roč. 13, č. 6, [online] [tlačená forma]. ISSN 1661-6596. ISSN (online) 1422-0067. - SCIE ; WOS CC, s. 7466 - 7482

2011 [01/12] / Aqua, T. - Cohen, H. - Sinai, O. - Frydman, V. - Bendikoy, T. - Krepel, D. - Hod, O. - Kronik, L. - Naaman, R. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 50. - SCIE ; WOS CC, s. 24888 - 24892

2011 [01/12] / **USA** - Krzeminski, L. - Cronin, S. - Ndamba, L. - Canters, G.W. - Aartsma, T.J. - Evans, S.D. - Jeuken, L.J.C. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2011, Roč. 115, č. 43, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 12607 - 12614

ADC_020: / Grybos, Robert (Autor) (25%) - Benco, Ľubomír (Autor) (25%) - Bučko, Tomáš (Autor) (25%) - Hafner, Jürgen (Autor) (25%): **Interaction of NO Molecules with Pd Clusters: Ab Initio Density-Functional Study**. – [recenzované]. – DOI 10.1002/jcc.21174. – CCC ; SCO ; WOS CC.
In: *Journal of computational chemistry* [textový dokument (print)] [elektronický dokument] . – Hoboken (USA) : John Wiley & Sons. – ISSN 0192-8651. – ISSN (online) 1096-987X. – Roč. 30, č. 12 (2009), s. 1910-1922 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (19):
2025 [01/20] / **NLD** - Jiang, Tianyan - Li, Shiqi - Liu, Chenmeng - Wu, Hao - He, Haibing - Lei, Shaolan - Bi, Maoqiang. **Adsorption and sensing properties of Pdn (n=1- 4) doped Janus WSSe for characteristic gases (CO, CO2, CH4, C2H4) in power transformer: A DFT study** [elektronický dokument]. DOI 10.1016/j.susc.2025.122840 In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2025, Roč. 762, art. no. 122840 [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 122840

2022 [01/20] / **USA** - Prates, L.M. - de M. Carneiro, J.W. - de M. Cruz, M.T. **Influence of the metal - support and metal - metal interactions on Pd nucleation and NO adsorption in a Pd4/gamma-Al2O3 (110D) model** [elektronický dokument] In: **Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2022, Roč. 28, č. 12, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCO, s. Art. No. 394

2022 [01/20] / **NLD** - Pangh, A. - Esrafili, M.D. - Nejad, M.R. **A DFT investigation of CO and NO adsorption on Cu5Sc and Cu6Sc+ metallic clusters** [elektronický dokument] In: **Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2022, Roč. 1210, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCO, s. Art. No. 113657

2018 [01/12] / **FRA** - Tielens, F. - Bazin, D. **In: Comptes Rendus Chimie**. [s.l.]: Elsevier, 2018, Roč. 21, č. 3-4, [tlačená forma] [online]. ISSN 1631-0748. ISSN (online) 1878-1543. - SCIE ; WOS CC, s. 174 - 181

2018 [01/12] / **GBR** - Dutta, A. - Mondal, P. **In: New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2018, Roč. 42, č. 2, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCIE ; WOS CC, s. 1121 - 1132

2017 [01/12] / **USA** - Begum, P. - Deka, R.C. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2017, Roč. 147, č. 2, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 581 - 591

2017 [01/12] / **USA** - Salazar-Villanueva, M. - Hernandez, A.B. - Mendez, J.F. - Cid, A.A.P. - Valdez, S. **In: Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2017, Roč. 23, č. 12, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCIE ; WOS CC, s. Art. No. 332

2016 [01/12] / **BRA** - Prates, L.M. - Ferreira, G.B. - Carneiro, J.W.M. - de Almeida, W.B. - Carauta, A.N.M. - Correia, J.C.G. - Cruz, M.T.M. **In: Journal of the Brazilian Chemical Society**. São Paulo: Sociedade Brasileira de Química, 2016, Roč. 27, č. 11, [tlačená forma] [online]. ISSN 0103-5053. ISSN (online) 1678-4790. - SCIE ; WOS CC, s. 2062 - 2069

2015 [01/12] / Begum, P. - Gogoi, P. - Mishra, B.K. - Deka, R.C. **In: : International journal of quantum chemistry,** 2015, Roč. 115, č. 13. - SCIE ; WOS CC, s. 837 - 845

2014 [01/12] / Zhao, S. - Li, G.Z. - Liu, J.N. - Ren, Y.L. - Lu, W.W. - Wang, J.J. **In: European Physical Journal D**, 2014,

Roč. 68, č. 9. - SCIE ; WOS CC, s. Art. No. 254

2013 [01/12] / **NLD** - Muir, J.M.R. - Idriss, H. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2013, Roč. 617, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 60 - 67

2013 [01/12] / **USA** - Xu, Q.Q. - Yang, H.Q. - Gao, C. - Hu, C.W. **In: Structural Chemistry**: an international journal concerned with energy, structure, and their relationships to chemical, physical, and biological properties: Computational and Experimental Studies of Chemical and Biological Systems. New York: Springer Nature, 2013, Roč. 24, č. 1, [tlačená forma]. ISSN 1040-0400. ISSN (online) 1572-9001. - SCIE ; WOS CC, s. 13 - 23

2012 [01/12] / Piotrowski, M.J. - Piquini, P. - Zeng, Z.H. - Da Silva, J.L.F. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 38. - SCIE ; WOS CC, s. 20540 - 20549

2012 [01/12] / **USA** - Wu, G.F. - Yang, M.L. - Guo, X.Y. - Wang, J.L. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2012, Roč. 33, č. 23, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 1854 - 1861

2012 [01/12] / **NLD** - Zhao, S. - Lu, W.W. - Ren, Y.L. - Ren, Y.L. - Wang, J.J. - Yin, W.P. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2012, Roč. 993, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 90 - 96

2012 [01/12] / **USA** - Xie, H.J. - Lei, Q.F. - Fang, W.J. **In: Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2012, Roč. 18, č. 2, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCIE ; WOS CC, s. 645 - 652

2011 [01/12] / Lacaze-Dufaure, C. - Roques, J. - Mijoule, C. - Sicilia, E. - Russo, N. - Alexiev, V. - Mineva, T. **In: Journal of Molecular Catalysis A-Chemical**, 2011, Roč. 341, č. 1-2. - SCIE ; WOS CC, s. 28 - 34

2011 [01/12] / **NLD** - Zhao, S.A. - Ren, Y.L. - Ren, Y.L. - Wang, J.J. - Yin, W.P. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2011, Roč. 964, č. 1-3, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 298 - 303

2009 [01/12] / Mehmood, F. - Greeley, J. - Curtiss, L.A. **In: Journal of Physical Chemistry C**, 2009, Roč. 113, č. 52. - SCIE ; WOS CC, s. 21789 - 21796

ADC_021: / Bučko, Tomáš (Autor) [UKOPRCFZ] (20%) - Benco, Ľubomír (Autor) (20%) - Dubay, Orest (Autor) (20%) - Dellago, Christoph (Autor) (20%) - Hafner, Jürgen (Autor) (20%): **Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: Ab initio transition path sampling**. – text, obr. – [recenzované]. – DOI 10.1063/1.3265715. – SCO ; SCIE ; WOS CC ; CCC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 131, č. 21 (2009), art. no. 214508 [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 47
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
Nordic List: 1 - 2009

Ohlasy (45):

2025 [01/20] / **DEU** - Göltl, Florian. **Exploring Quality Criteria for the Computational Modeling of Heterogeneous Catalysts** [elektronický dokument]. DOI 10.1002/cphc.202401123 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 11, art. no. e202401123 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Chen, Weixin - Muhtar, Dilxat - Li, Kaili - Xiao, Gaofei - Cao, Jun - Tang, Yueyuan - Qian, Guoyu - Lu, Xueyi - Sun, Yang - Lu, Xia. **Regulating Cation Disorder Triggered-Electronic Reshuffling for Sustainable Conventional Layered Oxide Cathodes** [elektronický dokument]. DOI 10.1021/acs.chemmater.3c02219 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2024, Roč. 36, č. 3, s. 1249-1261 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC, s. 1249 - 1261

2024 [01/20] / **NLD** - Fo, Yumeng - Song, Shaojia - Yang, Kun - Ji, Xiangyang - Yang, Luyuan - Huang, Liusai - Chen, Xinyu - Wu, Xueqiu - Liu, Jian - Zhao, Zhen - Song, Weiyu. **Ab initio molecular dynamics simulation reveals the influence of entropy effect on Co@BEA zeolite-catalyzed dehydrogenation of ethane** [elektronický dokument]. DOI 10.1016/S1872-2067(24)60116-6 In: **Chinese Journal of Catalysis**: the Journal of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and the Chinese Chemical Society. Amsterdam: Elsevier, 2024, Roč. 65, s. 195-205 [tlačená forma]. ISSN 1872-2067. ISSN (online) 0253-9837. - SCO ; CCC, s. 195 - 205

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **GBR** - Hutton, Daniel J. - Göltl, Florian. **Free and internal energies for the adsorption of short alkanes into the zeolite SSZ-13 from ab initio molecular dynamics simulations** [elektronický dokument]. DOI 10.1039/d3cp02523c In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 39, s. 26604-26612 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 26604 - 26612

2023 [01/20] / **USA** - Pigeon, Thomas - Stoltz, Gabriel - Corral-Valero, Manuel - Anciaux-Sedrakian, Ani - Moreaud, Maxime - Lelièvre, Tony - Raybaud, Pascal. **Computing Surface Reaction Rates by Adaptive Multilevel Splitting Combined with Machine Learning and Ab Initio Molecular Dynamics** [elektronický dokument]. DOI 10.1021/acs.jctc.3c00280 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2023, Roč. 19, č. 12, s. 3538-3550 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 3538 - 3550

2022 [01/20] / **USA** - Ma, S. - Liu, Z.-P. **The Role of Zeolite Framework in Zeolite Stability and Catalysis from Recent Atomic Simulation** [elektronický dokument] In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, č. 1-4, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 59 - 68

2021 [01/20] / **USA** - Van der Mynsbrugge, J. - Bell, A.T. **Challenges for the theoretical description of the mechanism and kinetics of reactions catalyzed by zeolites** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 404, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 832 - 849

2021 [01/20] / **USA** - Smith, A.T. - Plessow, P.N. - Studt, F. **Trends in the Reactivity of Proximate Aluminum Sites in H-SSZ-13** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 30. - SCO, s. 16508 - 16515

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2019 [01/12] / **CHE** - Quesne, M.G. - Silveri, F. - de Leeuw, N.H. - Catlow, C.R.A. **In: Frontiers in Chemistry**. Lausanne: Frontiers Media, 2019, Roč. 7, [online]. ISSN (online) 2296-2646. - SCIE ; WOS CC, s. Art. No. 182

2019 [01/12] / **USA** - Li, G.N. - Pidko, E.A. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano-Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 134 - 156

2018 [01/12] / Van der Mynsbrugge, J. - Janda, A. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ChemPhysChem**, 2018, Roč. 19, č. 4. - SCIE ; WOS CC, s. 341 - 358

2018 [01/12] / **GBR** - Grajciar, L. - Heard, C.J. - Bondarenko, A.A. - Polynski, M.V. - Meeprasert, J. - Pidko, E.A. - Nachtigall, P. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 47, č. 22, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 8307 - 8348

2018 [01/12] / **USA** - Plessow, P.N. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 2, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 981 - 990

2018 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Vanduyfhuys, L. - Demuynck, R. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 10, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 9579 - 9595

2017 [01/12] / **USA** - Hu, B. - Kim, W.G. - Sulmonetti, T.P. - Sarazen, M.L. - Tan, S. - So, J. - Liu, Y.J. - Dixit, R.S. - Nair, S. - Jones, C.W. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017, Roč. 9, č. 17, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 3330 - 3337

2017 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 345, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 53 - 69

2017 [01/12] / **USA** - Van der Mynsbrugge, J. - Janda, A. - Sharada, S.M. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ACS Catalysis**. Washington: American Chemical Society, 2017, Roč. 7, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2685 - 2697

2016 [01/12] / **USA** - Lin, F. - Chin, Y.H. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2016, Roč. 341, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 136 - 148

2016 [01/12] / **USA** - Janda, A. - Vlaisavljevich, B. - Lin, L.C. - Smit, B. - Bell, A.T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 14, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 4739 - 4756

2016 [01/12] / **USA** - Tan, S. - Hu, B. - Kim, W.G. - Pang, S.H. - Moore, J.S. - Liu, Y.J. - Dixit, R.S. - Pendergast, J.G. - Sholl, D.S. - Nair, S. - Jones, C.W. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 9,

[online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 5673 - 5683

2016 [01/12] / De Wispelaere, K. - Bailleul, S. - Van Speybroeck, V. **In: Catalysis Science & Technology**, 2016, Roč. 6, č. 8. - SCIE ; WOS CC, s. 2686 - 2705

2015 [01/12] / **USA** - Erichsen, M.W. - De Wispelaere, K. - Hemelsoet, K. - Moors, S.L.C. - Deconinck, T. - Waroquier, M. - Svelle, S. - Van Speybroeck, V. - Olsbye, U. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2015, Roč. 328, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 186 - 196

2015 [01/12] / De Wispelaere, K. - Ensing, B. - Ghysels, A. - Meijer, E.J. - Van Speybroeck, V. **In: Chemistry-A European Journal**, 2015, Roč. 21, č. 26. - SCIE ; WOS CC, s. 9385 - 9396

2015 [01/12] / Tranca, D.C. - Keil, F.J. - Tranca, I. - Calatayud, M. - Dzwigaj, S. - Trejda, M. - Tielens, F. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 24. - SCIE ; WOS CC, s. 13619 - 13631

2015 [01/12] / Janda, A. - Vlaisavljevich, B. - Lin, L.C. - Sharada, S.M. - Smit, B. - Head-Gordon, M. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 19. - SCIE ; WOS CC, s. 10427 - 10438

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2014 [01/12] / **USA** - Jiang, T. - Goltl, F. - Bulo, R.E. - Sautet, P. **In: ACS Catalysis**. Washington: American Chemical Society, 2014, Roč. 4, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2351 - 2358

2014 [01/12] / **GBR** - Van Speybroeck, V. - De Wispelaere, K. - Van der Mynsbrugge, J. - Vandichel, M. - Hemelsoet, K. - Waroquier, M. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 43, č. 21, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7326 - 7357

2013 [01/12] / **USA** - Borghese, S. - Haouas, M. - Sommer, J. - Taulelle, F. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2013, Roč. 305, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 130 - 134

2013 [01/12] / Patrylak, K.I. - Patrylak, L.K. - Repetskyi, I.A. **In: Theoretical and Experimental Chemistry**, 2013, Roč. 49, č. 3. - SCIE ; WOS CC, s. 143 - 157

2013 [01/12] / Sharada, S.M. - Zimmerman, P.M. - Bell, A.T. - Head-Gordon, M. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 24. - SCIE ; WOS CC, s. 12600 - 12611

2013 [01/12] / Hemelsoet, K. - Van der Mynsbrugge, J. - De Wispelaere, K. - Waroquier, M. - Van Speybroeck, V. **In: ChemPhysChem**, 2013, Roč. 14, č. 8. - SCIE ; WOS CC, s. 1526 - 1545

2013 [01/12] / **USA** - Goldsmith, B.R. - Sanderson, E.D. - Bean, D. - Peters, B. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 138, č. 20, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 204105

2013 [01/12] / **USA** - Moors, S.L.C. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 11, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2556 - 2567

2012 [01/12] / Bai, C. - Liu, L.C. - Sun, H. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 12. - SCIE ; WOS CC,

s. 7029 - 7039

2012 [01/12] / **USA** - Gounder, R. - Iglesia, E. **In: Accounts of Chemical Research**. Washington: American Chemical Society, 2012, Roč. 45, č. 2, [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCIE ; WOS CC, s. 229 - 238

2012 [01/12] / **GBR** - Cao, F.L. - Sun, H. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2012, Roč. 2, č. 19, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 7561 - 7568

2012 [01/12] / Hansen, N. - Keil, F.J. **In: Soft Materials**, 2012, Roč. 10, č. 1-3. ISSN 1539445X. ISSN (online) 15394468. - SCIE ; WOS CC, s. 179 - 201

2012 [01/12] / **USA** - Zimmerman, P.M. - Tranca, D.C. - Gomes, J. - Lambrecht, D.S. - Head-Gordon, M. - Bell, A.T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2012, Roč. 134, č. 47, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 19468 - 19476

2012 [01/12] / Tranca, D.C. - Hansen, N. - Swisher, J.A. - Smit, B. - Keil, F.J. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 44. - SCIE ; WOS CC, s. 23408 - 23417

2011 [01/12] / Keil, F.J. **In: Chemie Ingenieur Technik**: Verfahrenstechnik, technische Chemie, Apparatewesen, Biotechnologie, 2011, Roč. 83, č. 12, [tlačená forma]. ISSN 0009-286X. ISSN (online) 1522-2640. - SCIE ; WOS CC, s. 2188 - 2210

2010 [01/12] / **USA** - Hansen, N. - Kerber, T. - Sauer, J. - Bell, A.T. - Keil, F.J. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2010, Roč. 132, č. 33, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 11525 - 11538

ADC_022: / Grybos, Robert (Autor) (25%) - Benco, Ľubomír (Autor) (25%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (25%) - Hafner, Jürgen (Autor) (25%): **Molecular adsorption and metal-support interaction for transition-metal clusters in zeolites: NO adsorption on Pd-n (n=1-6) clusters in mordenite**. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 130, č. 10 (2009), Art. No. 104503 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
Nordic List: 1 - 2009

Ohlasy (30):
2025 [01/20] / **NLD** - Wang, Yilin - Zhao, Wenru - Wu, Yiqing - Walter, Eric D. - Rappé, Kenneth G. - Wang, Yong - Hong, Suk Bong - Mei, Donghai - Gao, Feng. **Mechanistic insights into N2O formation as a side product in NH3-SCR over small pore Cu-zeolites**. DOI 10.1016/j.apcatb.2025.125540 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2025, Roč. 378, art. no. 125540 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s. art. no. 125540

2024 [01/20] / **GBR** - Boekfa, Bundet - Maihom, Thana - Ehara, Masahiro - Limtrakul, Jumras. **Investigation of the Suzuki–Miyaura cross-coupling reaction on a palladium H-beta zeolite with DFT calculations** [elektronický

dokument]. DOI 10.1038/s41598-023-51116-x In: **Scientific reports**. Londýn: Springer Nature. Nature Publishing Group, 2024, Roč. 14, č. 1, art. no. 611 [online]. ISSN (online) 2045-2322. - SCO ; CCC ; WOS CC, s. art. no. 611

2024 [01/20] / **USA** - He, Guangyuan - Mei, Donghai. **Deciphering reaction mechanism network of n-heptane dehydrocyclization over H-ZSM-5 zeolite** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115623 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 436, art. no. 115623 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. art. no. 115623

2024 [01/20] / **GBR** - He, Guangyuan - Mei, Donghai. **The critical role of the active [GaH]2+ site in n-heptane dehydrocyclization over Ga/H-ZSM-5 zeolite** [elektronický dokument]. DOI 10.1039/d4cy00648h In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 18, s. 5450-5463 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 5450 - 5463

2023 [01/20] / **CHE** - Yang, Xiao Xu - Wu, Shao Yi - Guo, Tian Hao - Su, Jie - Wu, Mei - Zhu, Qin Sheng. **Density functional theory studies on the structures and NO molecule adsorption and dissociation of RhmPdn (m + n = 13) clusters** [elektronický dokument]. DOI 10.1007/s11051-023-05884-2 In: **Journal of Nanoparticle Research**: An Interdisciplinary Forum for Nanoscale Science and Technology. Cham: Springer Nature, 2023, Roč. 25, č. 11, art. no. 236 [tlačená forma] [online]. ISSN 1388-0764. ISSN (online) 1572-896X. - SCO ; WOS CC, s. art. no. 236

2022 [01/20] / **USA** - Prates, L.M. - de M. Carneiro, J.W. - de M. Cruz, M.T. **Influence of the metal - support and metal - metal interactions on Pd nucleation and NO adsorption in a Pd4/gamma-Al2O3 (110D) model** [elektronický dokument] In: **Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2022, Roč. 28, č. 12, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCO, s. Art. No. 394

2022 [01/20] / **NLD** - Diaz Soto, L.J. - Nascimento, M.A.C. **The impact of the zeolite local environment on the stability and spectroscopy features of the (CO, NO, NO2)-Pd-(H-MOR, MOR) systems** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 344, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 112228

2022 [01/20] / **CHE** - Xue, W. - Mei, D. **Mechanistic understanding of methane combustion over H-SSZ-13 zeolite encapsulated palladium nanocluster catalysts** [elektronický dokument] In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2022, Roč. 444, [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO, s. Art. No. 136671

2021 [01/20] / **USA** - Hatayama, S. - Kobayashi, K. - Saito, Y. - Fons, P. - Shuang, Y. - Mori, S. - Kolobov, A.V. - Sutou, Y. **Understanding the low resistivity of the amorphous phase of Cr2Ge2Te6 phase-change material: Experimental evidence for the key role of Cr clusters** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 5, č. 8, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 085601

2021 [01/20] / **GBR** - Liu, L. - Corma, A. **Confining isolated atoms and clusters in crystalline porous materials for catalysis** [elektronický dokument] In: **Nature Reviews Materials**. [s.l.]: Springer Nature. Nature Publishing Group, 2021, Roč. 6, č. 3, [online]. ISSN (online) 2058-8437. - SCO, s. 244 - 263

2021 [01/20] / **GBR** - Van der Mynsbrugge, J. - Head-Gordon, M. - Bell, A.T. **Computational modeling predicts the stability of both Pd+and Pd2+ion-exchanged into H-CHA** [elektronický dokument] In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2021, Roč. 9, č. 4, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 2161 - 2174

2020 [01/12] / Rimsza, J.M. - Chapman, K.W. - Nenoff, T.M. **Energetics and Structure of Ag-Water Clusters Formed in**

Mordenite In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 8. - SCO, s. 4517 - 4524

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2019 [01/12] / Mei, D.H. - Gao, F. - Szanyi, J. - Wang, Y. **In: Applied Catalysis A-General**, 2019, Roč. 569. - SCIE ; WOS CC, s. 181 - 189

2017 [01/12] / Huo, P.Y. - Zhang, X.R. - Zhu, J. - Yu, Z.C. **In: Bulletin of Materials Science**, 2017, Roč. 40, č. 6, [tlačená forma] [online]. ISSN 0250-4707. ISSN (online) 0973-7669. - SCIE ; WOS CC, s. 1087 - 1096

2016 [01/12] / **USA** - Rabelo, A.C. - Rosario, A.V. - Trapp, M.A. - Rodrigues, E. - Forim, M. - Pereira, E.C. **In: Journal of Nanoscience and Nanotechnology**. Valencia: American Scientific Publishers, 2016, Roč. 16, č. 9, [tlačená forma] [online]. ISSN 1533-4880. ISSN (online) 1533-4899. - SCIE ; WOS CC, s. 10040 - 10047

2016 [01/12] / **BRA** - Prates, L.M. - Ferreira, G.B. - Carneiro, J.W.M. - de Almeida, W.B. - Carauta, A.N.M. - Correia, J.C.G. - Cruz, M.T.M. **In: Journal of the Brazilian Chemical Society**. São Paulo: Sociedade Brasileira de Química, 2016, Roč. 27, č. 11, [tlačená forma] [online]. ISSN 0103-5053. ISSN (online) 1678-4790. - SCIE ; WOS CC, s. 2062 - 2069

2015 [01/12] / Begum, P. - Gogoi, P. - Mishra, B.K. - Deka, R.C. **In: : International journal of quantum chemistry,** 2015, Roč. 115, č. 13. - SCIE ; WOS CC, s. 837 - 845

2014 [01/12] / Zhao, S. - Li, G.Z. - Liu, J.N. - Ren, Y.L. - Lu, W.W. - Wang, J.J. **In: European Physical Journal D**, 2014, Roč. 68, č. 9. - SCIE ; WOS CC, s. Art. No. 254

2011 [01/12] / **PRK** - Kang, D. - Eum, M.S. - Lee, B. - Bae, T.S. - Lee, K.R. - Lim, H.B. - Hur, N.H. **In: Bulletin of the Korean Chemical Society**. Soul: The Korean Chemical Society, 2011, Roč. 32, č. 10, [online]. ISSN (online) 1229-5949. - SCIE ; WOS CC, s. 3712 - 3719

2011 [01/12] / Guesmi, H. - Costa, D. - Berthomieu, D. - Massiani, P. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 13. - SCIE ; WOS CC, s. 5607 - 5618

2011 [01/12] / **USA** - Rosch, N. - Petrova, G.P. - Petkov, P.S. - Genest, A. - Kruger, S. - Aleksandrov, H.A. - Vayssilov, G.N. **In: Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2011, Roč. 54, č. 5-7, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCIE ; WOS CC, s. 363 - 377

2011 [01/12] / **NLD** - Zhao, S.A. - Ren, Y.L. - Ren, Y.L. - Wang, J.J. - Yin, W.P. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2011, Roč. 964, č. 1-3, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 298 - 303

2011 [01/12] / Kuang, X.J. - Wang, X.Q. - Liu, G.B. **In: European Physical Journal D**, 2011, Roč. 61, č. 1. - SCIE ; WOS CC, s. 71 - 80

2011 [01/12] / **GBR** - Jin, R. - Zhang, S.L. - Zhang, Y.H. - Huang, S.P. - Wang, P. - Tian, H.P. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2011, Roč. 36, č. 15, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 9069 - 9078

2010 [01/12] / **GBR** - Petrova, G.P. - Vayssilov, G.N. - Rosch, N. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2010, Roč. 12, č. 36, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 11015 - 11020

2010 [01/12] / **GBR** - Kowal, A.T. **In: Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2010, Roč. 108, č. 12, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCIE ; WOS CC, s. 1665 - 1675

2010 [01/12] / **DEU** - Khemthong, P. - Klysubun, W. - Prayoonpokarach, S. - Wittayakun, J. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2010, Roč. 121, č. 1-2, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 131 - 137

2010 [01/12] / **USA** - Kalita, B. - Deka, R.C. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2010, Roč. 140, č. 3-4, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 205 - 211

2010 [01/12] / **USA** - Solis-Calero, C. - Ortega-Castro, J. - Munoz, F. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2010, Roč. 114, č. 48, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 15879 - 15885

ADC_023: / East, Allan L.L. (Autor) (33.333%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (33.334%) - Hafner, Jürgen (Autor) (33.333%): **On the structure and dynamics of secondary n-alkyl cations**. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 131, č. 10 (2009), Art. No. 104314, s. [1-1] [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
Nordic List: 1 - 2009

Ohlasy (10):
2023 [01/20] / **GBR** - Cnudde, Pieter - Waroquier, Michel - Van Speybroeck, Veronique. **Universal descriptors for zeolite topology and acidity to predict the stability of butene cracking intermediates** [elektronický dokument]. DOI 10.1039/d3cy00642e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 16, s. 4857-4872 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4857 - 4872

2022 [01/20] / **NLD** - Gros, A. **Hot atom chemistry: Oxygen at stepped platinum surfaces** In: **Applied surface science advances**: an Open Access Journal Devoted to the Physics and Chemistry of Surfaces and Interfaces. Amsterdam: Elsevier, 2022, Roč. 9, [online]. ISSN 2666-5239. - SCO, s. Art. No. 100240

2018 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Vanduyfhuys, L. - Demuynck, R. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 10, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 9579 - 9595

2018 [01/12] / **USA** - Bockisch, C. - Lorance, E.D. - Hartnett, H.E. - Shock, E.L. - Gould, I.R. **In: ACS Earth and Space Chemistry**. Washington: American Chemical Society, 2018, Roč. 2, č. 8, [online]. ISSN (online) 2472-3452. - SCIE ; WOS

CC, s. 821 - 832

2017 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 345, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 53 - 69

2017 [01/12] / Chibani, S. - Medlej, I. - Lebegue, S. - Angyan, J.G. - Cantrel, L. - Badawi, M. **In: ChemPhysChem**, 2017, Roč. 18, č. 12. - SCIE ; WOS CC, s. 1642 - 1652

2016 [01/12] / **DEU** - Hare, S.R. - Tantillo, D.J. **In: Beilstein Journal of Organic Chemistry**. Frankfurt nad Mohanom: Beilstein-Institut zur Förderung der Chemischen Wissenschaften, 2016, Roč. 12, [tlačená forma]. ISSN 2195-951X. ISSN (online) 1860-5397. - SCIE ; WOS CC, s. 377 - 390

2016 [01/12] / **NLD** - Gross, A. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2016, Roč. 260, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 60 - 65

2012 [01/12] / **USA** - Gounder, R. - Iglesia, E. **In: Accounts of Chemical Research**. Washington: American Chemical Society, 2012, Roč. 45, č. 2, [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCIE ; WOS CC, s. 229 - 238

2011 [01/12] / **USA** - Genaev, A.M. - Sal'nikov, G.E. - Shubin, V.G. **In: Russian Journal of Organic Chemistry**. New York: Pleiades Publishing, 2011, Roč. 47, č. 6, [tlačená forma] [online]. ISSN 1070-4280. ISSN (online) 1608-3393. - SCIE ; WOS CC, s. 862 - 868

2010 - **spolu** : **6**

ADC_024: / Karhánek, David (Autor) (33.333%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (33.334%) - Hafner, Jürgen (Autor) (33.333%): **A density functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: I. Molecular and dissociative adsorption**. – text. – DOI 10.1088/0953-8984/22/26/265005. – CCC ; WOS CC ; SCO.
In: *Journal of Physics* [textový dokument (print)] [elektronický dokument] : Condensed Matter. – Bristol (Veľká Británia) : Institute of Physics. IOP Publishing. – ISSN 0953-8984. – ISSN (online) 1361-648X. – Roč. 22, č. 26 (2010), s. 65005-65005 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (24):
2019 [01/12] / **USA** - Gawraczynski, J. - Kurzydlowski, D. - Ewings, R.A. - Bandaru, S. - Gadomski, W. - Mazej, Z. - Ruani, G. - Bergenti, I. - Jaron, T. - Ozarowski, A. - Hill, S. - Leszczynski, P.J. - Tokar, K. - Derzsi, M. - Barone, P. - Wohlfeld, K. - Lorenzana, J. - Grochala, W. **In: Proceedings of the National Academy of Sciences of the United States of America**. Washington: National Academy of Sciences of the United States of America, 2019, Roč. 116, č. 5, [tlačená forma] [online]. ISSN 0027-8424. ISSN (online) 1091-6490. - SCIE ; WOS CC, s. 1495 - 1500

2019 [01/12] / **NLD** - Yang, C. - Kobayashi, H. - Fukuoka, A. **In: Fuel Processing Technology**. Amsterdam: Elsevier, 2019, Roč. 196, [tlačená forma] [online]. ISSN 0378-3820. ISSN (online) 1873-7188. - SCIE ; WOS CC, s. Art. No. 106155

2018 [01/12] / **NLD** - Ahmad, T. - Mahmood, R. - Georgieva, I. - Zahariev, T. - Tahir, M.N. - Shaheen, M.A. - Gilani, M.A.

- Ahmad, S. **In: Journal of Molecular Structure**. Amsterdam: Elsevier, 2018, Roč. 1153, [tlačená forma] [online]. ISSN 0022-2860. ISSN (online) 1872-8014. - SCIE ; WOS CC, s. 179 - 186

2018 [01/12] / **CHE** - Hu, W. - Cao, X.R. **In: Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2018, Roč. 23, č. 1, [online]. ISSN (online) 1420-3049. - SCIE ; WOS CC, s. Art. No. 126

2018 [01/12] / Wurger, T. - Heckel, W. - Sellschopp, K. - Muller, S. - Stierle, A. - Wang, Y.M. - Noei, H. - Feldbauer, G. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 34. - SCIE ; WOS CC, s. 19481 - 19490

2017 [01/12] / **NLD** - Akhtar, M. - Alharthi, A.I. - Alotaibi, M.A. - Trendafilova, N. - Georgieva, I. - Tahir, M.N. - Mazhar, M. - Isab, A.A. - Hanif, M. - Ahmad, S. **In: Polyhedron**: The International Journal for Research in Inorganic Chemistry. Amsterdam: Elsevier, 2017, Roč. 122, [tlačená forma] [online]. ISSN 0277-5387. ISSN (online) 1873-3719. - SCIE ; WOS CC, s. 105 - 115

2017 [01/12] / **NLD** - Wang, Q.Q. - Huang, J.B. - Li, G.R. - Lin, Z. - Liu, B.H. - Li, Z.P. **In: Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2017, Roč. 339, [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCIE ; WOS CC, s. 20 - 26

2017 [01/12] / Hu, W. - Duan, S. - Luo, Y. **In: Wiley Interdisciplinary Reviews-Computational Molecular Science**, 2017, Roč. 7, č. 2. - SCIE ; WOS CC, s. Art. No. 1293

2017 [01/12] / **GBR** - Hu, W. - Duan, S. - Zhang, Y.J. - Ren, H. - Jiang, J. - Luo, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 32389 - 32397

2016 [01/12] / **NLD** - Li, A.X. - Piquemal, J.P. - Richardi, J. - Calatayud, M. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2016, Roč. 646, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 247 - 252

2016 [01/12] / Raouafi, F. - Seydou, M. - Lassoued, K. - Taleb, A. - Diawara, B. **In: Journal of Physics-Condensed Matter**, 2016, Roč. 28, č. 17. - SCIE ; WOS CC, s. Art. No. 175001

2016 [01/12] / Romo, A.I.B. - Abreu, D.S. - Paulo, T.D. - Carepo, M.S.P. - Sousa, E.H.S. - Lemus, L. - Aliaga, C. - Batista, A.A. - Nascimento, O.R. - Abruna, H.D. - Diogenes, I.C.N. **In: Chemistry-A European Journal**, 2016, Roč. 22, č. 29. - SCIE ; WOS CC, s. 10081 - 10089

2015 [01/12] / Becerril, D. - Noguez, C. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 20. - SCIE ; WOS CC, s. 10824 - 10835

2015 [01/12] / Hu, W. - Duan, S. - Zhang, G.P. - Ma, Y. - Tian, G.J. - Luo, Y. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 52. - SCIE ; WOS CC, s. 28992 - 28998

2014 [01/12] / Altmann, L. - Kunz, S. - Baumer, M. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 17. - SCIE ; WOS CC, s. 8925 - 8932

2014 [01/12] / **GBR** - Vericat, C. - Vela, M.E. - Corthey, G. - Pensa, E. - Cortes, E. - Fonticelli, M.H. - Ibanez, F. - Benitez, G.E. - Carro, P. - Salvarezza, R.C. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 4, č. 53, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 27730 - 27754

2013 [01/12] / Addato, M.A.F. - Rubert, A. - Benitez, G. - Zelaya, E. - Cabello, G. - Cuesta, A. - Thomas, J.E. - Visintin, A. - Salvarezza, R.C. - Fonticelli, M.H. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 15. - SCIE ; WOS CC, s.

7589 - 7597

2013 [01/12] / Quintero, Y.C. - Zhu, H. - Ramprasad, R. **In: Journal of Materials Science**, 2013, Roč. 48, č. 5. ISSN 0022-2461, 1573-4803. - SCIE ; WOS CC, s. 2277 - 2283

2013 [01/12] / **USA** - Kim, C.M. - Bechhoefer, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 138, č. 1, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 014707

2012 [01/12] / Breuer, T. - Celik, M.A. - Jakob, P. - Tonner, R. - Witte, G. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 27. - SCIE ; WOS CC, s. 14491 - 14503

2012 [01/12] / Hockendorf, R.F. - Hao, Q. - Sun, Z. - Fox-Beyer, B.S. - Cao, Y.L. - Balaj, O.P. - Bondybey, V.E. - Siu, C.K. - Beyer, M.K. **In: Journal of Physical Chemistry A**, 2012, Roč. 116, č. 15. - SCIE ; WOS CC, s. 3824 - 3835

2012 [01/12] / **GBR** - Fresch, B. - Boyen, H.G. - Remacle, F. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2012, Roč. 4, č. 14, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 4138 - 4147

2011 [01/12] / Addato, M.A.F. - Rubert, A.A. - Benitez, G.A. - Fonticelli, M.H. - Carrasco, J. - Carro, P. - Salvarezza, R.C. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 36. - SCIE ; WOS CC, s. 17788 - 17798

2010 [01/12] / **USA** - Martin, D.S. - Lane, P.D. - Isted, G.E. - Cole, R.J. - Blanchard, N.P. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2010, Roč. 82, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075428

ADC_025: / Karhánek, David (Autor) (33.333%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (33.334%) - Hafner, Jürgen (Autor) (33.333%): **A density functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: II. Vibrational spectroscopy**. – text. – [recenzované]. – DOI 10.1088/0953-8984/22/26/265006. – CCC ; WOS CC.
In: *Journal of Physics* [textový dokument (print)] [elektronický dokument] : Condensed Matter. – Bristol (Veľká Británia) : Institute of Physics. IOP Publishing. – ISSN 0953-8984. – ISSN (online) 1361-648X. – Roč. 22, č. 26 (2010), s. 65006-65006 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (62):
2020 [01/12] / Xu, K. - Liu, H. - Shi, Y.C. - You, J.Y. - Ma, X.Y. - Cui, H.J. - Yan, Q.B. - Chen, G.C. - Su, G. **In: Carbon**, 2020, Roč. 157. - SCIE ; WOS CC, s. 270 - 276

2019 [01/12] / **GBR** - Kang, S.H. - Park, J. - Woo, S. - Kwon, Y.K. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 43, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 24206 - 24211

2019 [01/12] / **NLD** - Ouasri, A. - Elyoubi, M.S.D. - Rhandour, A. - Georgieva, I. - Zahariev, T. - Trendafilova, N. - Roussel, P. **In: Journal of Molecular Structure**. Amsterdam: Elsevier, 2019, Roč. 1177, [tlačená forma] [online]. ISSN 0022-2860. ISSN (online) 1872-8014. - SCIE ; WOS CC, s. 55 - 67

2019 [01/12] / Xiao, T.T. - Zhang, Z.Y. - Guo, C.B. - Wang, G. - Liao, Y. **In: Spectroscopy and spectral analysis**, 2019, Roč. 39, č. 1. - SCIE ; WOS CC, s. 50 - 55

2019 [01/12] / Akhtar, M. - Georgieva, I. - Zahariev, T. - Trendafilova, N. - Ahmad, T. - Noor, A. - Tahir, M.N. - Mazhar, M. - Isab, A.A. - Ahmad, S. **In: Monatshefte fur Chemie**, 2019, Roč. 150, č. 2. - SCIE ; WOS CC, s. 219 - 231

2019 [01/12] / Therrien, A.J. - Hensley, A.J.R. - Hannagan, R.T. - Schilling, A.C. - Marcinkowski, M.D. - Larson, A.M. - McEwen, J.S. - Sykes, E.C.H. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 5. - SCIE ; WOS CC, s. 2911 - 2921

2019 [01/12] / **USA** - Gan, Z.X. - Yu, Z.Z. - Meng, M. - Xia, W. - Zhang, X.W. **In: APL materials**. Melville: ACA and AIP Publishing, 2019, Roč. 7, č. 3, [online]. ISSN (online) 2166-532X. - SCIE ; WOS CC, s. Art. No. 031107

2019 [01/12] / **USA** - Ahmad, S. - Georgieva, I. - Hanif, M. - Monim-ul-Mehboob, M. - Munir, S. - Sohail, A. - Isab, A.A. **In: Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2019, Roč. 25, č. 4, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCIE ; WOS CC, s. Art. No. 90

2019 [01/12] / **NLD** - Didelot, E. - Sadikin, Y. - Lodziana, Z. - Cerny, R. **In: Solid State Sciences**. Amsterdam: Elsevier. Elsevier Masson, 2019, Roč. 90, [tlačená forma]. ISSN 1293-2558. ISSN (online) 1873-3085. - SCIE ; WOS CC, s. 86 - 94

2019 [01/12] / Lazar, P. - Mach, R. - Otyepka, M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 16. - SCIE ; WOS CC, s. 10695 - 10702

2019 [01/12] / **GBR** - Xu, Y.D. - Wang, C. - Lv, Y.Y. - Chen, Y.B. - Yao, S.H. - Zhou, J. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 31, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 18042 - 18049

2019 [01/12] / **GBR** - Arndt, B. - Sellschopp, K. - Creutzburg, M. - Granaes, E. - Krausert, K. - Vonk, V. - Muller, S. - Noei, H. - Feldbauer, G.B.V. - Stierle, A. **In: Communications chemistry**. [London]: Springer Nature, 2019, Roč. 2, [online]. ISSN (online) 2399-3669. - SCIE ; WOS CC, s. Art. No. 92

2019 [01/12] / **USA** - Torres, J.A.G. - Gotze, J.P. - Grillo, F. - Richardson, N.V. - Fruchtl, H.A. - Hooley, C.A. - Schaub, R. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 3, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 035433

2019 [01/12] / Harvey, J.A. - McEntee, M.L. - Garibay, S.J. - Durke, E.M. - DeCoste, J.B. - Greathouse, J.A. - Gallis, D.F.S. **In: Journal of Physical Chemistry Letters**, 2019, Roč. 10, č. 17. - SCIE ; WOS CC, s. 5142 - 5147

2019 [01/12] / **USA** - Matz, O. - Calatayud, M. **In: Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2019, Roč. 62, č. 12-16, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCIE ; WOS CC, s. 956 - 967

2019 [01/12] / **GBR** - Romero-Muniz, C. - Paredes-Roibas, D. - Hernanz, A. - Gavira-Vallejo, J.M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 35, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 19538 - 19547

2019 [01/12] / **USA** - Bailleul, S. - Yarulina, I. - Hoffman, A.E.J. - Dokania, A. - Abou-Hamad, E. - Chowdhury, A.D. - Pieters, G. - Hajek, J. - De Wispelaere, K. - Waroquier, M. - Gascon, J. - Van Speybroeck, V. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2019, Roč. 141, č. 37, [tlačená forma] [CD-ROM] [online].

ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 14823 - 14842

2018 [01/12] / **USA** - Hensley, A.J.R. - Zhang, J.H. - Vincon, I. - Hernandez, X.P. - Tranca, D. - Seifert, G. - McEwen, J.S. - Wang, Y. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2018, Roč. 361, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 414 - 422

2018 [01/12] / **NLD** - Busch, M. - Mehar, V. - Merte, L.R. - Shipilin, M. - Lundgren, E. - Weaver, J.F. - Gronbeck, H. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2018, Roč. 693, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 84 - 87

2018 [01/12] / **GBR** - Vishwanathan, K. - Springborg, M. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 8, č. 21, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 11357 - 11366

2018 [01/12] / **CHE** - Hu, W. - Cao, X.R. **In: Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2018, Roč. 23, č. 1, [online]. ISSN (online) 1420-3049. - SCIE ; WOS CC, s. Art. No. 126

2018 [01/12] / **GBR** - Gallis, D.F.S. - Harvey, J.A. - Pearce, C.J. - Hall, M.G. - DeCoste, J.B. - Kinnan, M.K. - Greathouse, J.A. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2018, Roč. 6, č. 7, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 3038 - 3045

2018 [01/12] / **NLD** - Ahmad, S. - Saleem, M. - Georgieva, I. - Ruffer, T. - Schaarschmidt, D. - Lang, H. - Murtaza, G. - Hussain, I. - R. - Isab, A.A. - Malik, M.R. - Ali, S. **In: Polyhedron**: The International Journal for Research in Inorganic Chemistry. Amsterdam: Elsevier, 2018, Roč. 149, [tlačená forma] [online]. ISSN 0277-5387. ISSN (online) 1873-3719. - SCIE ; WOS CC, s. 126 - 133

2018 [01/12] / **USA** - Plazanet, M. - Tasseva, J. - Bartolini, P. - Taschin, A. - Torre, R. - Combes, C. - Rey, C. - Di Michele, A. - Verezhak, M. - Gourrier, A. **In: PLoS One**. San Francisco: Public Library of Science, 2018, Roč. 13, č. 8, [online]. ISSN (online) 1932-6203. - SCIE ; WOS CC, s. Art. No. 0201745

2018 [01/12] / **USA** - Speiser, E. - Baumann, A. - Chandola, S. - Esser, N. - Zahedifar, M. - Kratzer, P. - Tegenkamp, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 19, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 195427

2018 [01/12] / Moller, A. - George, J. - Dronskowski, R. **In: Zeitschrift fur Anorganische und Allgemeine Chemie**, 2018, Roč. 644, č. 22. - SCIE ; WOS CC, s. 1485 - 1491

2017 [01/12] / **NLD** - Ouasri, A. - Lambarki, F. - Rhandour, A. - Zahariev, T.K. - Trendafilova, N. - Georgieva, I. **In: Vibrational Spectroscopy**. Amsterdam: Elsevier, 2017, Roč. 88, [tlačená forma] [online]. ISSN 0924-2031. ISSN (online) 1873-3697. - SCIE ; WOS CC, s. 83 - 93

2017 [01/12] / **CHE** - Gorne, A.L. - George, J. - van Leusen, J. - Dronskowski, R. **In: Inorganics**. Bazilej: Multidisciplinary Digital Publishing Institute, 2017, Roč. 5, č. 1, [online]. ISSN (online) 2304-6740. - SCIE ; WOS CC, s. Art. No. 10

2017 [01/12] / Hu, W. - Duan, S. - Luo, Y. **In: Wiley Interdisciplinary Reviews-Computational Molecular Science**, 2017, Roč. 7, č. 2. - SCIE ; WOS CC, s. Art. No. 1293

2017 [01/12] / Wang, B. - Konig, M. - Bromley, C.J. - Yoon, B. - Treanor, M.J. - Torres, J.A.G. - Caffio, M. - Grillo, F. - Fruchtl, H. - Richardson, N.V. - Esch, F. - Heiz, U. - Landman, U. - Schaub, R. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 17. - SCIE ; WOS CC, s. 9413 - 9423

2017 [01/12] / **USA** - Chabungbam, S. - Sen, P. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 96, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045404

2017 [01/12] / **GBR** - Hu, W. - Duan, S. - Zhang, Y.J. - Ren, H. - Jiang, J. - Luo, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 32389 - 32397

2017 [01/12] / Yang, G.Y. - Wu, K.C. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 48. - SCIE ; WOS CC, s. 27139 - 27146

2017 [01/12] / **USA** - Nishino, H. - Fujita, T. - Cuong, N.T. - Tominaka, S. - Miyauchi, M. - Iimura, S. - Hirata, A. - Umezawa, N. - Okada, S. - Nishibori, E. - Fujino, A. - Fujimori, T. - Ito, S. - Nakamura, J. - Hosono, H. - Kondo, T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2017, Roč. 139, č. 39, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 13761 - 13769

2017 [01/12] / Kong, Y. - Hou, D. - Zhang, H.D. - Zheng, X. - Xu, R.X. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 34. - SCIE ; WOS CC, s. 18867 - 18875

2017 [01/12] / Inerbaev, T. - Dauletbekova, A. - Abdrakhmetova, A. **In: Physica B-Condensed Matter**, 2017, Roč. 521. - SCIE ; WOS CC, s. 258 - 263

2017 [01/12] / **USA** - Hu, L. - Wei, D.S. - Huang, X. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 147, č. 24, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 244701

2016 [01/12] / **NLD** - Sicolo, S. - Albe, K. **In: Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2016, Roč. 331, [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCIE ; WOS CC, s. 382 - 390

2016 [01/12] / **GBR** - Rybakov, A.A. - Larin, A.V. **In: Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2016, Roč. 114, č. 15, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCIE ; WOS CC, s. 2299 - 2304

2016 [01/12] / **GBR** - Mu, Y. - Li, S.D. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2016, Roč. 4, č. 30, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 7339 - 7344

2016 [01/12] / Oreskova, G. - Chrappova, J. - Puskelova, J - Simunek, J. - Schwendt, P. - Noga, J. - Gyepes, R. **In: Structral Chemistry Vol. 27, No. 2, 2016**, 2016. - SCIE ; WOS CC, s. 605 - 615

2016 [01/12] / Davantes, A. - Costa, D. - Lefevre, G. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 22. - SCIE ; WOS CC, s. 11871 - 11881

2016 [01/12] / **USA** - Monyoncho, E.A. - Steinmann, S.N. - Michel, C. - Baranova, E.A. - Woo, T.K. - Sautet, P. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 8, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 4894 - 4906

2015 [01/12] / **NLD** - Choi, J. - Pan, L. - Zhang, F. - Diulus, J.T. - Asthagiri, A. - Weaver, J.F. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2015, Roč. 640, [tlačená forma]. ISSN 0039-6028. ISSN (online)

1879-2758. - SCIE ; WOS CC, s. 150 - 158

2015 [01/12] / Davantes, A. - Costa, D. - Lefevre, G. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 22. - SCIE ; WOS CC, s. 12356 - 12364

2015 [01/12] / **USA** - Huang, X. - Beck, M.J. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2015, Roč. 27, č. 8, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 2965 - 2972

2015 [01/12] / **USA** - Casto, L.D. - Clune, A.J. - Yokosuk, M.O. - Musfeldt, J.L. - Williams, T.J. - Zhuang, H.L. - Lin, M.W. - Xiao, K. - Hennig, R.G. - Sales, B.C. - Yan, J.Q. - Mandrus, D. **In: APL materials**. Melville: ACA and AIP Publishing, 2015, Roč. 3, č. 4, [online]. ISSN (online) 2166-532X. - SCIE ; WOS CC, s. Art. No. 041515

2015 [01/12] / **USA** - Buchholz, M. - Li, Q. - Noei, H. - Nefedov, A. - Wang, Y.M. - Muhler, M. - Fink, K. - Woll, C. **In: Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2015, Roč. 58, č. 2-3, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCIE ; WOS CC, s. 174 - 183

2015 [01/12] / **USA** - Herklotz, F. - Hupfer, A. - Johansen, K.M. - Svensson, B.G. - Koch, S.G. - Lavrov, E.V. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 92, č. 15, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 155203

2015 [01/12] / Hu, W. - Duan, S. - Zhang, G.P. - Ma, Y. - Tian, G.J. - Luo, Y. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 52. - SCIE ; WOS CC, s. 28992 - 28998

2015 [01/12] / Bocquet, M.L. - Coasne, B. - Pellenq, R. - Ulm, F.J. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 12. - SCIE ; WOS CC, s. 6511 - 6517

2014 [01/12] / **USA** - Mattsson, A. - Hu, S.L. - Hermansson, K. - Osterlund, L. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 3, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 034705

2014 [01/12] / **GBR** - Seydou, M. - Teyssandier, J. - Battaglini, N. - Kenfack, G.T. - Lang, P. - Tielens, F. - Maurel, F. - Diawara, B. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 4, č. 49, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 25698 - 25708

2014 [01/12] / Zhang, F. - Pan, L. - Li, T. - Diulus, J.T. - Asthagiri, A. - Weaver, J.F. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 49. - SCIE ; WOS CC, s. 28647 - 28661

2014 [01/12] / **CHE** - Oemry, F. - Nakanishi, H. - Kasai, H. - Maekawa, H. - Osumi, K. - Sato, K. **In: Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2014, Roč. 594, [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCIE ; WOS CC, s. 93 - 101

2014 [01/12] / **NLD** - Ravi, C. - Kaur, G. - Bharathi, A. **In: Computational Materials Science**. Amsterdam: Elsevier, 2014, Roč. 90, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 177 - 181

2014 [01/12] / Lee, S.S. - Kim, B. - Lee, S. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 36. - SCIE ; WOS CC, s. 20840 - 20847

2013 [01/12] / Kamali, K. - Ravi, C. - Ravindran, T.R. - Sarguna, R.M. - Sairam, T.N. - Kaur, G. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 48. - SCIE ; WOS CC, s. 25704 - 25713

2013 [01/12] / **USA** - Kim, C.M. - Bechhoefer, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 138, č. 1, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 014707

2012 [01/12] / **USA** - Chiavarino, B. - Crestoni, M.E. - Fornarini, S. - Taioli, S. - Mancini, I. - Tosi, P. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2012, Roč. 137, č. 2, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 024307

2012 [01/12] / **USA** - Kamali, K. - Ravindran, T.R. - Ravi, C. - Sorb, Y. - Subramanian, N. - Arora, A.K. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 86, č. 14, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 144301

2012 [01/12] / Breuer, T. - Celik, M.A. - Jakob, P. - Tonner, R. - Witte, G. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 27. - SCIE ; WOS CC, s. 14491 - 14503

ADC_026: / Bučko, Tomáš (Autor) [UKOPRCFZ] (50%) - Hafner, Jürgen (Autor) (50%): **Entropy effects in hydrocarbon conversion reactions: free-energy integrations and transition-path sampling**. – text, ilustr., graf. – [recenzované]. – DOI 10.1088/0953-8984/22/38/384201. – CCC ; SCO ; WOS CC ; SCIE ; CPCI-S.
In: *Journal of Physics* [textový dokument (print)] [elektronický dokument] : Condensed Matter. – Bristol (Veľká Británia) : Institute of Physics. IOP Publishing. – ISSN 0953-8984. – ISSN (online) 1361-648X. – Roč. 22, č. 38 (2010), art no. 384201, s. [1-10] [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
Lit.: 50
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]

Ohlasy (30):
2025 [01/20] / **USA** - Carrillo, J. Luis - Ezazi, Andrew A. - Perez-Beltran, Saul - Larriuz, Carlos A. - Kohl, Harris - Ayala, Jaime A. - Maji, Arnab - Verkhoturov, Stanislav - Al-Hashimi, Mohammed - Bazzi, Hassan - Weiland, Conan - Jaye, Cherno - Fischer, Daniel A. - Zuin, Lucia - Wang, Jian - Banerjee, Sarbajit. **Electrochemical 6Li isotope enrichment based on selective insertion in 1D tunnel-structured V2O5** [elektronický dokument]. DOI 10.1016/j.chempr.2025.102486 In: **Chem**. Cambridge, MA: Elsevier. Cell Press, 2025, Roč. 11, č. 8, art. no. 102486 [tlačená forma] [online]. ISSN 2451-9308. ISSN (online) 2451-9294. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 102486

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **USA** - Perez-Beltran, Saul - Zaheer, Wasif - Sun, Zeyang - Defliese, William F. - Banerjee, Sarbajit - Grossman, Ethan L. **Density functional theory and ab initio molecular dynamics reveal atomistic mechanisms for carbonate clumped isotope reordering** [elektronický dokument]. DOI 10.1126/sciadv.adf1701 In: **Science advances**. Washington: American Association for the Advancement of Science, 2023, Roč. 9, č. 26, art. no. eadf1701 [online]. ISSN (online) 2375-2548. - SCO ; CCC ; WOS CC, s.

2022 [01/20] / **NLD** - DeLuca, M. - Hibbitts, D. **Predicting diffusion barriers and diffusivities of C6-C12 methylbenzenes in MFI zeolites** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 333, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 111705

2022 [01/20] / **NLD** - Kollias, L. - Collinge, G. - Zhang, D. - Allec, S.I. - Gurunathan, P.K. - Piccini, G. - Yuk, S.F. - Nguyen, M.-T. - Lee, M.-S. - Glezakou, V.-A. - Rousseau, R. **Assessing entropy for catalytic processes at complex reactive interfaces** [elektronický dokument] In: **Annual Reports in Computational Chemistry**. Amsterdam: Elsevier, 2022, [tlačená forma] [online]. ISBN 978-0-323-99092-9. ISBN (online) 978-0-323-99093-6. ISSN 1574-1400. ISSN (online) 1875-5232. - SCO, s. 3 - 51

2022 [01/20] / **NLD** - Wirth, L.J. - Woodward, C. - Farajian, A.A. **Ab initio molecular dynamics of pipe diffusion in fcc Ni beyond transition state theory** [elektronický dokument] In: **Acta Materialia**. Amsterdam: Acta Materialia, 2022, Roč. 222, [tlačená forma] [online]. ISSN 1359-6454. ISSN (online) 1873-2453. - SCO, s. Art. No. 117357

2021 [01/20] / **GBR** - Ayestaran Latorre, C. - Remias, J.E. - Moore, J.D. - Spikes, H.A. - Dini, D. - Ewen, J.P. **Mechanochemistry of phosphate esters confined between sliding iron surfaces** [elektronický dokument] In: **Communications chemistry**. [London]: Springer Nature, 2021, Roč. 4, č. 1, [online]. ISSN (online) 2399-3669. - SCO, s. Art. No. 178

2020 [01/12] / **NLD** - Liu, M. - Vesely, O. - Eliasova, P. - Shamzhy, M. - Lyu, P. - Grajciar, L. **Identification of the most active sites for tetrahydropyranylation in zeolites: MFI as a test case** [elektronický dokument] In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 345, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; SCIE ; WOS CC, s. 165 - 174

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2019 [01/12] / **USA** - Li, G.N. - Pidko, E.A. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano-Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 134 - 156

2018 [01/12] / Li, G.N. - Liu, C. - Rohling, R. - Hensen, E.J.M. - Pidko, E.A. **In: Modelling and Simulation in the Science of Micro- and Meso-Porous Materials**, 2018. - SCIE ; WOS CC, s. 229 - 263

2018 [01/12] / **NLD** - Katada, N. **In: Molecular Catalysis**. Amsterdam: Elsevier, 2018, Roč. 458, [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCIE ; WOS CC, s. 116 - 126

2018 [01/12] / **GBR** - Grajciar, L. - Heard, C.J. - Bondarenko, A.A. - Polynski, M.V. - Meeprasert, J. - Pidko, E.A. - Nachtigall, P. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 47, č. 22, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 8307 - 8348

2017 [01/12] / **USA** - Van der Mynsbrugge, J. - Janda, A. - Sharada, S.M. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ACS Catalysis**. Washington: American Chemical Society, 2017, Roč. 7, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2685 - 2697

2016 [01/12] / **USA** - Janda, A. - Vlaisavljevich, B. - Lin, L.C. - Smit, B. - Bell, A.T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 14, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 4739 - 4756

2016 [01/12] / **USA** - Petraglia, R. - Nicolai, A. - Wodrich, M.D. - Ceriotti, M. - Corminboeuf, C. **In: Journal of**

computational chemistry. Hoboken: John Wiley & Sons, 2016, Roč. 37, č. 1, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 83 - 92

2016 [01/12] / **USA** - Ghorbanpour, A. - Rimer, J.D. - Grabow, L.C. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2287 - 2298

2015 [01/12] / Tranca, D.C. - Keil, F.J. - Tranca, I. - Calatayud, M. - Dzwigaj, S. - Trejda, M. - Tielens, F. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 24. - SCIE ; WOS CC, s. 13619 - 13631

2015 [01/12] / Janda, A. - Vlaisavljevich, B. - Lin, L.C. - Sharada, S.M. - Smit, B. - Head-Gordon, M. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 19. - SCIE ; WOS CC, s. 10427 - 10438

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2015 [01/12] / Yun, J.H. - Lobo, R.F. **In: Catalysis Science & Technology**, 2015, Roč. 5, č. 1. - SCIE ; WOS CC, s. 264 - 273

2014 [01/12] / Jones, A.J. - Iglesia, E. **In: Angewandte Chemie-International Edition**, 2014, Roč. 53, č. 45. - SCIE ; WOS CC, s. 12177 - 12181

2014 [01/12] / **CHE** - Abrams, C. - Bussi, G. **In: Entropy**. Bazilej: Multidisciplinary Digital Publishing Institute, 2014, Roč. 16, č. 1, [online]. ISSN (online) 1099-4300. - SCIE ; WOS CC, s. 163 - 199

2013 [01/12] / Patrylak, K.I. - Patrylak, L.K. - Repetskyi, I.A. **In: Theoretical and Experimental Chemistry**, 2013, Roč. 49, č. 3. - SCIE ; WOS CC, s. 143 - 157

2013 [01/12] / Keil, F.J. **In: Computers & Mathematics with Applications**, 2013, Roč. 65, č. 10. - SCIE ; WOS CC, s. 1674 - 1697

2012 [01/12] / **USA** - Gounder, R. - Iglesia, E. **In: Accounts of Chemical Research**. Washington: American Chemical Society, 2012, Roč. 45, č. 2, [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCIE ; WOS CC, s. 229 - 238

2012 [01/12] / Hansen, N. - Keil, F.J. **In: Soft Materials**, 2012, Roč. 10, č. 1-3. ISSN 1539445X. ISSN (online) 15394468. - SCIE ; WOS CC, s. 69 - 107

2012 [01/12] / **USA** - Zimmerman, P.M. - Tranca, D.C. - Gomes, J. - Lambrecht, D.S. - Head-Gordon, M. - Bell, A.T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2012, Roč. 134, č. 47, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 19468 - 19476

2012 [01/12] / Tranca, D.C. - Hansen, N. - Swisher, J.A. - Smit, B. - Keil, F.J. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 44. - SCIE ; WOS CC, s. 23408 - 23417

2011 [01/12] / Keil, F.J. **In: Chemie Ingenieur Technik**: Verfahrenstechnik, technische Chemie, Apparatewesen, Biotechnologie, 2011, Roč. 83, č. 12, [tlačená forma]. ISSN 0009-286X. ISSN (online) 1522-2640. - SCIE ; WOS CC, s. 2188 - 2210

ADC_027: / Bučko, Tomáš (Autor) [UKOPRCFZ] (25%) - Hafner, Juergen (Autor) (25%) - Lebegue, Sebastien (Autor) (25%) - Ángyán, János G. (Autor) (25%): **Improved Description of the Structure of Molecular and Layered Crystals** : ab Initio DFT Calculations with van der Waals Corrections. – text, tab., obr. – DOI 10.1021/jp106469x. – SCIE ; SCO ; CCC ; WOS CC.
In: *The Journal of Physical Chemistry A* [textový dokument (print)] [elektronický dokument] : Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. – Washington (USA) : American Chemical Society. – ISSN 1089-5639. – ISSN (online) 1520-5215. – Roč. 114, č. 43 (2010), s. 11814-11824 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 85
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (933):
2025 [01/20] / **NLD** - Hastuti, Dian Putri - Kitaoka, Yukie - Imamura, Hiroshi. **Magnetic anisotropy of Co/h-BN heterostructures: First principles calculations** [elektronický dokument]. DOI 10.1016/j.jmmm.2025.173282 In: **Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2025, Roč. 629, art. no. 173282 [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 173282

2025 [01/20] / **GBR** - Jiang, Yuncai - Lei, Shuangying - Li, Zixian - Zhou, Zaifa. **Step-by-step HF etching on the Si(0001) and C(000$\bar{1}$) crystal faces of 4H-SiC with OH or F-OH terminations: a first-principles study of the atomic-scale etching mechanism** [elektronický dokument]. DOI 10.1039/d5cp03118d In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 44, s. 23706-23721 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; WOS CC ; SCIE, s. 23706 - 23721

2025 [01/20] / **GBR** - Zhou, Tao - Fan, Jibin - Duan, Weiwei - Wei, Xing - Liu, Jian - Tian, Ye - Duan, Li. **Highly catalytic Z-scheme GaAs/GeTe heterojunction photocatalysts: A first-principles study** [elektronický dokument]. DOI 10.1016/j.ijhydene.2025.06.203 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 149, art. no. 150013 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; SCIE, s. art. no. 150013

2025 [01/20] / **NLD** - Jiang, Yuncai - Lei, Shuangying - Zhou, Zaifa - Hung, Chiahsiang - Li, Zixian. **Initial dissociative absorption study of HF etchants on Si (0001) and C (000$\bar{1}$) faces with differently terminated 4H–SiC** [elektronický dokument]. DOI 10.1016/j.surfin.2025.105949 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2025, Roč. 59, art. no. 105949 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 105949

2025 [01/20] / **NLD** - Li, Zhen - You, Yang - Zhu, Zhiqi - Wang, Lianghua - Ou, Shengwen - Xu, Jingyue - Yuan, Mingliang. **The synergistic enhancement of electrochemical performance in LiMn0.5Fe0.5PO4 through V doping and V2CTx MXene coating** [elektronický dokument]. DOI 10.1016/j.est.2024.115111 In: **Journal of Energy Storage**. Amsterdam: Elsevier, 2025, Roč. 110, art. no. 115111 [tlačená forma] [online]. ISSN 2352-152X. ISSN (online) 2352-1538. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 115111

2025 [01/20] / **DEU** - Karmakar, Sreejani - Biswas, Shneha - Dutta, Sudipta. **Bandgap Modulation of Graphene Using B3C2N3 as Substrate** [elektronický dokument]. DOI 10.1002/pssr.202500058 In: **Physica Status Solidi**: Rapid Research Letters. Weinheim: John Wiley & Sons. Wiley Blackwell, 2025, Roč. 19, č. 10, art. no. 2500058 [tlačená forma] [online]. ISSN 1862-6254. ISSN (online) 1862-6270. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **GBR** - Karamanis, Ioannis - Dell'Angelo, David - Monnier, Hubert - Badawi, Michael. **Computational screening analysis of iron zeolites for selectively capturing NOx and CO over H2O and CO2** [elektronický dokument]. DOI 10.1039/d5me00003c In: **Molecular Systems Design and Engineering**. [s.l.]: The Royal Society of Chemistry, 2025, Roč. 10, č. 10, s. 855-867 [online]. ISSN (online) 20589689. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 855 - 867

2025 [01/20] / **USA** - Yao, Zhibo - Liu, Yachao - Zheng, Tongxing - Liu, Jiang - Jia, Wanli - Wang, Vei. **Low Ferroelectric Switching Barriers and Stacking-Insensitive Electronic Structures in CrX2(X = S, Se, Te) Bilayers Enabled by Weak Interlayer Coupling** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c04939 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 42, s. 19134-19144 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO, s. 19134 - 19144

2025 [01/20] / **USA** - Carneiro Queiroz da Silva, G. - Salazar, J. Marcos. **Emergence of an Icosahedral (H2)13 Cluster inside a Pure Silica Faujasite** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c08679 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 14, s. 7031-7039 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 7031 - 7039

2025 [01/20] / **USA** - Sulaiman, Nura M. - Weikun, Liu - Yunhan, Zhen - Douxing, Pan. **Lennard-Jones Potential Parameters and Cut-Off Modifications for Layered Transition Metal Dichalcogenides** [elektronický dokument]. DOI 10.1115/1.4068957 In: **Journal of applied mechanics**. NewYork: American Society of Mechanical Engineers, 2025, Roč. 92, č. 10, art. no. 101010 [tlačená forma]. ISSN 0021-8936. ISSN (online) 1528-9036. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 101010

2025 [01/20] / **USA** - Jinghan, Li - Yutian, Li - Sulaiman, Nura M. - Douxing, Pan. **Lennard-Jones interfacial parameters and cut-off modifications for layered buckled honeycomb bi-elemental crystals** [elektronický dokument]. DOI 10.1063/5.0277888 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2025, Roč. 138, č. 7, art. no. 075303 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 075303

2025 [01/20] / **SGP** - Yang, Xiaotong - Liu, Guili - Liu, Yuan - Zhang, Guoying. **Harnessing strain engineering for adaptive optoelectronics in Janus Ga2SX (X= Se, Te) monolayers** [elektronický dokument]. DOI 10.1142/S0217979225502285 In: **International Journal of Modern Physics B**: Condensed Matter Physics; Statistical Physics; Atomic, Molecular and Optical Physics. Singapur: World Scientific Publishing, 2025, Roč. 39, č. 24, art. no. 2550228 [tlačená forma] [online]. ISSN 0217-9792. ISSN (online) 1793-6578. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **USA** - Gao, Yue - Zou, Wenli - Zhang, Chunmei. **Vacancy-Driven Sizable Shift Current in Centrosymmetric Materials** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c04498 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 37, s. 16855-16862 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 16855 - 16862

2025 [01/20] / **USA** - Wang, Tongtong - Zheng, Jian - Wei, Xin - Shu, Dajun. **Phase diagram of growth modes in graphene growth on copper by vapor deposition** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.9.L021001 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 9, č. 2, art. no. L021001 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. L021001

2025 [01/20] / **GBR** - McIntyre, Samantha M. - Garden, Anna L. **Computational modelling of nanoparticle catalysis** [elektronický dokument]. DOI 10.1039/d4nr04364b In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 24, s. 14491-14520 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC ;

SCIE, s. 14491 - 14520

2025 [01/20] / **USA** - Xiong, Lixin - Su, Neil Qiang. **From Li2CO3 to Li2C2O4: Understanding Discharge Product Decomposition in Li-CO2 Batteries** [elektronický dokument]. DOI 10.1021/acs.inorgchem.5c00832 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2025, Roč. 64, č. 16, s. 8376-8385 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC ; SCIE, s. 8376 - 8385

2025 [01/20] / **NLD** - Liu, Pengfei - Wang, Mingqian - Hu, Wanfei - Feng, Xiaoying - Gao, Xing - Qian, Wei - Wang, Qiang - Zhang, Junying. **Embedded nickel-metallofullerenes (Nin@C60) as an effective catalyst for controlled C-C coupling of CO** [elektronický dokument]. DOI 10.1016/j.mcat.2025.115242 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2025, Roč. 583, art. no. 115242 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 115242

2025 [01/20] / **CHE** - Li, Fajun - Ma, Yuqi - Xu, Rui - Chen, Jingyang - Kan, Shujin - Wang, Guizhi - Xu, Haifeng - Jin, Zhong. **Electrochemically synthesized MoS2 with enhanced S-bonds for hydrogen evolution** [elektronický dokument]. DOI 10.1016/j.jelechem.2024.118906 In: **Journal of Electroanalytical Chemistry**. Lausanne: Elsevier, 2025, Roč. 979, art. no. 118906 [tlačená forma] [online]. ISSN 1572-6657. ISSN (online) 1873-2569. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 118906

2025 [01/20] / **CHE** - Zhang, Ren yun - Liu, Yan - Fan, Zhi yu - Li, Ji dong - Wang, Yi yong - Zhang, Ting an - Xing, Hong xuan - Liu, Yi feng - Gong, Xue qiang. **Leaching kinetics combined with DFT simulation to explore the mechanism of differential phase transformation of calcium in magnesium slag induced by HCl and the preparation of calcium carbonate by electrolytic carbonization** [elektronický dokument]. DOI 10.1016/j.cej.2024.159082 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2025, Roč. 505, art. no. 159082 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 159082

2025 [01/20] / **CHE** - Han, Wei - Xie, You - Hao, Jia Yu - Du, Chen - Li, Jia Qi - Zhang, Miao - Hao, Li Mei - Li, Shao Rong - Wang, Su Fang - Chen, Li Yong - Zhang, Tao. **Ultrahigh photocurrents and polarization sensitivity of BC6N/Janus MoSSe heterostructure photodetector with asymmetric contacts** [elektronický dokument]. DOI 10.1016/j.diamond.2025.111965 In: **Diamond and Related Materials**: international journal on the science and technology of diamond and related materials. Lausanne: Elsevier, 2025, Roč. 152, art. no. 111965 [tlačená forma] [online]. ISSN 0925-9635. ISSN (online) 1879-0062. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 111965

2025 [01/20] / **NLD** - Liu, Xianqing - Liang, Fei - Liu, Shule - Pan, Gechuanqi - Ding, Jing - Lu, Jianfeng. **NaCl-KCl-CaCl2 molten salts for high temperature heat storage: Experimental and deep learning molecular dynamics simulation study** [elektronický dokument]. DOI 10.1016/j.solmat.2024.113275 In: **Solar Energy Materials & Solar Cells**: an International Journal Devoted to Photovoltaic, Photothermal, and Photochemical Solar Energy Conversion. Amsterdam: Elsevier, 2025, Roč. 280, art. no. 113275 [tlačená forma]. ISSN 0927-0248. ISSN (online) 1879-3398. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 113275

2025 [01/20] / **NLD** - Duan, Weiwei - Wei, Xing - Liang, Kanghao - Zhang, Yan - Yang, Yun - Liu, Jian - Tian, Ye - Duan, Li. **The tunable electronic and optical properties of WS2/PtO2 heterojunctions are calculated by first principles** [elektronický dokument]. DOI 10.1016/j.chemphys.2024.112524 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2025, Roč. 591, art. no. 112524 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 112524

2025 [01/20] / **NLD** - shi, Weiqi - Ding, Yifang - Fang, Shaojun - Zhou, Hong - Qi, Jiao - Fan, Jiajie - Zhang, Rongjun - Zhang, Guoqi - Tang, Hongyu. **High-performance type II WSOx/WS2-based heterojunction photodetectors** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.161848 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 683, art. no. 161848 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 161848

2025 [01/20] / **NLD** - Chen, Li Yong - Liu, Yan Yan - Wang, Su Fang - Xie, You - Zhang, Jian Min. **Tuning sensitivity of twin T-graphene towards harmful gas via synergistic effects of doping and strain** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.161857 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 684, art. no. 161857 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 161857

2025 [01/20] / **GBR** - Zheng, Xiao - Han, Xiaoqi - Yao, Wenjiao - Wei, Liangming - Zhu, Jie - Tang, Yongbing. **A bifunctional heterostructure promoting the kinetics and stability of sulfur cathodes in advanced aluminum-sulfur batteries** [elektronický dokument]. DOI 10.1039/d4qi02117g In: **Inorganic Chemistry Frontiers**. London: The Royal Society of Chemistry, 2025, Roč. 12, č. 7, s. 2747-2758 [tlačená forma] [online]. ISSN 2052-1545. ISSN (online) 2052-1553. - SCO ; CCC ; WOS CC ; SCIE, s. 2747 - 2758

2025 [01/20] / **USA** - Yan, Guihua - Pršlja, Paulina - Chen, Gaofeng - Kang, Jiahui - Liu, Yongde - Caro, Miguel A. - Chen, Xi - Zeng, Xianhai - Peng, Bo. **Syngas Conversion to Higher Alcohols via Wood-Framed Cu/Co-Carbon Catalyst** [elektronický dokument]. DOI 10.1021/acscatal.4c07156 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, č. 3, s. 2492-2503 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 2492 - 2503

2025 [01/20] / **NLD** - Li, Lin - Zhang, Zhang - Wang, Jianpei - Yang, Ping. **ZnO/Gra/Si structure to improve photoelectric properties** [elektronický dokument]. DOI 10.1016/j.jpcs.2024.112321 In: **Journal of Physics and Chemistry of Solids**: an International Journal. Amsterdam: Elsevier, 2025, Roč. 196, art. no. 112321 [tlačená forma]. ISSN (online) 0022-3697. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 112321

2025 [01/20] / **NLD** - Liang, Jing - Wang, Su Fang - Chen, Li Yong - Xue, Dan - Xie, You - Zheng, Chunli - Song, Yu Ling. **Enhancing sensitivity of C3N monolayer to CH4 molecule through doping 3d transition metal: A first-principles study** [elektronický dokument]. DOI 10.1016/j.surfin.2024.105671 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2025, Roč. 56, art. no. 105671 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 105671

2025 [01/20] / **GBR** - Liu, Rong - Han, Bing - Li, Fengyu - Chen, Zhongfang. **A cluster-assembled B26 monolayer and its inverse-sandwiched derivative B24P4: stable 2D boron-based materials with topological properties, superconductivity, and electrocatalytic activity** [elektronický dokument]. DOI 10.1039/d5ta03928b In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2025, s. 34659-34670 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC ; SCIE, s. 34659 - 34670

2025 [01/20] / **CHN** - Gao, Peng - Zhang, Yanping - Wang, Min - Yu, Wanfei - Yan, Zihao - Li, Jianbao. **Cost-efficient sunlight-driven thermoelectric electrolysis over Mo-doped Ni5P4 nanosheets for highly efficient alkaline water/seawater splitting** [elektronický dokument]. DOI 10.1016/j.jmst.2024.05.019 In: **Journal of materials science & technology**. Wenhua: Chinese Society of Metals, 2025, Roč. 211, s. 134-144 [tlačená forma] [online]. ISSN 1005-0302. ISSN (online) 1941-1162. - SCO ; WOS CC ; SCIE, s. 134 - 144

2025 [01/20] / **NLD** - Gebru, Medhanie Gebremedhin - Pitussi, Itay - Teller, Hanan - Marammurian Chathoth, Achyuth - Kornweitz, Haya - Medlín, Rostislav - Bělský, Petr - Subramanian, Palaniappan - Schechter, Alex. **Multiphase PtPdSb nanoparticles for direct electrochemical energy conversion using hydrogen-rich dimethyl ether** [elektronický dokument]. DOI 10.1016/j.jpowsour.2025.236301 In: **Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2025, Roč. 632, art. no. 236301 [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 236301

2025 [01/20] / **GBR** - Amairi, Rania - Smiri, Adlen - Jaziri, Sihem. **Layer-number and strain effects on the structural and electronic properties of PtSe2 material** [elektronický dokument]. DOI 10.1088/1361-648X/ad8697 In: **Journal of Physics**: Condensed Matter. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 37, č. 3, art. no. 035501 [tlačená forma]

[online]. ISSN 0953-8984. ISSN (online) 1361-648X. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 035501

2025 [01/20] / **USA** - Zeng, Yan - Ou, Zhenwei - Li, Zhe - Wang, Cheng - Yan, Jiakai - Li, Wenbo - Li, Yan - Dai, Wei - Zhang, Huiting - Taniguchi, Takashi - Watanabe, Kenji - Jiang, Haoqing - Guo, Hongli - Lu, Gang - Zhu, Tong - Wang, Ti - Xu, Hongxing. **Small Twist Angles Accelerate Electron and Hole Transfer in MoSe2/WSe2 Heterostructures** [elektronický dokument]. DOI 10.1021/acsnano.4c18675 In: **ACS Nano**. Washington: American Chemical Society, 2025, Roč. 19, č. 12, s. 12138-12145 [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO ; CCC ; WOS CC ; SCIE, s. 12138 - 12145

2025 [01/20] / **GBR** - Yang, Mei - Wang, Changxin - Song, Minhui - Xie, Lu - Qian, Ping - Su, Yanjing. **Machine learning assisted screening of non-metal doped MXenes catalysts for hydrogen evolution reaction** [elektronický dokument]. DOI 10.1016/j.ijhydene.2025.02.469 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 113, s. 740-748 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC ; SCIE, s. 740 - 748

2025 [01/20] / **USA** - Ren, Fei - Xu, Zongwei. **Atomistic Simulations of Carbon Implantation into hBN for Creating Color Centers** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c07558 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 10, s. 5054-5064 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 5054 - 5064

2025 [01/20] / **USA** - Li, Jialin - Liang, Tao - Sun, Qihua - Sun, Jun - Xu, Yan - Li, Aolin - Duan, Haiming. **Weak Interfacial Coupling Effect on In-Plane Thermal Conductivity of BoronP/JTMD van der Waals Heterostructures** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c07381 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 7, s. 3826-3836 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 3826 - 3836

2025 [01/20] / **NLD** - Li, Zhen - You, Yang - Zhu, Zhiqi - Wang, Lianghua - Ou, Shengwen - Xu, Jingyue - Yuan, Mingliang. **Surface iron concentration gradient: A strategy to suppress Mn3+ Jahn-Teller effect in lithium manganese iron phosphate** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.161689 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 682, art. no. 161689 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 161689

2025 [01/20] / **CHE** - Qu, Li Hua - Wang, Yu - Xia, Si Wen - Nie, Ran - Yin, Le - Zhong, Chong Gui - Zhang, Sheng Li - Zhang, Jian Min - Xie, You. **Interface Effects on the Electronic and Optical Properties of Graphitic Carbon Nitride (g-C3N4)/SnS2: First-Principles Studies** [elektronický dokument]. DOI 10.3390/ma18040892 In: **Materials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 18, č. 4, art. no. 892 [online]. ISSN (online) 1996-1944. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 892

2025 [01/20] / **NLD** - Alrebdi, Tahani A. - Amin, B. **Vertical stacking approach for tailoring electronic and optical properties of ultrathin two-dimensional vdW heterostructures of P-MAB (M=Ti, Zr, Hf; A=S, B=Se)** [elektronický dokument]. DOI 10.1016/j.chemphys.2024.112493 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2025, Roč. 588, art. no. 112493 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **CHE** - Huang, Haishen - Liu, Xiaoying - Sun, Li - Shang, Zhenzhen - Zhou, Tingyan - Li, Ping - Wu, Bo. **First-Principles Investigation of the Structural, Magnetic, and Electronic Properties of Janus MXene Material CrScCO2** [elektronický dokument]. DOI 10.3390/coatings15050580 In: **Coatings**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 5, art. no. 580 [online]. ISSN (online) 2079-6412. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 580

2025 [01/20] / **NLD** - Nikmanesh, Samira - Srinivasan, Seshasai - Safaiee, Rosa. **Ti-decorated SiC2 as a high-performance anode material for Li-ion batteries: A DFT-D2 approach** [elektronický dokument]. DOI 10.1016/j.mtphys.2025.101734 In: **Materials Today Physics**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 54, art. no. 101734 [online]. ISSN (online) 2542-5293. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101734

2025 [01/20] / **NLD** - Nam, Jeong Uk - Kim, Bo Hyeon - Hong, Sung Jin - Jeon, Gi Hong - Park, Jae Won - Kim, Un Jeong - Choi, Yong Seok - Woo, Yun Sung. **Toward selecting optimal support layer for CVD-grown graphene transfer onto arbitrary substrate by surface energy engineering** [elektronický dokument]. DOI 10.1016/j.apsusc.2025.162528 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 689, art. no. 162528 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 162528

2025 [01/20] / **GBR** - Song, Lingling - Su, Chen - Wang, Yixian - Chen, Dongdong - Yang, Yu - Zheng, Xiaohong. **Designing 2D h-BN/MnO2 heterostructure for enhanced spintronic MTJs: half-metallicity induction and high tunnel magnetoresistance performance** [elektronický dokument]. DOI 10.1088/1361-6463/adbcba In: **Journal of Physics D**: Applied Physics. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 58, č. 16, art. no. 165303 [tlačená forma] [online]. ISSN 0022-3727. ISSN (online) 1361-6463. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 165303

2025 [01/20] / **GBR** - Yang, Xiaotong - Liu, Guili - Dai, Ying - Ma, Mengting - Zhang, Guoying. **Reshaping photovoltaic efficiency: Characteristic regulation and future application exploration of GaS/MoTe2 van der Waals heterostructure** [elektronický dokument]. DOI 10.1016/j.mtcomm.2025.112162 In: **Materials today. Communications.**. Oxford: Elsevier, 2025, Roč. 45, art. no. 112162 [online]. ISSN (online) 2352-4928. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 112162

2025 [01/20] / **NLD** - Dang, Minh Triet - Long, Nguyen Truong - Thi Phung, Viet Bac - Trang, Nguyen Thi Bao - Nguyen, Truc Anh - Tran, Thi Nhan - Duy, Nguyen Vo Anh - Van, Nguyen To - Nghia, Nguyen Van - Schall, Peter. **Resolving adsorption mechanism of sodium polysulfides on Tim+1CmO2 MXenes for application in sodium-sulfur batteries: A first-principles study** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.162210 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 687, art. no. 162210 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 162210

2025 [01/20] / **NLD** - Rumthao, Phamei - Vaitheeswaran, G. **Exploring optical isotropy in halide double perovskites X2MgCl4 (X = Na, K, Rb, and Cs) with anisotropic structures**. DOI 10.1016/j.cocom.2025.e01016 In: **Computational condensed matter**. Amsterdam: Elsevier, 2025, Roč. 43, art. no. e01016 [tlačená forma]. ISSN 2352-2143. - SCO ; WOS CC ; ESCI, s. art. no. e01016

2025 [01/20] / **CHN** - Lv, Xiaodong - Han, Ting - Liu, Rong - Li, Fengyu - Gong, Jian - Chen, Zhongfang. **High-throughput theoretical exploration of multifunctional planar MBenes: Magnetism, topology, superconductivity, and anode applications** [elektronický dokument]. DOI 10.1016/j.apmate.2025.100297 In: **Advanced Powder Materials**. Peking: KeAi Communications Co., 2025, Roč. 4, č. 3, art. no. 100297. ISSN (online) 2772-834X. - SCO ; WOS CC ; ESCI ; OA, s. art. no. 100297

2025 [01/20] / **NLD** - Long, Yun - Martin, Jean Michel - Dubreuil, Frederic - Thiebaut, Benoit - Loehle, Sophie - Ta, Huong T.T. - Ferrario, Mauro - Clelia Righi, M. - De Barros Bouchet, Maria Isabel. **Reducing friction and wear with alkyl gallate additives in water-based lubricants**. DOI 10.1016/j.mtnano.2025.100629 In: **Materials Today Nano**. Amsterdam: Elsevier, 2025, Roč. 30, art. no. 100629. ISSN 2588-8420 (online). - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 100629

2025 [01/20] / **NLD** - Yang, Fan - Record, Marie Christine - Boulet, Pascal. **Self-defined monolayers, bilayers and trilayers of two-dimensional Janus MoSSe and Ga2SSe van der Waals homojunctions as potential photocatalysts for**

overall water splitting [elektronický dokument]. DOI 10.1016/j.renene.2025.122829 In: **Renewable Energy**: An International Journal: The Official Journal of WREN - The World Renewable Energy Network. Amsterdam: Elsevier, 2025, Roč. 245, art. no. 122829 [tlačená forma] [online]. ISSN 0960-1481. ISSN (online) 1879-0682. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 122829

2025 [01/20] / **NLD** - Ma, Chao - Li, Wei Yin - Xiao, Xue Feng - Liu, Ya Chao - Geng, Wen Tong - Wang, Vei. **A comparative first-principles study of the electronic and excitonic properties of 2H-CrX2 (X = S, Se, Te) monolayers** [elektronický dokument]. DOI 10.1016/j.physe.2025.116237 In: **Physica E**: Low-Dimensional Systems & Nanostructures. Amsterdam: Elsevier, 2025, Roč. 171, art. no. 116237 [tlačená forma] [online]. ISSN 1386-9477. ISSN (online) 1873-1759. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 116237

2025 [01/20] / **GBR** - Zheng, Zhifan - Yang, Shili - Yu, Shaohui - Cao, Tengfei - Zheng, Xiaohong - Wang, Weiyang - Liu, Yushen. **Switchable half-metallicity in anti-ferromagnetic bilayer NbS2** [elektronický dokument]. DOI 10.1039/d5cp01093d In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 20, s. 10556-10561 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 10556 - 10561

2025 [01/20] / **CHE** - Yang, Fan - Record, Marie Christine - Boulet, Pascal. **From Type II to Z-Scheme: A DFT Study of Enhanced Water Splitting in the SGa2Se/TeMoS Heterojunction** [elektronický dokument]. DOI 10.3390/cryst15050442 In: **Crystals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 5, art. no. 442 [online]. ISSN (online) 2073-4352. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 442

2025 [01/20] / **NLD** - Zhang, Shi Kai - Ye, Xiao Juan - Zheng, Xiao Hong - Liu, Chun Sheng. **Two-dimensional metallic TPHOD-graphene: surface and interface engineering toward a high-performance anode material for potassium-ion batteries** [elektronický dokument]. DOI 10.1016/j.surfin.2025.106468 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2025, Roč. 64, art. no. 106468 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 106468

2025 [01/20] / **GBR** - Xie, Luzhen - Yang, Wenhao - Zhou, Wensheng - Luo, Cheng - Peng, Zejiang - Xiao, Xianbo - Chen, Tong. **Research on hydrogen storage and its gas sensing modulation of two-dimensional BeN4 monolayer in relation to concentration, humidity, and metal modification** [elektronický dokument]. DOI 10.1016/j.fuel.2025.134430 In: **Fuel**: the science and technology of fuel and energy. Oxford: Elsevier, 2025, Roč. 387, art. no. 134430 [tlačená forma] [online]. ISSN 0016-2361. ISSN (online) 1873-7153. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 134430

2025 [01/20] / **GBR** - Zheng, Zhifan - Cao, Tengfei - Liu, Chun Sheng - Zheng, Xiaohong - Hao, Hua - Liu, Yushen - Yu, Shaohui. **Electrically switchable valley polarization and an anomalous valley Hall effect in monolayer and bilayer NbS2** [elektronický dokument]. DOI 10.1039/d5cp02481a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 35, s. 18658-18664 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 10658 - 18664

2025 [01/20] / **USA** - Zhang, Guanghui - Yi, Wencai - Cao, Yiqing - Zhang, Shengli - Liu, Xiaobing. **Activation of N≡N bonds by CN4 tetrahedron leading to energetic carbon polynitrides under high pressure** [elektronický dokument]. DOI 10.1063/5.0282879 In: **Matter and Radiation at Extremes**, 2025, Roč. 10, č. 5, art. no. 057801. ISSN 24682047. ISSN (online) 2468080X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 057801

2025 [01/20] / **DEU** - Li, Zhen - You, Yang - Wang, Lianghua - Ou, Shengwen - Xu, Jingyue - Yuan, Mingliang. **Achieving Ultrahigh Cycling Stability of LiMn0.5Fe0.5PO4 Through Oxygen Vacancy with Jahn-Teller Distortion Accommodation Induced by B-Doping at P-site** [elektronický dokument]. DOI 10.1002/smll.202504227 In: **Small**. Weinheim: John Wiley & Sons, 2025, Roč. 21, č. 33, art. no. 2504227 [tlačená forma] [online]. ISSN 1613-6810. ISSN (online) 1613-6829. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **USA** - Zhao, Zhengbo - Wang, Jie - Liu, Mengxue - Ding, Zihang - Xia, Jingxing - Ding, Jiaxin - Wu, Fang.

Tunable Electronic and Optical Properties of AlSb/In2Te2Se van der Waals Heterostructure via Ferroelectric Substrate [elektronický dokument]. DOI 10.1021/acsaelm.5c00909 In: **ACS Applied Electronic Materials**. Washington: American Chemical Society, 2025, Roč. 7, č. 15, s. 7082-7091 [online]. ISSN (online) 2637-6113. - SCO ; CCC ; WOS CC ; SCIE, s. 7082 - 7091

2025 [01/20] / **USA** - Jonuarti, Riri - Suprijadi - Hidayat, Rahmat - Ratnawulan - Fauzi, Ahmad - Jhora, Fadhila Ulfa - Nizar, Umar Kalmar - Nasra, Edi - Basri, Irma Yulia. **Insight Into Water Adsorption and Dissociation on Gen/hSi: A Density Functional Theory Study** [elektronický dokument]. DOI 10.1002/sia.7415 In: **Surface and Interface Analysis**. Hoboken: John Wiley & Sons, 2025, Roč. 57, č. 8, s. 567-575 [tlačená forma] [online]. ISSN 0142-2421. ISSN (online) 1096-9918. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 567 - 575

2025 [01/20] / **NLD** - Ye, Shengyun - Zhou, Baichuan - Wang, Xuewen - Zhang, Weibin - Feng, Xiaobo - Ahmad, Syed Awais. **First principles exploration of tunable electronic properties in MoSi2N4/AlSb heterostructures via interlayer spacing, external electric fields, and biaxial strain** [elektronický dokument]. DOI 10.1016/j.commatsci.2025.114102 In: **Computational Materials Science**. Amsterdam: Elsevier, 2025, Roč. 258, art. no. 114102 [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 114102

2025 [01/20] / **USA** - Hou, Changsheng - Xin, Jiaqi - Shen, Yiheng - Guo, Yaguang - Wang, Qian. **Giant Bulk Photovoltaic Effect in Penta-PdTe2Induced by Layer Stacking** [elektronický dokument]. DOI 10.1021/acs.jpclett.5c01522 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2025, Roč. 16, č. 28, s. 7177-7186 [online]. ISSN (online) 1948-7185. - SCO ; WOS CC ; SCIE, s. 7177 - 7186

2025 [01/20] / **USA** - Abdukayumov, Khasan - Paull, Oliver - Mičica, Martin - Ibrahim, Fatima - Vojáček, Libor - Wright, Adrien - Massabeau, Sylvain - Mazzola, Federico - Polewczyk, Vincent - Jego, Cyriack - Sharma, Rahul - Vergnaud, Céline - Marty, Alain - De Moraes, Isabelle Gomes - Ouerghi, Abdelkarim - Okuno, Hanako - Jana, Anupam - Kar, Indrani - Fujii, Jun - Vobornik, Ivana - Costa, Leticia Melo - Renault, Olivier - Li, Jing - Bonell, Frédéric - Chshiev, Mairbek. **Monolayer Control of Spin-Charge Conversion in van der Waals Heterostructures** [elektronický dokument]. DOI 10.1103/l41n-qxpd In: **Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 135, č. 1, art. no. 016702 [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 016702

2025 [01/20] / **NLD** - Ta, Huong Thi Thuy - Ferrario, Mauro - Loehlé, Sophie - Righi, Maria Clelia. **Probing additives for green lubricants with the aid of machine learning molecular dynamics: The case of gallate molecules for aqueous solutions** [elektronický dokument]. DOI 10.1016/j.apsusc.2025.162836 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 695, art. no. 162836 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; WOS CC ; SCIE ; OA, s. art. no. 162836

2025 [01/20] / **NLD** - Wu, Huan - Zhu, Huaze - Li, Shaorong - Zhang, Pengli - Xie, You - Zhao, Pengxiang - Wang, Chengyue - Zhang, Chengfu - Qiao, Dongwei - Wang, Hao - Zhang, Lin - Cao, Chuhan - Zhang, Tao. **Effects of biaxial strain on the electronic structure and optical absorptivity of van der Waals heterostructures stacked by MoSTe and ZnO monolayers** [elektronický dokument]. DOI 10.1016/j.apsusc.2025.162861 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 695, art. no. 162861 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 162861

2025 [01/20] / **USA** - Xiong, Lixin - Su, Neil Qiang. **Exploring the Catalytic Role of Mo2C in Lithium-Nitrogen Batteries** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c01110 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 24, s. 10886-10899 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 10886 - 10899

2025 [01/20] / **GBR** - Zhang, Chao - Xiang, Jing - Tian, Liangliang - Hu, Lei - Tang, Hua - Zhu, Pengshu. **Investigation on**

the hydrogen storage properties of alkali-metal-decorated (X = Li, Na, K) B7N5 based on the first-principles [elektronický dokument]. DOI 10.1016/j.ijhydene.2025.05.254 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 139, s. 145-156 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC ; SCIE, s. 145 - 156

2025 [01/20] / **GBR** - Chen, Zheng Yong - Xie, You - Li, Shao Rong - Wang, Su Fang - Chen, Li Yong - Zhang, Tao. **Tunable contact types of VSe2/BC6N van der Waals heterostructures via vertical strain and electric field** [elektronický dokument]. DOI 10.1016/j.mssp.2025.109416 In: **Materials Science in Semiconductor Processing**: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2025, Roč. 192, art. no. 109416 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 109416

2025 [01/20] / **NLD** - Liu, Xianqing - Huang, Fochao - Liang, Fei - Liang, Wenshuo - Liu, Shule - Pan, Gechuanqi - Ding, Jing - Lu, Jianfeng. **Thermal properties and structural evolution of Na2SO4-MgSO4 eutectic molten salts for large-scale energy storage: Unveiling mechanisms through deep potential molecular dynamics** [elektronický dokument]. DOI 10.1016/j.solmat.2025.113505 In: **Solar Energy Materials & Solar Cells**: an International Journal Devoted to Photovoltaic, Photothermal, and Photochemical Solar Energy Conversion. Amsterdam: Elsevier, 2025, Roč. 285, art. no. 113505 [tlačená forma]. ISSN 0927-0248. ISSN (online) 1879-3398. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 113505

2025 [01/20] / **USA** - Dong, Xushiyao - Jiang, Jie - Liu, Zhen - Lin, Shaoliang - Zhao, Ling - Xi, Zhenhao. **Architecting CO2-Based Tri-Segmented Polyols via the Cerium-Modified Double Metal Cyanide Catalyst for Sustainable Polyurethane Elastomers**. DOI 10.1021/acsapm.5c00902 In: **ACS Applied Polymer Materials**. Washington DC: American Chemical Society, 2025, Roč. 7, č. 11, s. 7337-7349 [online]. ISSN 2637-6105. - SCO ; CCC ; WOS CC ; SCIE, s. 7337 - 7349

2025 [01/20] / **DEU** - Chen, Xinyu - Bi, Min - Yan, Qingdian - Fan, Deqi - Huang, Biao - Sun, Bianjing - Qin, Chenchen - Chen, Chuntao - Sun, Dongping - He, Qian - Zhao, Ming. **Ce Single Atom-Engineered Amorphous/Crystalline Nanosheets for Enhanced Alkaline Water Electrolysis** [elektronický dokument]. DOI 10.1002/adma.202508893 In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 37, č. 50, art. no. e08893 [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. e08893

2025 [01/20] / **NLD** - Xie, You - Chen, Zheng Yong - Jin, Xin Wen - Liu, Yi An - Wang, Jia Hao - Chen, Li Yong - Zhang, Tao. **Atomic vacancy effects on enhanced photoresponse in 2D MoS2/VSe2 lateral heterostructure** [elektronický dokument]. DOI 10.1016/j.physb.2025.417775 In: **Physica B**: Condensed Matter. Amsterdam: Elsevier, 2025, Roč. 717, art. no. 417775 [tlačená forma] [online]. ISSN 0921-4526. ISSN (online) 1873-2135. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 417775

2025 [01/20] / **GBR** - EL Fatouaki, Zakaria - Hrida, El Mustapha - Jabar, Abderrahim - Tahiri, Abdellah - Idiri, Mohamed. **Study by DFT and AIMD: Structural, mechanic, electronic and thermodynamic properties of AZrF6 for application solid electrolyte** [elektronický dokument]. DOI 10.1016/j.ssc.2025.116155 In: **Solid State Communications**: an International Journal. Oxford: Elsevier, 2025, Roč. 405, art. no. 116155 [tlačená forma] [online]. ISSN 0038-1098. ISSN (online) 1879-2766. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 116155

2025 [01/20] / **USA** - Lin, Lisha - Li, Jing. **Strain regulation of the optoelectronic characteristics of arsenene/PtSeS heterostructure: promoting smart diagnosis** [elektronický dokument]. DOI 10.1007/s00894-025-06548-9 In: **Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2025, Roč. 31, č. 11, art. no. 315 [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 315

2025 [01/20] / **USA** - Dattila, Federico - López, Núria. **The Potential of Cations for Carbon Dioxide Electroreduction** [elektronický dokument]. DOI 10.1002/cctc.202500749 In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- &

Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2025, Roč. 17, č. 20, art. no. e00749 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **DEU** - Sosa, Raul Ian - Galante, Mario - Tkatchenko, Alexandre. **Power of the Many-Body Force: Magnitudes and Angles of Atomic Van der Waals Dispersion Forces in Extended Molecular Systems** [elektronický dokument]. DOI 10.1002/sstr.202500226 In: **Small Structures**. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 6, č. 10, art. no. 2500226 [online]. ISSN (online) 26884062. - SCO ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **DEU** - Li, Shu Long - Zhou, Hongyuan - Zhou, Zuhui - Gan, Li Yong - Cai, Fanggong - Zhao, Yong - Long, Jianping - Qiao, Liang. **Synergizing Machine Learning with High-Throughput DFT to Design Efficient Single-Atom Catalysts for Hydrogen Evolution Reaction** [elektronický dokument]. DOI 10.1002/smtd.202501271 In: **Small methods**. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 9, č. 10, art. no. e01271 [online]. ISSN (online) 2366-9608. - SCO ; WOS CC ; SCIE, s. art. no. e01271

2025 [01/20] / **DEU** - Wang, Qiuying - Sang, Zhiyuan - Liu, Wei - Li, Zhenxin - Li, Jun - Nie, Jiahuan - Wang, Qichen - Yang, De'an - Hou, Feng - Liang, Ji. **Industrial-Level H2O2 Electrosynthesis via Defect-Induced Strain in Laser-Fabricated Nickel-Carbon Catalysts and Gas-Diffusion Electrodes** [elektronický dokument]. DOI 10.1002/adfm.202502458 In: **Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 35, č. 40, art. no. 2502458 [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **GBR** - Yang, Xiaotong - Liu, Guili - Zhang, Guoying. **Electric field and strain-driven Janus graphene/Ga2SX (X = Se, Te)/graphene heterostructure: performance optimization and innovative regulation** [elektronický dokument]. DOI 10.1088/1402-4896/ae09dd In: **Physica Scripta**: an international journal for experimental and theoretical physics. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 100, č. 10, art. no. 105909 [tlačená forma] [online]. ISSN 0031-8949. ISSN (online) 1402-4896. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 105909

2025 [01/20] / **GBR** - Jiang, Yuncai - Lei, Shuangying - Hung, Chiahsiang - Li, Zixian. **S-scheme MoSTe/WSeTe heterostructures induced by stacking engineering: A switch-like strategy for efficient photocatalytic hydrogen evolution** [elektronický dokument]. DOI 10.1016/j.ijhydene.2025.151246 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 170, art. no. 151246 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 151246

2025 [01/20] / **USA** - Sheng, Mengqi - Dai, Yuting - Wu, Xian - Zhang, Zhen - Diao, Yu - Xia, Sihao. **Machine Learning Accelerated Calculations of Alkali Metal Adsorption on AlGaN: Mixed Adatoms, Multiple Coverage, and Variable Components** [elektronický dokument]. DOI 10.1021/acs.langmuir.5c02731 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2025, Roč. 41, č. 36, s. 24512-24523 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC ; SCIE, s. 24512 - 24523

2025 [01/20] / **NLD** - Xiao, Xiao Sa - Xie, You - Hao, Li Mei - Liu, Qi Chao - Zou, Yu - Wang, Su Fang - Zhang, Tao. **Biaxial strain engineering of electronic structure and photovoltaic performance in Janus MoSTe-boron phosphide heterostructure** [elektronický dokument]. DOI 10.1016/j.micrna.2025.208191 In: **Micro and Nanostructures**. Amsterdam: Elsevier, 2025, Roč. 205, art. no. 208191 [online]. ISSN (online) 2773-0123. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 208191

2025 [01/20] / **DEU** - Rumthao, Phamei - Mukherjee, Supratik - Muñoz, Alfonso - Singh, David J. - Vaitheeswaran, G. **Optical properties and isotropy in anisotropic alkali tetrafluoroborates** [elektronický dokument]. DOI 10.1016/j.ijleo.2025.172542 In: **Optik**: international journal for light and electron optics. Jena: Elsevier. Urban & Fischer, 2025, Roč. 339, art. no. 172542 [tlačená forma] [online]. ISSN 0030-4026. ISSN (online) 1618-1336. - SCO, s. art. no. 172542

2025 [01/20] / **USA** - Lazaar, Koussai - Aouaini, Fatma - Basha, Beriham - Gueddida, Saber. **Ab initio study of spin-crossover mechanism in Fe(II) complexes with thiazole-based chelating ligands using density functional theory** [elektronický dokument]. DOI 10.1007/s00894-025-06502-9 In: **Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2025, Roč. 31, č. 12, art. no. 329 [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 329

2025 [01/20] / **NLD** - Lazaar, Koussai - Aouaini, Fatma - Alkallas, Fatemah H. - Alyousef, Haifa - Gueddida, Saber. **Exploring the two step spin transition of Fe(NCBH3)(4phpy)2(m-bpypz)2 with ab initio calculations** [elektronický dokument]. DOI 10.1016/j.jssc.2024.125167 In: **Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2025, Roč. 344, art. no. 125167 [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCO ; CCC ; WOS CC, s. art. no. 125167

2024 [01/20] / **NLD** - Hastuti, Dian Putri - Nawa, Kenji - Rhim, S. H. - Nakamura, Kohji. **Theoretical investigation of spin Hall conductivity in graphene/MoS<inf>2</inf> van der Waals heterostructure under external electric field** [elektronický dokument]. DOI 10.1016/j.cap.2023.12.012 In: **Current Applied Physics**. Amsterdam: Elsevier. Elsevier Science, 2024, Roč. 59, s. 71-76 [tlačená forma] [online]. ISSN 1567-1739. ISSN (online) 1878-1675. - SCO ; WOS CC, s. 71 - 76

2024 [01/20] / **NLD** - Diao, Yu - Xia, Sihao - Dai, Yuting - Shi, Hongkai - Wang, Yuyan - Wu, Xian. **Gas adsorption on activated AlGaN photocathode: A first-principle study on charge redistribution, work function variation and emission performance attenuation** [elektronický dokument]. DOI 10.1016/j.surfin.2024.104665 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2024, Roč. 51, art. no. 104665 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC, s. art. no. 104665

2024 [01/20] / **NLD** - He, Shihao - Gao, Lei - Fan, Xiao - Zhou, Hangjing - Xue, Yufei - Zeng, Chunhua. **Thickness-dependent mechanical, electronic, and optical properties of λ-Cu2Se and ζ-Cu2Se: First-principles calculations** [elektronický dokument]. DOI 10.1016/j.cjph.2024.04.042 In: **Chinese Journal of Physics**. Amsterdam: Elsevier, 2024, Roč. 90, s. 83-89 [tlačená forma] [online]. ISSN 0577-9073. ISSN (online) 2309-9097. - SCO, s. 83 - 89

2024 [01/20] / **NLD** - Kitaoka, Yukie - Ueda, Akiko - Imamura, Hiroshi. **Tuning the electronic and magnetic properties of MoS2 bilayers by transition-metal intercalation** [elektronický dokument]. DOI 10.1016/j.jmmm.2024.172168 In: **Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2024, Roč. 602, art. no. 172168 [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCO ; CCC ; WOS CC, s. art. no. 172168

2024 [01/20] / **GBR** - Yang, Fan - Boulet, Pascal - Record, Marie Christine. **Electronic structure and photocatalytic performance of Janus MoSSe/Ga2SSe van der Waals heterostructures** [elektronický dokument]. DOI 10.1016/j.ijhydene.2024.06.042 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2024, Roč. 73, s. 536-546 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC, s. 536 - 546

2024 [01/20] / **GBR** - Guo, Yimeng - Li, Jiangxu - Zhan, Xuepeng - Wang, Chunwen - Li, Min - Zhang, Biao - Wang, Zirui - Liu, Yueyang - Yang, Kaining - Wang, Hai - Li, Wanying - Gu, Pingfan - Luo, Zhaoping - Liu, Yingjia - Liu, Peitao - Chen, Bo - Watanabe, Kenji - Taniguchi, Takashi - Chen, Xing Qiu - Qin, Chengbing - Chen, Jiezhi - Sun, Dongming - Zhang, Jing - Wang, Runsheng - Liu, Jianpeng. **Van der Waals polarity-engineered 3D integration of 2D complementary logic** [elektronický dokument]. DOI 10.1038/s41586-024-07438-5 In: **Nature**. London: Springer Nature. Nature Publishing Group, 2024, Roč. 630, č. 8016, s. 346-352 [tlačená forma] [online]. ISSN 0028-0836. ISSN (online) 1476-4687. - SCO ; CCC ; WOS CC, s. 346 - 352

2024 [01/20] / **USA** - Jiang, Yuncai - Lei, Shuangying - Wang, Mingyuan. **S-Scheme Boron Phosphide/MoS2**

Heterostructure with Excellent Light Conversion Ability for Solar Cells and Water Splitting Photocatalysts [elektronický dokument]. DOI 10.1021/acsami.4c03567 In: **ACS applied materials and interfaces**. Washington: American Chemical Society, 2024, Roč. 16, č. 23, s. 30521-30533 [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCO ; CCC ; WOS CC, s. 30521 - 30533

2024 [01/20] / **GBR** - Niu, Yuan - Ren, Yi - Zhao, Zhenghua - Xu, Yuanpu - He, Wenhao - Lu, Zhibin. **Robustness of frictional anisotropy under high load due to self-folding** [elektronický dokument]. DOI 10.1016/j.triboint.2024.109524 In: **Tribology international**. Guildford: Butterworth Scientific, 2024, Roč. 194, art. no. 109524 [tlačená forma] [online]. ISSN 0301-679X. ISSN (online) 1879-2464. - SCO ; CCC ; WOS CC, s. art. no. 109524

2024 [01/20] / **USA** - Pan, Douxing - Li, Jinghan - Voon, Lok C.Lew Yan - Wei, Peijun. **Determination of Lennard-Jones potential parameters for interfacial interaction in elemental layered crystals** [elektronický dokument]. DOI 10.1063/5.0213582 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2024, Roč. 135, č. 20, art. no. 204301 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC, s. art. no. 204301

2024 [01/20] / **GBR** - Zhang, Guanghui - Yi, Wencai - Cao, Yiqing - Zhang, Shengli - Liu, Xiaobing. **Achieving ultrahigh energy density and excellent stability in carbon pentazole** [elektronický dokument]. DOI 10.1039/d4ta01837k In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2024, Roč. 12, č. 24, s. 14801-14808 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 14801 - 14808

2024 [01/20] / **DEU** - Zhao, Yifei - Li, Zhongyao. **Tuning the Bandgap and Topological Phase Transition in Bilayer Van der Waals Stanane by Electric Field** [elektronický dokument]. DOI 10.1002/pssr.202300496 In: **Physica Status Solidi**: Rapid Research Letters. Weinheim: John Wiley & Sons. Wiley Blackwell, 2024, Roč. 18, č. 5, art. no. 2300496 [tlačená forma] [online]. ISSN 1862-6254. ISSN (online) 1862-6270. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Liu, Min - Tian, Yali - Zhang, Lifang - Zhou, Yan - Wu, Ping. **First-principles study on the properties of Cu-doped in 2H-WSe2** [elektronický dokument]. DOI 10.1557/s43578-024-01311-x In: **Journal of Materials Research**. Warrendale: Materials Research Society, 2024, Roč. 39, č. 8, s. 1300-1312 [tlačená forma] [online]. ISSN 0884-2914. ISSN (online) 2044-5326. - SCO ; CCC ; WOS CC, s. 1300 - 1312

2024 [01/20] / **USA** - Choudhuri, Deep - Rinehart, Alex J. **Interaction between water and point defects inside volume-constrained α-quartz: An ab initio molecular dynamics study at 300 K** [elektronický dokument]. DOI 10.1063/5.0190356 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2024, Roč. 135, č. 16, art. no. 165103 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC, s. art. no. 165103

2024 [01/20] / **GBR** - Li, Shu Long - Song, Xiaogui - Zhou, Zuhui - Zhou, Hongyuan - Qiao, Liang - Zhao, Yong - Gan, Li Yong. **Rational design of single-atom catalysts for efficient H2O2 production via a four-step strategy** [elektronický dokument]. DOI 10.1039/d4ma00732h In: **Materials advances**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 5, č. 20, s. 8223-8232 [online]. ISSN (online) 2633-5409. - SCO ; WOS CC, s. 8223 - 8232

2024 [01/20] / **USA** - Zheng, Xiaohong - Zheng, Zhifan - Yang, Shili - Liu, Chun Sheng - Zhang, Lei - Hao, Hua. **Ferroelectrically induced half-metallicity, giant tunnel electroresistance, and giant tunnel magnetoresistance in spin-semiconducting LaBr2** [elektronický dokument]. DOI 10.1103/PhysRevB.110.115439 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2024, Roč. 110, č. 11, art. no. 115439 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 115439

2024 [01/20] / **USA** - Piliai, Lesia - Castro-Latorre, Pablo - Pchálek, František - Oveysipoor, Shiva - Kosto, Yuliia - Khalakhan, Ivan - Skála, Tomáš - Neyman, Konstantin M. - Alemany, Pere - Vorochta, Michael - Bruix, Albert - Matvija, Peter - Matolínová, Iva. **Electronic and Structural Properties of Thin Iron Oxide Films on CeO2** [elektronický dokument]. DOI 10.1021/acsami.4c05542 In: **ACS applied materials and interfaces**. Washington: American Chemical

Society, 2024, Roč. 16, č. 35, s. 46858-46871 [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCO ; CCC ; WOS CC, s. 46858 - 46871

2024 [01/20] / **USA** - Yang, Jing - Todorova, Mira - Neugebauer, Jörg. **Comparative analysis of surface phase diagrams in aqueous environment: Implicit vs explicit solvation models** [elektronický dokument]. DOI 10.1063/5.0190304 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2024, Roč. 160, č. 16, art. no. 164715 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 164715

2024 [01/20] / **DEU** - Abdukayumov, Khasan - Mičica, Martin - Ibrahim, Fatima - Vojáček, Libor - Vergnaud, Céline - Marty, Alain - Veuillen, Jean Yves - Mallet, Pierre - de Moraes, Isabelle Gomes - Dosenovic, Djordje - Gambarelli, Serge - Maurel, Vincent - Wright, Adrien - Tignon, Jérôme - Mangeney, Juliette - Ouerghi, Abdelkarim - Renard, Vincent - Mesple, Florie - Li, Jing - Bonell, Frédéric - Okuno, Hanako - Chshiev, Mairbek - George, Jean Marie - Jaffrès, Henri - Dhillon, Sukhdeep. **Atomic-Layer Controlled Transition from Inverse Rashba–Edelstein Effect to Inverse Spin Hall Effect in 2D PtSe2 Probed by THz Spintronic Emission** [elektronický dokument]. DOI 10.1002/adma.202304243 In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 36, č. 14, art. no. 2304243 [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **CHE** - Wang, Xiulin - Gao, Yue - Xie, You - Song, Yuling - Gan, Jiangjie. **Adsorption of potassium atoms on twin T-graphene and twin-graphene surfaces for K-ion batteries** [elektronický dokument]. DOI 10.1016/j.diamond.2024.111023 In: **Diamond and Related Materials**: international journal on the science and technology of diamond and related materials. Lausanne: Elsevier, 2024, Roč. 144, art. no. 111023 [tlačená forma] [online]. ISSN 0925-9635. ISSN (online) 1879-0062. - SCO ; CCC ; WOS CC, s. art. no. 111023

2024 [01/20] / **GBR** - Lu, Zhaohu - Jia, Shaolei - Li, Guanghao - Sun, Pingwei - Jiang, Shangrui - Cao, Yingying - Li, Jiayu - Jing, Shiwei. **Calculation of tunable optical and electronic properties of two-dimensional AlSb/BAs heterojunction based on first principles** [elektronický dokument]. DOI 10.1016/j.mssp.2024.108163 In: **Materials Science in Semiconductor Processing**: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2024, Roč. 173, art. no. 108163 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC, s. art. no. 108163

2024 [01/20] / **NLD** - Han, Wei - Xie, You - Song, Yu Ling - Jiang, Ning Ning - Jin, Xin Wen - Wang, Su Fang - Chen, Li Yong - Xiao, Xiao Sa - Chen, Zheng Yong - Gan, Jiang Jie. **Effect of tensile strain on the electronic structure, optical absorptivity, and power conversion efficiency of the BC6N/ZnO van der Waals heterostructure** [elektronický dokument]. DOI 10.1016/j.physe.2024.115908 In: **Physica E**: Low-Dimensional Systems & Nanostructures. Amsterdam: Elsevier, 2024, Roč. 158, art. no. 115908 [tlačená forma] [online]. ISSN 1386-9477. ISSN (online) 1873-1759. - SCO ; CCC ; WOS CC, s. art. no. 115908

2024 [01/20] / **DEU** - Lian, Zan - Dattila, Federico - López, Núria. **Stability and lifetime of diffusion-trapped oxygen in oxide-derived copper CO2 reduction electrocatalysts** [elektronický dokument]. DOI 10.1038/s41929-024-01132-5 In: **Nature Catalysis**. Berlín: Springer Nature, 2024, Roč. 7, č. 4, s. 401-411. ISSN (online) 2520-1158. - SCO ; CCC ; WOS CC, s. 401 - 411

2024 [01/20] / **CHN** - Li, Fengyu - Liu, Yu - Yu, Linke - Lv, Xiaodong - Jin, Peng - Chen, Zhongfang. **Expanding the landscape of anti-MoS2 monolayers: computational exploration of stability and multifaceted properties across the periodic table** [elektronický dokument]. DOI 10.1007/s40843-024-2861-2 In: **Science China materials**. Beijing: Science China Press, 2024, Roč. 67, č. 4, s. 1260-1272 [tlačená forma] [online]. ISSN 2095-8226. ISSN (online) 2199-4501. - SCO ; CCC ; WOS CC, s. 1260 - 1272

2024 [01/20] / **USA** - Yakovlev, Ilya V. - Shubin, Aleksandr A. - Papulovskiy, Evgeniy S. - Toktarev, Alexander V. - Lapina, Olga B. **Repulsive Lateral Interaction of Water Molecules at the Initial Stages of Adsorption in Microporous AlPO4-11 According to 27Al NMR and DFT** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c03969 In:

Langmuir: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2024, Roč. 40, č. 12, s. 6384-6393 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 6384 - 6393

2024 [01/20] / **NLD** - Kitaoka, Yukie - Ueda, Akiko - Imamura, Hiroshi. **Magnetism of MoS2 bilayers with intercalated and surface adsorbed Fe** [elektronický dokument]. DOI 10.1016/j.jmmm.2024.171895 In: **Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2024, Roč. 594, art. no. 171895 [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCO ; CCC ; WOS CC, s. art. no. 171895

2024 [01/20] / **USA** - Paschoal, Vitor H. - Ribeiro, Mauro C.C. **Phase transitions of choline dihydrogen phosphate: A vibrational spectroscopy and periodic DFT study** [elektronický dokument]. DOI 10.1063/5.0189049 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2024, Roč. 160, č. 9, art. no. 094507 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 094507

2024 [01/20] / **NLD** - Lu, Xiuyuan - Roldan, Alberto. **Ammonia cracking on single-atom catalysts: A mechanistic and microkinetic study**. DOI 10.1016/j.apcata.2024.119589 In: **Applied catalysis A, General**: An International Journal Devoted to Catalytic Science and its Applications. Amsterdam: Elsevier, 2024, Roč. 673, art. no. 119589 [tlačená forma]. ISSN 0926-860X. - SCO ; CCC ; WOS CC, s. art. no. 119589

2024 [01/20] / **USA** - González, José E. - Besse, Rafael - Lima, Matheus P. - Da Silva, Juarez L.F. **Decoding Van der Waals Impact on Chirality Transfer in Perovskite Structures: Density Functional Theory Insights** [elektronický dokument]. DOI 10.1021/acs.jcim.3c01895 In: **Journal of Chemical Information and Modeling**. Washington, D.C.: American Chemical Society, 2024, Roč. 64, č. 4, s. 1306-1318 [tlačená forma] [online]. ISSN 1549-9596. ISSN (online) 1549-960X. - SCO ; CCC ; WOS CC, s. 1306 - 1318

2024 [01/20] / **USA** - Shao, Ketong - Mesbah, Ali. **A Study on the Role of Electric Field in Low-Temperature Plasma Catalytic Ammonia Synthesis via Integrated Density Functional Theory and Microkinetic Modeling** [elektronický dokument]. DOI 10.1021/jacsau.3c00654 In: **JACS Au**. Washington: American Chemical Society, 2024, Roč. 4, č. 2, s. 525-544 [online]. ISSN (online) 2691-3704. - SCO ; WOS CC, s. 525 - 544

2024 [01/20] / **GBR** - Torkashvand, Ziba - Mirabbaszadeh, Kavoos - Shayeganfar, Farzaneh - Srivastava, Pawan Kumar - Lee, Changgu - Beigtan, Mohadese. **Current-in-plane tunneling measurement of oxygen-functionalized few-layer boron nitride lateral barriers** [elektronický dokument]. DOI 10.1039/d3tc03527a In: **Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2024, Roč. 12, č. 21, s. 7615-7626 [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO ; CCC ; WOS CC, s. 7615 - 7626

2024 [01/20] / **USA** - Qiu, Jian - Li, Dongling - Wen, Quan. **Piezoelectricity of lead-free hybrid perovskite monolayer (ATHP)2XY4 (X = Ge, Sn; Y = Cl, Br, I): Cross-scale calculation and simulation** [elektronický dokument]. DOI 10.1063/5.0190029 In: **AIP Advances**. Melville: American Institute of Physics, 2024, Roč. 14, č. 2, art. no. 025328 [online]. ISSN (online) 2158-3226. - SCO ; CCC ; WOS CC, s. art. no. 025328

2024 [01/20] / **GBR** - Wang, Jianpei - Yang, Ping. **Building efficient photoelectric properties with Si/Graphene/ZnO interface structure** [elektronický dokument]. DOI 10.1016/j.vacuum.2023.112844 In: **Vacuum**. Oxford: Elsevier. Pergamon Press, 2024, Roč. 220, art. no. 112844 [tlačená forma] [online]. ISSN 0042-207X. ISSN (online) 1879-2715. - SCO ; CCC ; WOS CC, s. art. no. 112844

2024 [01/20] / **GBR** - Qi, Chenchen - Yan, Cuixia - Li, Qiuyang - Yang, Ting - Qiu, Shi - Cai, Jinming. **Two-dimensional Janus chalcogenides: candidates for efficient photocatalysts and piezoelectric materials** [elektronický dokument]. DOI 10.1039/d3ta06340b In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2024, Roč. 12, č. 6, s. 3542-3556 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 3542 - 3556

2024 [01/20] / **GBR** - Wan, Zicheng - Zhou, Chen - Lin, Yichao - Chen, Liang - Tian, Ziqi. **Computational understanding of Na-LTA for ethanol-water separation** [elektronický dokument]. DOI 10.1039/d3cp06046b In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2024, Roč. 26, č. 5, s. 4505-4510 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 4505 - 4510

2024 [01/20] / **GBR** - Zhang, Peipei - Sun, Hanlei - Lu, Xiuyuan - Oh, Rena - Zhang, Nuowei - Akdim, Ouardia - Roldan, Alberto - Huang, Xiaoyang - Chen, Binghui. **Tandem reactions on phase separated MnO2 and C to enhance formaldehyde conversion to hydrogen** [elektronický dokument]. DOI 10.1016/j.ijhydene.2023.10.281 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2024, Roč. 51, s. 982-992 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC, s. 982 - 992

2024 [01/20] / **NLD** - Sun, Yue - Luan, Lijun - Ye, Linshen - Zhao, Jiaheng - Zhang, Yan - Wei, Xing - Fan, Jibin - Ni, Lei - Liu, Chen - Yang, Yun - Liu, Jian - Tian, Ye - Duan, Li. **Tunable electronic and optical properties of AlSb/InSe heterojunction and As and Te doped AlSb/InSe heterojunction based on first principles** [elektronický dokument]. DOI 10.1016/j.chemphys.2023.112087 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2024, Roč. 576, art. no. 112087 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO ; CCC ; WOS CC, s. art. no. 112087

2024 [01/20] / **CHE** - Elomrani, Abdelali - Lamhani, Mohammed - Oukahou, Said - Maymoun, Mohammad - Etrini, Ayoub - Sbiaai, Khalid - Hasnaoui, Abdellatif. **Theoretical Investigations of Layered Anode Materials** [elektronický dokument]. DOI 10.1007/978-3-031-47303-6_16 In: **Novel Aspects of Diamond II**: Science and Technology. Cham: Springer Nature, 2024, s. 437-468. ISBN 978-3-031-47558-0. ISBN (online) 978-3-031-47556-6. ISSN 0303-4216. ISSN (online) 1437-0859. - SCO, s. 437 - 468

2024 [01/20] / **GBR** - Zhang, Xinge - Jiang, Yuqian - Tian, Yuping - Zhang, Binyuan - Li, Linyang - Gong, Wei Jiang - Kong, Xiangru. **Strain-engineering quantized spin Hall conductivity in sliding multiferroic RuCl2 bilayers** [elektronický dokument]. DOI 10.1039/d4tc03680h In: **Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2024, Roč. 13, č. 7, s. 3352-3361 [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO, s. 3352 - 3361

2024 [01/20] / **NLD** - Li, Kang - Gao, Yue - Dong, Zhongxin - Zhang, Huibo - Fan, Xudong - Xu, Lei - Huang, Jie - Teng, Feng - Fan, Haibo - Song, Jiaming - Zhang, Chunmei - He, Xuexia - Hu, Peng. **SbSeI for high-efficient photocatalytic degradation of multiple pollutants** [elektronický dokument]. DOI 10.1016/j.envres.2024.120209 In: **Environmental research**. Amsterdam : Elsevier, 2024, Roč. 263, art. no. 120209 [tlačená forma] [online]. ISSN 0013-9351. ISSN (online) 1096-0953. - SCO ; CCC ; WOS CC, s. art. no. 120209

2024 [01/20] / **DEU** - Mukherjee, Supratik - Vaitheeswaran, G. **Beyond Traditional Perovskites: Xenon's Influence on the Vibrational and Electronic Properties of K4Xe3O12** [elektronický dokument]. DOI 10.1002/adts.202400545 In: **Advanced theory and simulations**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 7, č. 12, art. no. 2400545 [online]. ISSN (online) 2513-0390. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Shi, Junjie - Pršlja, Paulina - Suominen, Milla - Jin, Benjin - Lahtinen, Jouko - Moumaneix, Lilian - Kong, Xiangze - Kallio, Tanja. **Mn-doped Bi2O3 grown on PTFE-treated carbon paper for electrochemical CO2-to-formate production** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115798 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 440, art. no. 115798 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. art. no. 115798

2024 [01/20] / **GBR** - Zhan, Chao - Dattila, Federico - Rettenmaier, Clara - Herzog, Antonia - Herran, Matias - Wagner, Timon - Scholten, Fabian - Bergmann, Arno - López, Núria - Roldan Cuenya, Beatriz. **Key intermediates and Cu active sites for CO2 electroreduction to ethylene and ethanol** [elektronický dokument]. DOI 10.1038/s41560-024-01633-4 In:

Nature energy. Londýn: Springer Nature. Macmillan Education, 2024, Roč. 9, č. 12, s. 1485-1496 [online]. ISSN (online) 2058-7546. - SCO ; CCC ; WOS CC, s. 1485 - 1496

2024 [01/20] / **GBR** - Jason J, Ian - Pal, Yash - Lee, Hoonkyung - Kaewmaraya, Thanayut - Aguey-Zinsou, K. F. - Hussain, Tanveer - Panigrahi, Puspamitra. **Enhanced hydrogen storage properties of light metals dispersed boron hydride monolayer** [elektronický dokument]. DOI 10.1016/j.ijhydene.2024.10.347 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2024, Roč. 92, s. 1389-1400 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC, s. 1389 - 1400

2024 [01/20] / **USA** - Ma, Haibin - Ibáñez-Alé, Enric - You, Futian - López, Núria - Yeo, Boon Siang. **Electrochemical Formation of C2+ Products Steered by Bridge-Bonded *CO Confined by *OH Domains** [elektronický dokument]. DOI 10.1021/jacs.4c08755 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2024, Roč. 146, č. 44, s. 30183-30193 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC, s. 30183 - 30193

2024 [01/20] / **NLD** - Adloo, S. - Nasresfahani, Sh - Safaiee, R. **A DFT screening of CH4 detection by (8,0) single-walled carbon nanotubes decorated with small tin oxide clusters** [elektronický dokument]. DOI 10.1016/j.surfin.2024.105123 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2024, Roč. 54, art. no. 105123 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC, s. art. no. 105123

2024 [01/20] / **GBR** - Wang, Shukai - Shi, Kai - Li, Jie - Lyu, Juan - Li, Fengyu. **First-principles explorations on 2D transition metal diborides featuring inverse sandwich structures and their gas sensing properties** [elektronický dokument]. DOI 10.1088/1361-6463/ad6331 In: **Journal of Physics D**: Applied Physics. Bristol: Institute of Physics. IOP Publishing, 2024, Roč. 57, č. 42, art. no. 425301 [tlačená forma] [online]. ISSN 0022-3727. ISSN (online) 1361-6463. - SCO ; CCC ; WOS CC, s. art. no. 425301

2024 [01/20] / **USA** - Dong, Hui - Mu, Junzheng - Peng, Jinfeng - Zheng, Xuejun - Chu, Liang. **Mechanism of local electric oxidation on two-dimensional MoS2 for resistive memory application** [elektronický dokument]. DOI 10.1016/j.isci.2024.110819 In: **iScience**. [Cambridge]: Elsevier. Cell Press, 2024, Roč. 27, č. 10, art. no. 110819 [online]. ISSN (online) 2589-0042. - SCO ; CCC ; WOS CC, s. art. no. 110819

2024 [01/20] / **NLD** - Wang, Mengbo - Wei, Xing - Duan, Li - Zhu, Yongheng - Fan, Jibin. **A Type-II InP/MoTe2 van der waals heterostructure with adjustable electronic properties under external electric field and biaxial strain** [elektronický dokument]. DOI 10.1016/j.physleta.2024.129788 In: **Physics Letters A**: General Physics, Nonlinear Science, Statistical Physics, Atomic, Molecular and Cluster Physics, Plasma and Fluid Physics, Condensed Matter, Cross-disciplinary Physics, Biological Physics, Nanosciences, Quantum Physics, Optical physics. Amsterdam: Elsevier, 2024, Roč. 522, art. no. 129788 [tlačená forma] [online]. ISSN 0375-9601. ISSN (online) 1873-2429. - SCO ; CCC ; WOS CC, s. art. no. 129788

2024 [01/20] / **USA** - Ding, Cheng - Zhu, Yun Lai - Qu, Zihan - Dai, Yuehua. **Electrostatic Gating-Dependent Multiple Band Alignments in Ferroelectric α-In2Se3/α-Te van der Waals Heterostructures** [elektronický dokument]. DOI 10.1021/acs.langmuir.4c02225 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2024, Roč. 40, č. 41, s. 21453-21459 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 21453 - 21459

2024 [01/20] / **USA** - Zhao, Dianlong - Wang, Xinjiang - Wang, Xiaoyu - Wang, Xueting - He, Xin - Fu, Yuhao - Singh, David J. - Zhang, Lijun. **Layer Stacking-Induced Transition to a Kane-Band Semiconductor in Sb2Te3** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c03409 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 40, s. 17081-17090 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO, s. 17081 - 17090

2024 [01/20] / **USA** - Gao, Yue - Yang, Mengtong - Zou, Wenli - Zhou, Jian - Zhang, Chunmei. **Band-Edge Mixture Engineered Giant and Switchable Shift Current Generation** [elektronický dokument]. DOI 10.1021/acs.nanolett.4c03520 In: **Nano letters**. Washington: American Chemical Society, 2024, Roč. 24, č. 40, s. 12560-12567 [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCO ; CCC ; WOS CC, s. 12560 - 12567

2024 [01/20] / **NLD** - Duan, Weiwei - Liang, Kanghao - Wei, Xing - Zhang, Yan - Chen, Huaxin - Yang, Yun - Liu, Jian - Tian, Ye - Wei, Shijie - Duan, Li. **First-principles calculation of the tunable electronic and optical properties of the BP/ZrS2 heterojunction** [elektronický dokument]. DOI 10.1016/j.chemphys.2024.112364 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2024, Roč. 586, art. no. 112364 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO ; CCC ; WOS CC, s. art. no. 112364

2024 [01/20] / **DEU** - Liang, Hao - Lv, Yangbo - Tang, Kui - Chai, Yuxin - Yang, Yu - Yang, Zhi - Liu, Yuyang - Sun, Jianping. **Enhanced Oxygen Evolution Reaction Catalytic Properties of Novel Nanowire Structures from FeCo-MOFs/GO via Low-Temperature Annealing** [elektronický dokument]. DOI 10.1002/ente.202400058 In: **Energy Technology**: generation, conversion, storage, distribution. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 12, č. 10, art. no. 2400058 [tlačená forma] [online]. ISSN 2194-4288. ISSN (online) 2194-4296. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **AUT** - Yakovlev, Ilya V. - Papulovskiy, Evgeniy S. - Shubin, Aleksandr A. - Toktarev, Aleksandr V. - Lapina, Olga B. **Hydration and Hydrolysis of Boron-Substituted Aluminophosphate BAPO-5 According to Solid-State NMR and DFT Calculations** [elektronický dokument]. DOI 10.1007/s00723-024-01673-9 In: **Applied Magnetic Resonance**. Viedeň: Springer Nature. Springer International Publishing AG, 2024, Roč. 55, č. 10, s. 1245-1261 [tlačená forma]. ISSN 0937-9347. ISSN (online) 1613-7507. - SCO ; CCC ; WOS CC, s. 1245 - 1261

2024 [01/20] / **GBR** - Dai, Zhuangzhuang - Wei, Xing - Sun, Yue - Zhang, Yan - Chen, Huaxin - Yang, Yun - Liu, Jian - Tian, Ye - Duan, Li. **The optical and tunable electronic properties of WTe2/ZnI2 heterostructures under the influence of strain and electric field** [elektronický dokument]. DOI 10.1016/j.mssp.2024.108620 In: **Materials Science in Semiconductor Processing**: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2024, Roč. 181, art. no. 108620 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC, s. art. no. 108620

2024 [01/20] / **NLD** - Wang, Hewen - Luo, Wenwei - Wu, Musheng - Ouyang, Chuying. **First principles study of two-dimensional penta-germagraphene as good anode material for potassium ion batteries** [elektronický dokument]. DOI 10.1016/j.ssi.2024.116605 In: **Solid State Ionics**: Diffusion and Reactions. Amsterdam: Elsevier, 2024, Roč. 412, art. no. 116605 [tlačená forma] [online]. ISSN 0167-2738. ISSN (online) 1872-7689. - SCO ; CCC ; WOS CC, s. art. no. 116605

2024 [01/20] / **CHE** - Li, Shu Long - Peng, Ming - Song, Yu - Chen, Yutao - Qiao, Liang - Feng, Yong - Zhao, Yong - Gan, Li Yong. **Screening transition metal and nonmetal atoms co-doped graphyne as efficient single-atom catalysts for nitrogen reduction** [elektronický dokument]. DOI 10.1016/j.cej.2024.153275 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2024, Roč. 495, art. no. 153275 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 153275

2024 [01/20] / **NLD** - Xie, You - Jiang, Ning Ning - Han, Wei - Wang, Su Fang - Chen, Li Yong - Jin, Xin Wen - Chen, Zheng Yong - Xiao, Xiao Sa - Zhou, Zi Xuan - Song, Yu Ling. **Electric field tunable electronic structures and ultrahigh power conversion efficiency of BC6N/MoSe2 van der Waals heterostructure: A promising material for high-efficiency solar cell applications** [elektronický dokument]. DOI 10.1016/j.jpcs.2024.112067 In: **Journal of Physics and Chemistry of Solids**: an International Journal. Amsterdam: Elsevier, 2024, Roč. 192, art. no. 112067 [tlačená forma]. ISSN (online) 0022-3697. - SCO, s. art. no. 112067

2024 [01/20] / **USA** - Jiang, Yuncai - Lei, Shuangying - Gao, Ran - Wang, Mingyuan - He, Longbing - Xu, Feng - Huang, Qingan - Sun, Litao. **First-Principles Calculations of Black Phosphorene-Like MX (M = Ge, Sn; X = S, Se) Bilayers: Implications for Photovoltaic Solar Cells** [elektronický dokument]. DOI 10.1021/acsanm.4c04015 In: **ACS applied nano**

materials. Washington: American Chemical Society, 2024, Roč. 7, č. 16, s. 19745-19754 [online]. ISSN (online) 2574-0970. - SCO ; CCC ; WOS CC, s. 19745 - 19754

2024 [01/20] / **USA** - Su, Jingnan - Yu, Linke - Han, Bing - Li, Fengyu - Chen, Zhongfang - Zeng, Xiao Cheng. **Enhanced CO2 Reduction on a Cu-Decorated Single-Atom Catalyst via an Inverse Sandwich M-Graphene-Cu Structure** [elektronický dokument]. DOI 10.1021/acs.jpclett.4c01858 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2024, Roč. 15, č. 33, s. 8600-8607 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 8600 - 8607

2024 [01/20] / **DEU** - Nachawaty, Abir - Chen, Tongxin - Ibrahim, Fatima - Wang, Yuchen - Hao, Yafei - Dalla Francesca, Kevin - Tyagi, Priyanka - Da Costa, Antonio - Ferri, Anthony - Liu, Chuanchuan - Li, Xiaoguang - Chshiev, Mairbek - Migot, Sylvie - Badie, Laurent - Jahjah, Walaa - Desfeux, Rachel - Le Breton, Jean Christophe - Schieffer, Philippe - Le Pottier, Arnaud - Gries, Thomas - Devaux, Xavier - Lu, Yuan. **Voltage-Driven Fluorine Motion for Novel Organic Spintronic Memristor** [elektronický dokument]. DOI 10.1002/adma.202401611 In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 36, č. 33, art. no. 2401611 [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Dai, Zhuangzhuang - Wei, Xing - Sun, Yue - Zhang, Yan - Yang, Yun - Liu, Jian - Tian, Ye - Li, Ziyuan - Wei, Shijie - Duan, Li. **The optical and tunable electronic properties of BAs/ZnSe heterostructures under the influence of strain and electric field** [elektronický dokument]. DOI 10.1039/d4nj02635g In: **New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2024, Roč. 48, č. 34, s. 14958-14969 [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCO ; CCC ; WOS CC, s. 14958 - 14969

2024 [01/20] / **GBR** - Jin, Xin Wen - Xie, You - Han, Wei - Chen, Zheng Yong - Xiao, Xiao Sa - Hao, Jia Yu - Wang, Su Fang - Chen, Li Yong - Song, Yu Ling. **Biaxial strain-modulated power conversion efficiency, electronic structures, and optical properties of type-II MoS2/BC6N vdW heterostructure: A density functional theory study** [elektronický dokument]. DOI 10.1016/j.mtcomm.2024.110012 In: **Materials today. Communications.**. Oxford: Elsevier, 2024, Roč. 40, art. no. 110012 [online]. ISSN (online) 2352-4928. - SCO ; CCC ; WOS CC, s. art. no. 110012

2024 [01/20] / **USA** - Vrška, Dávid - Urban, Miroslav - Neogrády, Pavel - Pittner, Jiří - Blaško, Martin - Pitoňák, Michal. **DFT Modeling of Polyethylene Chains Cross-linked by Selected ns1 and ns2 Metal Atoms** [elektronický dokument]. DOI 10.1021/acs.jpca.4c04755 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2024, Roč. 128, č. 36, s. 7634-7647 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO ; WOS CC ; SCIE, s. 7634 - 7647

2023 [01/20] / **CHN** - Cheng, Beitong - Huang, Xingyong - Jiang, Ruomei - Huang, Shuai - Zhou, Yong - Zhang, Shan - Zhang, Wei - Dai, Qian - Song, Hai Zhi. **Structural and Electronic Properties of tri-layer Van der Waals Heterostructure**. DOI 10.1117/12.2663132 In: **Conference on Infrared, Millimeter, Terahertz Waves and Applications (IMT2022)**. Xian: The International Society for Optics and Photonics, 2023, art. no. 125653L. ISBN [9781510662476]. - SCO, s. art. no. 125653L

2023 [01/20] / **GBR** - Ghani, Awais - Ahmed, Shehzad - Murtaza, Adil - Muhammad, Imran - Rehman, Wasif ur - Zhou, Chao - Zuo, Wen Liang - Yang, Sen. **Bi-C monolayer as a promising 2D anode material for Li, Na, and K-ion batteries** [elektronický dokument]. DOI 10.1039/d2cp04712h In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 6, s. 4980-4986 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 4980 - 4986

2023 [01/20] / **NLD** - Fabiano, Eduardo - Cortona, Pietro. **Seeking widely applicable dispersion-corrected GGA functionals: The performances of TCA+D3 and RevTCA+D3 on solid-state systems** [elektronický dokument]. DOI 10.1016/j.commatsci.2022.111826 In: **Computational Materials Science**. Amsterdam: Elsevier, 2023, Roč. 216, art. no.

111826 [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO ; CCC ; WOS CC, s. art. no. 111826

2023 [01/20] / **NLD** - Xu, Yuanpu - Zhu, Xinghua - Cheng, Ziwen - Zhang, Guangan - He, Wenhao - Lu, Zhibin. **Anomalous strain-dependent charge density in honeycomb borophene** [elektronický dokument]. DOI 10.1016/j.commatsci.2022.111838 In: **Computational Materials Science**. Amsterdam: Elsevier, 2023, Roč. 216, art. no. 111838 [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO ; CCC ; WOS CC, s. art. no. 111838

2023 [01/20] / **CHE** - Ritzmann, Andrew M. - LaCount, Michael D. - Sassi, Michel - Johnson, Alyssa E. - Henson, Neil J. **A density functional theory analysis of the adsorption and surface chemistry of inorganic iodine species on graphite a** [elektronický dokument]. DOI 10.3389/fnuen.2023.1170424 In: **Frontiers in Nuclear Engineering**. Lausanne: Frontiers Media, 2023, Roč. 2, art. no. 1170424. ISSN (online) 2813-3412. - SCO, s.

2023 [01/20] / **GBR** - Ulian, Gianfranco - Valdrè, Giovanni. **Structural, elastic, electronic, optical and vibrational properties of single-layered, bilayered and bulk molybdenite MoS2-2H** [elektronický dokument]. DOI 10.1107/S1600576723002571 In: **Journal of applied crystallography**. Chester: International Union of Crystallography, 2023, Roč. 56, č. 3, s. 611-623 [tlačená forma] [online]. ISSN 0021-8898. ISSN (online) 1600-5767. - SCO ; CCC ; WOS CC, s. 611 - 623

2023 [01/20] / **CHE** - Wu, Feng - Wang, Zijin - He, Jiaqi - Li, Zhenzhe - Meng, Lijuan - Zhang, Xiuyun. **Effect of 3d Transition Metal Atom Intercalation Concentration on the Electronic and Magnetic Properties of Graphene/MoS2 Heterostructure: A First-Principles Study** [elektronický dokument]. DOI 10.3390/molecules28020509 In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 28, č. 2, art. no. 509 [online]. ISSN (online) 1420-3049. - SCO ; CCC ; WOS CC, s. art. no. 509

2023 [01/20] / **DEU** - Ruiz, Eliseo - Aravena, Daniel. **Theoretical Approaches for Electron Transport Through Magnetic Molecules** [elektronický dokument]. DOI 10.1007/978-3-031-31038-6_9 In: **Computational Modelling of Molecular Nanomagnets**. Cham: Springer Nature. Springer Science+Business Media, 2023, s. 445-494 [tlačená forma] [online]. ISBN 978-3-031-31037-9. ISBN 978-3-031-31040-9. ISBN (online) 978-3-031-31038-6. - SCO, s. 445 - 494

2023 [01/20] / **USA** - Mallet, P. - Ibrahim, F. - Abdukayumov, K. - Marty, A. - Vergnaud, C. - Bonell, F. - Chshiev, M. - Jamet, M. - Veuillen, J. Y. **Angular dependence of the interlayer coupling at the interface between two-dimensional materials 1 T-PtS e2 and graphene** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.7.L121001 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 7, č. 12, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; WOS CC, s.

2023 [01/20] / **USA** - Reji, Rence Painappallil - Balaji, Sarath Kumar Chedharla - Sivalingam, Yuvaraj - Kawazoe, Yoshiyuki - Velappa Jayaraman, Surya. **First-Principles Density Functional Theory Calculations on the Potential of Sc2CO2 MXene Nanosheets as a Dual-Mode Sensor for Detection of Volatile Organic Compounds in Exhaled Human Breath** [elektronický dokument]. DOI 10.1021/acsanm.2c05474 In: **ACS applied nano materials**. Washington: American Chemical Society, 2023, Roč. 6, č. 7, s. 5345-5356 [online]. ISSN (online) 2574-0970. - SCO ; CCC ; WOS CC, s. 5345 - 5356

2023 [01/20] / **CHE** - Young Jang, Won - Venkata Reddy, Ch - Daouli, Ayoub - Kakarla, Raghava Reddy - Bandaru, Narendra - Shim, Jaesool - Badawi, Michael - Aminabhavi, Tejraj M. **Novel 2D sulfur-doped V2O5 flakes and their applications in photoelectrochemical water oxidation and high-performance energy storage supercapacitors** [elektronický dokument]. DOI 10.1016/j.cej.2023.141935 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2023, č. 461, art. no. 141935 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 141935

2023 [01/20] / **IDN** - Hastuti, Dian Putri - Nawa, Kenji - Nakamura, Kohji. **Electronic Structures of Graphene/MoS2 Heterostructure: Effects of Stacking Orientation, Element Substitution, and Interlayer Distance** [elektronický

dokument]. DOI 10.22146/ijc.75538 In: **Indonesian Journal of Chemistry**. Depok: Universitas Gadjah Mada Master in Chemistry, 2023, Roč. 23, č. 1, s. 140-147 [tlačená forma] [online]. ISSN 1411-9420. ISSN (online) 2460-1578. - SCO ; WOS CC, s. 140 - 147

2023 [01/20] / **NLD** - Zhang, Xiaolin - Yang, Baishun - Guo, Xiaoyan - Liu, Yuheng - Han, Xiufeng - Yan, Yu. **Ferroelectric control of magnetic coupling of monolayer MnBr2 in semiconducting multiferroic van der Waals heterostructure** [elektronický dokument]. DOI 10.1016/j.apsusc.2022.156201 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, Roč. 614, art. no. 156201 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 156201

2023 [01/20] / **NLD** - Sun, Yue - Luan, Lijun - Zhao, Jiaheng - Zhang, Yan - Wei, Xing - Fan, Jibin - Ni, Lei - Liu, Chen - Yang, Yun - Liu, Jian - Tian, Ye - Duan, Li. **Calculation of tunable electronic and optical properties of AlSb/CdSe heterojunction based on first principles** [elektronický dokument]. DOI 10.1016/j.apsusc.2022.156261 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, Roč. 614, art. no. 156261 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 156261

2023 [01/20] / **GBR** - Li, Qiuyang - Yan, Cuixia - Qi, Chenchen - Qiu, Shi - Yang, Ting - Cai, Jinming. **A family of robust Dirac cone materials: two-dimensional hexagonal M3X2 (M = Zn/Cd/Hg, X = Si/Ge)** [elektronický dokument]. DOI 10.1039/d2cp05494a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 15, s. 10811-10819 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 10811 - 10819

2023 [01/20] / **GBR** - Li, Tianyu - Leonard, Matthew - Tsyshevsky, Roman - McEntee, Monica - Karwacki, Christopher - Durke, Erin M. - Kuklja, Maija M. - Rodriguez, Efrain E. **High reactivity of mesoporous CeO2 to dissociate chemical warfare agent sarin** [elektronický dokument]. DOI 10.1039/d2qm01253g In: **Materials chemistry frontiers**. Londýn: The Royal Society of Chemistry, 2023, Roč. 7, č. 9, s. 1855-1866 [online]. ISSN (online) 2052-1537. - SCO ; CCC ; WOS CC, s. 1855 - 1866

2023 [01/20] / **USA** - Al-Hamdani, Yasmine S. - Zen, Andrea - Michaelides, Angelos - Alfè, Dario. **Mechanisms of adsorbing hydrogen gas on metal decorated graphene** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.7.035402 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 7, č. 3, art. no. 035402 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC, s. art. no. 035402

2023 [01/20] / **NLD** - Rangarajan, Srinivas - Mavrikakis, Manos. **A comparative analysis of different van der Waals treatments for molecular adsorption on the basal plane of 2H-MoS2** [elektronický dokument]. DOI 10.1016/j.susc.2022.122226 In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2023, Roč. 729, art. no. 122226 [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO ; CCC ; WOS CC, s. art. no. 122226

2023 [01/20] / **NLD** - Nematollahi, Parisa. **Selectivity of Mo–N–C sites for electrocatalytic N2 reduction: A function of the single atom position on the surface and local carbon topologies** [elektronický dokument]. DOI 10.1016/j.apsusc.2022.155908 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, Roč. 612, art. no. 155908 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 155908

2023 [01/20] / **NLD** - Griffith, M. A.R. - Rufo, S. - Dias, Alexandre C. - Da Silva, Juarez L.F. **Enhancing topological Weyl Semimetals by Janus transition-metal dichalcogenides structures** [elektronický dokument]. DOI 10.1016/j.commatsci.2022.112004 In: **Computational Materials Science**. Amsterdam: Elsevier, 2023, Roč. 218, art. no. 112004 [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO ; CCC ; WOS CC, s. art. no. 112004

2023 [01/20] / **GBR** - Ai, Wen - Hu, Xiaohui - Yang, Jian - Lu, Chunhua - Sun, Litao. **Selective sensing properties and enhanced ferromagnetism in CrI3 monolayer via gas adsorption** [elektronický dokument]. DOI 10.1088/1361-6528/aca0fa In: **Nanotechnology**. Bristol : Institute of Physics. IOP Publishing, 2023, Roč. 34, č. 6, art. no. 065202 [tlačená forma] [online]. ISSN 0957-4484. ISSN (online) 1361-6528. - SCO ; CCC ; WOS CC, s. art. no. 065202

2023 [01/20] / **GBR** - Qi, Chenchen - Yan, Cuixia - Li, Qiuyang - Yang, Ting - Qiu, Shi - Cai, Jinming. **Two-dimensional Janus monolayers Al2XYZ (X/Y/Z = S, Se, Te, X ≠ Y ≠ Z): first-principles insight into the photocatalytic and highly adjustable piezoelectric properties** [elektronický dokument]. DOI 10.1039/d2tc04939b In: **Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2023, Roč. 11, č. 9, s. 3262-3274 [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO ; CCC ; WOS CC, s. 3262 - 3274

2023 [01/20] / **CHE** - Bai, Mengmeng - Li, Zuo - Shi, Mingxia - Tao, Minlong - Sun, Kai - Yang, Xiaotian - Zhang, Yufeng - Wang, Junzhong. **Reconstructed Cd(0001) Surface Induced by Adsorption of Triphenyl Bismuth** [elektronický dokument]. DOI 10.3390/coatings13020394 In: **Coatings**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 2, art. no. 394 [online]. ISSN (online) 2079-6412. - SCO ; CCC ; WOS CC, s. art. no. 394

2023 [01/20] / **USA** - Peng, Qiong - Rehman, Javed - Butt, Mehwish Khalid - Yang, Zhao - Wang, Shuanhu - Al-Ammar, Essam A. - Sillanpää, Mika - Dinh, Van An - Shibl, Mohamed F. **Adsorption and diffusion of potassium on layered SnO: a DFT analysis** [elektronický dokument]. DOI 10.1007/s10853-023-08224-w In: **Journal of Materials Science**. Norwell: Springer Nature. Springer International Publishing AG, 2023, Roč. 58, č. 7, s. 3208-3218 [tlačená forma] [online]. ISSN 0022-2461. ISSN (online) 1573-4803. - SCO ; WOS CC, s. 3208 - 3218

2023 [01/20] / **NLD** - Liu, Ting - He, Mengjie - Shen, Chenhai - Xia, Congxin - Li, Xueping. **Interface-controlled band alignments in Janus Ga2STe/MoSi2N4 vdWHs** [elektronický dokument]. DOI 10.1016/j.physb.2023.415061 In: **Physica B**: Condensed Matter. Amsterdam: Elsevier, 2023, Roč. 666, art. no. 415061 [tlačená forma] [online]. ISSN 0921-4526. ISSN (online) 1873-2135. - SCO ; CCC ; WOS CC, s. art. no. 415061

2023 [01/20] / **USA** - Ta, Huong Thi Thuy - Tran, Nam Van - Righi, Maria Clelia. **Nanotribological Properties of Oxidized Diamond/Silica Interfaces: Insights into the Atomistic Mechanisms of Wear and Friction by Ab Initio Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acsanm.3c02881 In: **ACS applied nano materials**. Washington: American Chemical Society, 2023, Roč. 6, č. 18, s. 16674-16683 [online]. ISSN (online) 2574-0970. - SCO ; CCC ; WOS CC, s. 16674 - 16683

2023 [01/20] / **USA** - van der Laan, Marco - Heemskerk, Edwin - Kienhuis, Floris - Diepeveen, Nella - Poonia, Deepika - Kinge, Sachin - Dang, Minh Triet - Dinh, Van An - Siebbeles, Laurens D.A. - Isaeva, Anna - van de Groep, Jorik - Schall, Peter. **Stacking-Order-Dependent Excitonic Properties Reveal Interlayer Interactions in Bulk ReS2** [elektronický dokument]. DOI 10.1021/acsphotonics.3c00477 In: **ACS Photonics**. Washington : American Chemical Society, 2023, Roč. 10, č. 9, s. 3115-3123 [online]. ISSN (online) 2330-4022. - SCO ; CCC ; WOS CC, s. 3115 - 3123

2023 [01/20] / **USA** - Zhang, Guang - Wang, Kai - Liu, Qiaoyu - Pan, Mingyuan - Shen, Ding - Yao, Yansun - Wu, Lailei - Gou, Huiyang. **Stability and Semiconducting Behavior of Magnesium Polysulfides by Nonequivalent sp3 Hybridizations** [elektronický dokument]. DOI 10.1021/acs.inorgchem.3c02398 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2023, Roč. 62, č. 37, s. 15226-15233 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 15226 - 15233

2023 [01/20] / **USA** - Feng, Li - Chen, Xiaofang - Qi, Jingshan. **Nonvolatile electric field control of spin-valley-layer polarized anomalous Hall effect in a two-dimensional multiferroic semiconductor bilayer** [elektronický dokument]. DOI 10.1103/PhysRevB.108.115407 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 108, č. 11, art. no. 115407 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 115407

2023 [01/20] / **USA** - Ye, Chunmiao - Dattila, Federico - Chen, Xiaoting - López, Núria - Koper, Marc T.M. **Influence of Cations on HCOOH and CO Formation during CO2 Reduction on a PdMLPt(111) Electrode** [elektronický dokument]. DOI 10.1021/jacs.3c03786 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2023, Roč. 145, č. 36, s. 19601-19610 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC, s. 19601 - 19610

2023 [01/20] / **USA** - Pastukh, Svitlana - Jochym, Paweł T. - Pastukh, Oleksandr - Łażewski, Jan - Legut, Dominik - Piekarz, Przemysław. **Anharmonicity and structural phase transition in the Mott insulator Cu2P2O7** [elektronický dokument]. DOI 10.1103/PhysRevB.108.104104 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 108, č. 10, art. no. 104104 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 104104

2023 [01/20] / **GBR** - Yan, Xiaoya - Shen, Tao - Liu, Xin - Liu, Chi - Gong, Aina. **Transition metal (Co, Ti) decorated graphene monolayer and their adsorption properties towards SO2: First-principle calculation** [elektronický dokument]. DOI 10.1016/j.ssc.2023.115196 In: **Solid State Communications**: an International Journal. Oxford: Elsevier, 2023, Roč. 369, art. no. 115196 [tlačená forma] [online]. ISSN 0038-1098. ISSN (online) 1879-2766. - SCO ; CCC ; WOS CC, s. art. no. 115196

2023 [01/20] / **USA** - Xiong, Lixin - Su, Neil Qiang - Fang, Wei Hai. **The Role of Self-Catalysis Induced by Co Doping in Nonaqueous Li-O Batteries** [elektronický dokument]. DOI 10.1021/acs.jpclett.3c02041 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 33, s. 7526-7540 [online]. ISSN (online) 1948-7185. - SCO, s. 7526 - 7540

2023 [01/20] / **GBR** - Idrees, M. - Khurami, M. W. - Amin, B. - Chen, Yuanping - Yan, Xiaohong. **Interfacial characteristics, metal-semiconductor contact and optical properties of CSe and BX (X=B, As and Sb) monolayers** [elektronický dokument]. DOI 10.1016/j.mssp.2023.107593 In: **Materials Science in Semiconductor Processing**: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2023, Roč. 163, art. no. 107593 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC, s. art. no. 107593

2023 [01/20] / **USA** - Oh, Rena - Huang, Xiaoyang - Lu, Xiuyuan - Chen, Chunhui - Lou, Yao Yin - Geng, Lili - Zhang, Xiang - Du, Delin - Li, Jianjun - Yan, Wei - Park, Gyeong Su - Akdim, Ouardia - Kim, Seong Keun - Sun, Shi Gang. **Enhanced Alcohol Electrochemical Oxidation by Using an Environmentally Friendly Xanthan Gum Binder** [elektronický dokument]. DOI 10.1021/acssuschemeng.3c03719 In: **ACS Sustainable Chemistry & Engineering**. Washington: American Chemical Society, 2023, Roč. 11, č. 31, s. 11681-11692 [online]. ISSN (online) 2168-0485. - SCO ; CCC ; WOS CC, s. 11681 - 11692

2023 [01/20] / **GBR** - Li, Yuqiang - Li, Yuhong - Zhang, Qiang - Su, Ningning - Sun, Jinlu - Xiao, Ningru - Liu, Yang - Liu, Yuyao - Zhang, Jianxin - Liu, Hongwei. **First-principles study of structural phase transitions and metallization of XPSe3 (X = Fe, Mn) under high pressure** [elektronický dokument]. DOI 10.1016/j.mtcomm.2023.106661 In: **Materials today. Communications.**. Oxford: Elsevier, 2023, Roč. 36, art. no. 106661 [online]. ISSN (online) 2352-4928. - SCO ; CCC ; WOS CC, s. art. no. 106661

2023 [01/20] / **DEU** - López-Galán, Oscar A. - Perez, Israel - Nogan, John - Ramos, Manuel. **Determining the Electronic Structure and Thermoelectric Properties of MoS2/MoSe2 Type-I Heterojunction by DFT and the Landauer Approach**. DOI 10.1002/admi.202202339 In: **Advanced Materials Interfaces**. Weinheim: John Wiley & Sons. Wiley-VCH, 2023, Roč. 10, č. 11, art. no. 2202339 [online]. ISSN 2196-7350. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **CHE** - Zhao, Xiaoyu - Zhang, Zhenghua. **FeOCl in Advanced Oxidization Processes for Water Purification: A Critical Review** [elektronický dokument]. DOI 10.1007/s40726-023-00256-9 In: **Current Pollution**

Reports. Cham: Springer Nature, 2023, Roč. 9, č. 2, s. 143-164 [online]. ISSN (online) 2198-6592. - SCO ; CCC ; WOS CC, s. 143 - 164

2023 [01/20] / **GBR** - Wang, Jiaming - Wu, Hao - Pan, Min - Liu, Zhixiao - Han, Lei - Huang, Zheng - Deng, Huiqiu. **Bilayer tetragonal AlN nanosheets as potential cathodes for Li-O2 batteries** [elektronický dokument]. DOI 10.1039/d2cp05794h In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 21, s. 15030-15039 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 15030 - 15039

2023 [01/20] / **CHE** - Cheng, Beitong - Zhou, Yong - Jiang, Ruomei - Wang, Xule - Huang, Shuai - Huang, Xingyong - Zhang, Wei - Dai, Qian - Zhou, Liujiang - Lu, Pengfei - Song, Hai Zhi. **Structural, Electronic and Optical Properties of Some New Trilayer Van de Waals Heterostructures** [elektronický dokument]. DOI 10.3390/nano13091574 In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 9, art. no. 1574 [online]. ISSN (online) 2079-4991. - SCO ; CCC ; WOS CC, s. art. no. 1574

2023 [01/20] / **NLD** - Jalili, Seifollah - Pakzadiyan, Atena. **Tensile strain as an efficient way to tune transport properties of Graphdiyne/Borophene hetero-bilayers; a first principle investigation** [elektronický dokument]. DOI 10.1016/j.commatsci.2023.112161 In: **Computational Materials Science**. Amsterdam: Elsevier, 2023, Roč. 224, art. no. 112161 [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO ; CCC ; WOS CC, s. art. no. 112161

2023 [01/20] / **NLD** - Wang, Lijing - Gao, Shan - Li, Wenting - Zhu, Ao - Li, Huan - Zhao, Chunning - Zhang, Haijun - Wang, Wei Hua - Wang, Weichao. **Machine learning assisted screening of MXenes pseudocapacitive materials** [elektronický dokument]. DOI 10.1016/j.jpowsour.2023.232834 In: **Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2023, Roč. 564, art. no. 232834 [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCO ; CCC ; WOS CC, s. art. no. 232834

2023 [01/20] / **USA** - Qiu, Yang - Li, Gaoyang - Zhou, Huimin - Zhang, Guoliang - Guo, Liang - Guo, Zhanhu - Yang, Ruonan - Fan, Yuqi - Wang, Weiliang - Du, Yong - Dang, Feng. **Highly Stable Garnet Fe2Mo3O12 Cathode Boosts the Lithium–Air Battery Performance Featuring a Polyhedral Framework and Cationic Vacancy Concentrated Surface** [elektronický dokument]. DOI 10.1002/advs.202300482 In: **Advanced Science**. Hoboken: John Wiley & Sons. Wiley Blackwell, 2023, Roč. 10, č. 12, art. no. 2300482 [online]. ISSN (online) 2198-3844. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Lazaar, Koussai - Aouaini, Fatma - Gueddida, Saber. **Binuclear spin-crossover [Fe(bt)(NCS)2]2(bpm) complex: A study using first principles calculations** [elektronický dokument]. DOI 10.1063/5.0147313 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 14, art. no. 144307 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 144307

2023 [01/20] / **USA** - Goldman, Nir - Fried, Laurence E. - Lindsey, Rebecca K. - Pham, C. Huy - Dettori, R. **Enhancing the accuracy of density functional tight binding models through ChIMES many-body interaction potentials** [elektronický dokument]. DOI 10.1063/5.0141616 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 14, art. no. 144112 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 144112

2023 [01/20] / **GBR** - Sun, Fu Li - Fang, Qiao Jun - Zhang, Wei - Lin, Cun Biao - Chen, Wen Xian - Zhuang, Gui Lin. **p-State of surface oxygen for mediating the s-band center of a single-atomic Ag catalyst for enhanced catalytic property for the oxygen reduction reaction** [elektronický dokument]. DOI 10.1039/d3ta04453j In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2023, Roč. 11, č. 46, s. 25399-25409 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 25399 - 25409

2023 [01/20] / **NLD** - Ren, Zhengfeng - Qi, Shandong - Zhou, Hua - Yan, Shishen - Xu, Mingchun - Hu, Shujun. **Tracking**

the atomic structure evolution of ZnO(0001¯) polar surface via carbon dioxide infrared probe [elektronický dokument]. DOI 10.1016/j.apsusc.2023.157730 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, č. 635, art. no. 157730 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 157730

2023 [01/20] / **GBR** - Sun, Yue - Luan, Lijun - Zhao, Jiaheng - Zhang, Yan - Wei, Xing - Fan, Jibin - Ni, Lei - Liu, Chen - Yang, Yun - Liu, Jian - Tian, Ye - Duan, Li. **Tunable properties of WTe2/GaS heterojunction and Se-doped WTe2/GaS heterojunction** [elektronický dokument]. DOI 10.1016/j.mssp.2023.107695 In: **Materials Science in Semiconductor Processing**: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2023, Roč. 166, art. no. 107695 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC, s. art. no. 107695

2023 [01/20] / **CHN** - Chen, Miao Miao - Li, Sheng Shi - Ji, Wei Xiao - Zhang, Chang Wen. **Two-dimensional transition metal halide PdX 2 (X = F, Cl, Br, I): A promising candidate of bipolar magnetic semiconductors** [elektronický dokument]. DOI 10.1088/1674-1056/ad04c3 In: **Chinese Physics B**. Peking: Chinese Physical Society, 2023, Roč. 32, č. 12, art. no. 127103 [tlačená forma] [online]. ISSN 1674-1056. ISSN (online) 2058-3834. - SCO, s. art. no. 127103

2023 [01/20] / **GBR** - Shao, Bin - Wang, Zhi Qiang - Gong, Xue Qing - Liu, Honglai - Qian, Feng - Hu, P. - Hu, Jun. **Synergistic promotions between CO2 capture and in-situ conversion on Ni-CaO composite catalyst** [elektronický dokument]. DOI 10.1038/s41467-023-36646-2 In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2023, Roč. 14, č. 1, art. no. 996 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s. art. no. 996

2023 [01/20] / **NLD** - Li, Yuqiang - Li, Yuhong - Zhang, Qiang - Su, Ningning - Sun, Jinlu - Xiao, Ningru - Liu, Yang - Liu, Yuyao - Ning, Pingfan - Liu, Hongwei. **First-principles study of electronic structure and metallization of Mg2Pb under high pressure** [elektronický dokument]. DOI 10.1016/j.physb.2023.415159 In: **Physica B**: Condensed Matter. Amsterdam: Elsevier, 2023, Roč. 667, art. no. 415159 [tlačená forma] [online]. ISSN 0921-4526. ISSN (online) 1873-2135. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Ganta, Prasanna Kumar - Chang, Chun Juei - Chen, Hsing Yin - Kamaraj, Rajiv - Sambandam, Anandan - Lai, Yi Chun - Chu, Yu Ting - Ding, Shangwu - Chen, Hsuan Ying. **Comparative Study of Aluminum Complexes Bearing N,N′-Diaryldioxalamidate and N,N′-Diaryldithiooxalamidate Ligands in Ring-Opening Polymerization of ϵ-Caprolactone** [elektronický dokument]. DOI 10.1021/acs.organomet.3c00317 In: **Organometallics**. Washington, D. C.: American Chemical Society. ACS Publications, 2023, Roč. 42, č. 19, s. 2856-2866 [tlačená forma] [online]. ISSN 0276-7333. ISSN (online) 1520-6041. - SCO, s. 2856 - 2866

2023 [01/20] / **USA** - Ta, Huong T.T. - Tran, Nam V. - Righi, M. C. **Atomistic Wear Mechanisms in Diamond: Effects of Surface Orientation, Stress, and Interaction with Adsorbed Molecules** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c01800 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 40, s. 14396-14403 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 14396 - 14403

2023 [01/20] / **NLD** - Jiang, Ningning - Xie, You - Wang, Sufang - Song, Yuling - Chen, Liyong - Han, Wei - Jin, Xinwen - Zhou, Zixuan - Yan, Zhengxin. **Electronic structure and carrier mobility of BC6N/BN van der Waals heterostructure induced by in-plane strains** [elektronický dokument]. DOI 10.1016/j.apsusc.2023.157007 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, Roč. 623, art. no. 157007 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 157007

2023 [01/20] / **USA** - Ma, Qingquan - Gao, Jianan - Moussa, Botamina - Young, Joshua - Zhao, Mengqiang - Zhang, Wen. **Electrosorption, Desorption, and Oxidation of Perfluoroalkyl Carboxylic Acids (PFCAs) via MXene-Based Electrocatalytic Membranes** [elektronický dokument]. DOI 10.1021/acsami.3c03991 In: **ACS applied materials and interfaces**. Washington: American Chemical Society, 2023, Roč. 15, č. 24, s. 29149-29159 [tlačená forma] [online]. ISSN

1944-8244. ISSN (online) 1944-8252. - SCO ; CCC ; WOS CC, s. 29149 - 29159

2023 [01/20] / **USA** - Han, Ting - Wang, Shuaiyu - Han, Bing - Liu, Yu - Li, Fengyu - Wang, Lei. **Two-dimensional potassium borides with hidden kagome-like lattice: Topological semimetals, van Hove singularities, and superconductivity** [elektronický dokument]. DOI 10.1103/PhysRevB.107.235154 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 107, č. 23, art. no. 235154 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 235154

2023 [01/20] / **GBR** - Sun, Yue - Luan, Lijun - Zhao, Jiaheng - Zhang, Yan - Wei, Xing - Fan, Jibin - Ni, Lei - Liu, Chen - Yang, Yun - Liu, Jian - Tian, Ye - Duan, Li. **Calculation of tunable electronic and optical properties of AlP/InSe heterostructure based on first principles** [elektronický dokument]. DOI 10.1016/j.mssp.2023.107443 In: **Materials Science in Semiconductor Processing**: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2023, Roč. 160, art. no. 107443 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC, s. art. no. 107443

2023 [01/20] / **CHE** - Lu, Shaohua - Lu, Enhao - Zhu, Kai - Hu, Xiaojun. **C4S Nanosheet: A Potential Anode Material for Potassium-Ion Batteries** [elektronický dokument]. DOI 10.3390/batteries9060288 In: **Batteries**. Basel: Multidisciplinary Digital Publishing Institute, 2023, Roč. 9, č. 6, art. no. 288 [online]. ISSN (online) 2313-0105. - SCO ; CCC ; WOS CC, s. art. no. 288

2023 [01/20] / **CHE** - Ren, Weiwei - Tian, Jintao - Pang, Rui - Shang, Yuanyuan. **Ferroelectric SnPz/In2Se3 as a Stable and Durable Non-Volatile 2D Ferroelectric Memory Material** [elektronický dokument]. DOI 10.3390/cryst13060940 In: **Crystals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 6, art. no. 940 [online]. ISSN (online) 2073-4352. - SCO ; CCC ; WOS CC, s. art. no. 940

2023 [01/20] / **USA** - Qiu, Jian - Lv, Qiaoya - Li, Dongling - Zhou, Yuanyuan - Wen, Quan. **2D Organic-Inorganic Perovskite (ATHP)2PbI4With Huge Out-of-Plane Piezoelectric Properties** [elektronický dokument]. DOI 10.1109/LED.2023.3266877 In: **IEEE Electron Device Letters**. Piscataway: Institute of Electrical and Electronics Engineers, 2023, Roč. 44, č. 6, s. 987-990 [tlačená forma] [online]. ISSN 0741-3106. ISSN (online) 1558-0563. - SCO, s. 987 - 990

2023 [01/20] / **GBR** - Nair, Heera T. - Jha, Prafulla K. - Chakraborty, Brahmananda. **High-capacity hydrogen storage in zirconium decorated psi-graphene: acumen from density functional theory and molecular dynamics simulations** [elektronický dokument]. DOI 10.1016/j.ijhydene.2022.08.084 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2023, Roč. 48, č. 96, s. 37860-37871 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC, s. 37860 - 37871

2023 [01/20] / **GBR** - Yan, Yuandong - Wang, Ruyi - Zheng, Qian - Zhong, Jiaying - Hao, Weichang - Yan, Shicheng - Zou, Zhigang. **Nonredox trivalent nickel catalyzing nucleophilic electrooxidation of organics** [elektronický dokument]. DOI 10.1038/s41467-023-43649-6 In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2023, Roč. 14, č. 1, art. no. 7987 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s. art. no. 7987

2023 [01/20] / **USA** - Liu, Yunhai - Zhang, Hu - Wang, Xiaowen - Luo, Yiyao. **Exploring the Key Mechanism of Superlubricity Behavior of DLC Film in Vacuum Environment Based on First-Principles Calculations and Molecular Dynamics Simulation** [elektronický dokument]. DOI 10.1007/s11249-023-01790-9 In: **Tribology Letters**. New York: Springer Nature. Springer, 2023, Roč. 71, č. 4, art. no. 113 [tlačená forma] [online]. ISSN 10238883. ISSN (online) 15732711. - SCO ; CCC ; WOS CC, s. art. no. 113

2023 [01/20] / **GBR** - Sun, Yue - Luan, Lijun - Zhao, Jiaheng - Zhang, Yan - Wei, Xing - Fan, Jibin - Ni, Lei - Liu, Chen - Yang, Yun - Liu, Jian - Tian, Ye - Duan, Li. **Efficient separation carrier structure of tunable two-dimensional AlSb/GaSe heterojunction** [elektronický dokument]. DOI 10.1016/j.mssp.2023.107822 In: **Materials Science in**

Semiconductor Processing: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2023, Roč. 168, art. no. 107822 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC, s. art. no. 107822

2023 [01/20] / **GBR** - Javed, Mehreen - Noureddine, Amrane - Benkraouda, Maamar. **Band gap tailoring with octahedral distortion and bader charge analysis for 2D-Ruddlesden–Popper monolayer tin halide perovskites** [elektronický dokument]. DOI 10.1016/j.mssp.2023.107490 In: **Materials Science in Semiconductor Processing**: Functional Materials for (Opto)electronics, Sensors, Detectors, Biotechnology, and Green Energy.. Amsterdam: Elsevier, 2023, Roč. 162, art. no. 107490 [tlačená forma] [online]. ISSN 1369-8001. ISSN (online) 1873-4081. - SCO ; CCC ; WOS CC, s. art. no. 107490

2023 [01/20] / **GBR** - Mohammadzaheri, Masoumeh - Jamehbozorgi, Saeed - Ganji, Maosud Darvish - Rezvani, Mahyar - Javanshir, Zahra. **Toward functionalization of ZnO nanotubes and monolayers with 5-aminolevulinic acid drugs as possible nanocarriers for drug delivery: a DFT based molecular dynamic simulation** [elektronický dokument]. DOI 10.1039/d3cp01490h In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 32, s. 21492-21508 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 21492 - 21508

2023 [01/20] / **USA** - Yu, Linke - Li, Fengyu - Huang, Jingsong - Sumpter, Bobby G. - Mustain, William E. - Chen, Zhongfang. **Double-Atom Catalysts Featuring Inverse Sandwich Structure for CO2 Reduction Reaction: A Synergetic First-Principles and Machine Learning Investigation** [elektronický dokument]. DOI 10.1021/acscatal.3c01584 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 14, s. 9616-9628 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 9616 - 9628

2023 [01/20] / **NLD** - Gorai, Deepak Kumar - Kuila, Saikat Kumar - Kumar, Anurag - Ahmad, Md Imteyaz - Kundu, Tarun Kumar. **Insight into the effect of Li/P co-doping on the electronic structure and photocatalytic performance of g-C3N4 by the first principle** [elektronický dokument]. DOI 10.1016/j.apsusc.2023.157031 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, Roč. 623, art. no. 157031 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 157031

2023 [01/20] / **NLD** - Ma, Pengju - Shu, Jiaohong - Zhao, Xinxin - Cao, Yunjiu - Wang, Lili - Chen, Guanglong - Wu, Jianbao - Mi, Yiming. **The CrBr3 monolayer: Two dimension sodium ion battery anode material to characterize state-of-charge by magnetism** [elektronický dokument]. DOI 10.1016/j.apsusc.2023.157074 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, Roč. 623, art. no. 157074 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. art. no. 157074

2023 [01/20] / **NLD** - Huang, Hao. **Advanced Materials for Electrochemical Devices** [textový dokument (print)] [elektronický dokument] . Amsterdam: Elsevier, 2023. 1. vyd. ISBN 9780443134883. ISBN (online) 9780443134890. - SCO, s. 1 - 892

2022 [01/20] / **GBR** - Wu, Tzu-Yi - Lai, Feng-Jie - Lee, Wei - Chang, Chun-Juei - Chang, Yu-Lun - Ding, Shangwu - Chen, Hsuan-Ying - Chang, Yung-Chi. **Guaiacolate derivatives-containing sodium complexes as catalysts for l-lactide polymerization** [elektronický dokument]. DOI 10.1002/aoc.6967 In: **Applied organometallic chemistry**. Harlow: Longman Scientific & Technical, 2022, s. [tlačená forma] [online]. ISSN 0268-2605. ISSN (online) 1099-0739. - WOS CC ; SCO, s.

2022 [01/20] / **GBR** - Chai, H. - Chen, W. - Li, Y. - Zhao, M. - Shi, J. - Tang, Y. - Dai, X. **Theoretical exploration of the structural, electronic and optical properties of g-C3N4/C3N heterostructures** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 25, č. 5, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 4081 - 4092

2022 [01/20] / **USA** - Wang, V. - Tang, G. - Liu, Y.-C. - Wang, R.-T. - Mizuseki, H. - Kawazoe, Y. - Nara, J. - Geng, W.T.

High-Throughput Computational Screening of Two-Dimensional Semiconductors In: **Journal of Physical Chemistry Letters**, 2022, Roč. 13, č. 50. - SCO, s. 11581 - 11594

2022 [01/20] / **USA** - Chen, Q. - Zheng, X. - Jiang, P. - Zhou, Y.-H. - Zhang, L. - Zeng, Z. **Electric field induced tunable half-metallicity in an A -type antiferromagnetic bilayer LaBr2** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 106, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 245423

2022 [01/20] / **USA** - Lu, S. - Zhang, S. - Hu, X. **Ab Initio Study of High-Capacity Hydrogen Storage in Lithium-Shrouded Honeycomb Borophene Oxide Nanosheet** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 49. - SCO, s. 20762 - 20772

2022 [01/20] / **NLD** - Gao, Y. - Wang, S. - Xie, Y. - Wang, X. - Yang, J. - Jiang, N. - Chen, L. - Zhang, J. **Effect of 4d transition metals on the electronic and magnetic properties of twin graphene** [elektronický dokument] In: **Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2022, Roč. 564, [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCO, s. Art. No. 170127

2022 [01/20] / **NLD** - Li, S.-L. - Li, Q. - Chen, Y. - Zhao, Y. - Gan, L.-Y. **Transition metal embedded graphynes as advanced bifunctional single atom catalysts for oxygen reduction and evolution reactions** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2022, Roč. 605, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 154828

2022 [01/20] / **GBR** - Ji, S. - Granas, O. - Kumar Prasad, A. - Weissenrieder, J. **Influence of strain on an ultrafast phase transition** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 15, č. 1, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 304 - 312

2022 [01/20] / **GBR** - Wang, Y. - Gao, X. - Yang, K. - Gu, P. - Lu, X. - Zhang, S. - Gao, Y. - Ren, N. - Dong, B. - Jiang, Y. - Watanabe, K. - Taniguchi, T. - Kang, J. - Lou, W. - Mao, J. - Liu, J. - Ye, Y. - Han, Z. - Chang, K. - Zhang, J. - Zhang, Z. **Quantum Hall phase in graphene engineered by interfacial charge coupling** [elektronický dokument] In: **Nature nanotechnology**. Londýn: Springer Nature. Nature Publishing Group, 2022, Roč. 17, č. 12, [tlačená forma] [online]. ISSN 1748-3387. ISSN (online) 1748-3395. - SCO, s. 1272 - 1279

2022 [01/20] / **DEU** - Cho, S.R. - Kim, D.-H. - Jeon, M. - Rani, P. - Gyeon, M. - Kim, Y. - Jo, M.-K. - Song, S. - Park, J.Y. - Kim, J. - Kim, I.-D. - Kang, K. **Overlaying Monolayer Metal-Organic Framework on PtSe2-Based Gas Sensor for Tuning Selectivity** [elektronický dokument] In: **Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2022, Roč. 32, č. 47, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCO, s. Art. No. 2207265

2022 [01/20] / **GBR** - Randrianandraina, J. - Badawi, M. - Ramseyer, C. - Cardey, B. - Groetz, J.-E. - Perreau, N. - Torrealba-Anzola, F. - Chambelland, C. - Ducret, D. - Grivet, M. **Effect of the water coverage on the interaction of O2 and H2 with the Na-LTA zeolite by first-principles simulations** [elektronický dokument] In: **Inorganic Chemistry Frontiers**. London: The Royal Society of Chemistry, 2022, Roč. 10, č. 2, [tlačená forma] [online]. ISSN 2052-1545. ISSN (online) 2052-1553. - SCO, s. 383 - 395

2022 [01/20] / **CHE** - Yu, L. - Li, F. **Pt2 Dimer Anchored Vertically in Defective BN Monolayer as an Efficient Catalyst for N2 Reduction: A DFT Study** In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 12, č. 11, [online]. ISSN 2073-4344. - SCO, s. Art. No. 1387

2022 [01/20] / **CHE** - Xue, S. - Ning, J. - Zhang, B. - Wu, Q. - Zhang, F. - Zhang, W. **The Electronic Structure and Optical Properties of CdGeAs2 Crystal: A DFT and HSE06 Study** [elektronický dokument] In: **Coatings**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 12, č. 11, [online]. ISSN (online) 2079-6412. - SCO, s. Art. No.

1778

2022 [01/20] / **NLD** - Wang, H. - Luo, W. - Wu, M. - Ouyang, C. **Two-dimensional penta-siligraphene with high performance for non-lithium metal ions batteries anode materials** [elektronický dokument] In: **Solid State Ionics**: Diffusion and Reactions. Amsterdam: Elsevier, 2022, Roč. 385, [tlačená forma] [online]. ISSN 0167-2738. ISSN (online) 1872-7689. - SCO, s. Art. No. 116020

2022 [01/20] / **NLD** - Gong, A. - Feng, Y. - Liu, C. - Chen, J. - Wang, Z. - Shen, T. **A promising ZnO/Graphene van der Waals heterojunction as solar cell devices: A first-principles study** [elektronický dokument] In: **Energy Reports**. Amsterdam: Elsevier, 2022, Roč. 8, [online]. ISSN (online) 2352-4847. - SCO, s. 904 - 910

2022 [01/20] / **NLD** - Tran, N.V. - Righi, M.C. **Ab initio insights into the interaction mechanisms between H2, H2O, and O2 molecules with diamond surfaces** In: **Carbon**, 2022, Roč. 199. - SCO, s. 497 - 507

2022 [01/20] / **USA** - Tiwari, N. - Hariharan, S. - Tiwari, A.K. **Effect of temperature on CO oxidation over Pt(111) in two-dimensional confinement** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2022, Roč. 157, č. 14, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 144701

2022 [01/20] / **USA** - Zhu, H. - Gao, Y. - Hou, Y. - Gui, Z. - Huang, L. **Tunable magnetic anisotropy in two-dimensional CrX3/AlN (X= I,Br,Cl) heterostructures** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 106, č. 13, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 134412

2022 [01/20] / **NLD** - Qin, X. - Zhao, J. - Wei, R. - Xu, X. - He, M. **Mechanical properties of pyrophyllite under the coupling of high temperature-pressure: A first-principle study** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2022, Roč. 228, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 106613

2022 [01/20] / **GBR** - Xu, Y. - Zhu, X. - Cheng, Z. - Lu, Z. - He, W. - Zhang, G. **Effect of strain on the tribological properties of honeycomb borophene/graphene heterostructures: An electronic hierarchical understanding of ultra-low friction** [elektronický dokument] In: **Tribology international**. Guildford: Butterworth Scientific, 2022, Roč. 174, [tlačená forma] [online]. ISSN 0301-679X. ISSN (online) 1879-2464. - SCO, s. Art. No. 107707

2022 [01/20] / **GBR** - Sandagiripathira, K. - Moghaddasi, M.A. - Shepard, R. - Smeu, M. **Investigating the role of structural water on the electrochemical properties of alpha-V2O5 through density functional theory** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 39, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 24271 - 24280

2022 [01/20] / **USA** - Nematollahi, P. - Neyts, E.C. **Identification of a Unique Pyridinic FeN4CxElectrocatalyst for N2Reduction: Tailoring the Coordination and Carbon Topologies** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 34. - SCO, s. 14460 - 14469

2022 [01/20] / **GBR** - Wang, Y. - He, M. - He, W. - Niu, Y. - Lu, Z. **The influences of atom relaxation on the DFT-calculated friction properties of the h-BN/h-BN and Gr/Gr interfaces** [elektronický dokument] In: **Tribology international**. Guildford: Butterworth Scientific, 2022, Roč. 173, [tlačená forma] [online]. ISSN 0301-679X. ISSN (online) 1879-2464. - SCO, s. Art. No. 107586

2022 [01/20] / **DEU** - Dong, Y. - Li, J. - Li, F. - Gong, J. **DFT Investigations on the Boron-Phosphorus Assembled Nanowires** [elektronický dokument] In: **Journal of Cluster Science**. Berlín: Springer Nature, 2022, Roč. 33, č. 5. ISSN 1040-7278. ISSN (online) 1572-8862. - SCO, s. 2157 - 2166

2022 [01/20] / **CHE** - Peng, Q. - Rehman, J. - Eid, K. - Alofi, A.S. - Laref, A. - Albaqami, M.D. - Alotabi, R.G. - Shibl, M.F. **Vanadium Carbide (V4C3) MXene as an Efficient Anode for Li-Ion and Na-Ion Batteries** [elektronický dokument] In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 12, č. 16, [online]. ISSN (online) 2079-4991. - SCO, s. Art. No. 2825

2022 [01/20] / **GBR** - Ma, Q. - Young, J. - Basuray, S. - Cheng, G. - Gao, J. - Yao, N. - Zhang, W. **Elucidating facet dependent electronic and electrochemical properties of Cu2O nanocrystals using AFM/SCEM and DFT** [elektronický dokument] In: **Nano today**. Londýn: Elsevier. Elsevier Science, 2022, Roč. 45, [tlačená forma] [online]. ISSN 1748-0132. ISSN (online) 1878-044X. - SCO, s. Art. No. 101538

2022 [01/20] / **USA** - Lv, X. - Chen, X. - Zhang, B. - Jiang, P. - Zhong, Z. **Thickness-Dependent Magnetism and Topological Properties of EuSn2As2** [elektronický dokument] In: **ACS Applied Electronic Materials**. Washington: American Chemical Society, 2022, Roč. 4, č. 7, [online]. ISSN (online) 2637-6113. - SCO, s. 3212 - 3219

2022 [01/20] / **GBR** - Li, J. - Liu, Y. - Yu, L. - Meng, H. - Gu, J. - Li, F. **Lithium stabilizes square-two-dimensional metal sheets: a computational exploration** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 14, č. 32, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 11770 - 11778

2022 [01/20] / **USA** - Xu, B. - Zhang, D. - Chang, S. - Hou, M. - Peng, C. - Xue, D. - Yang, B. - Lei, Y. - Liang, F. **Fabrication of long-life quasi-solid-state Na-CO2 battery by formation of Na2C2O4 discharge product** [elektronický dokument] In: **Cell Reports Physical Science**. Cambridge: Elsevier. Cell Press, 2022, Roč. 3, č. 7, [tlačená forma] [online]. ISSN (online) 2666-3864. - SCO, s. Art. No. 100973

2022 [01/20] / **NLD** - Gorai, D.K. - Kundu, T.K. **NO adsorption on the Os, Ir, and Pt embedded tri-s-triazine based graphitic carbon nitride: A DFT study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2022, Roč. 590, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 153104

2022 [01/20] / **USA** - O'Connor, D. - Bier, I. - Hsieh, Y.-T. - Marom, N. **Performance of Dispersion-Inclusive Density Functional Theory Methods for Energetic Materials** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 7, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 4456 - 4471

2022 [01/20] / **GBR** - Yang, M. - Ren, X. - Li, S. - Zhang, Y. - Li, X. - Pang, R. - Shang, Y. **Electrocatalytic activity of a beta-Sb two-dimensional surface for the hydrogen evolution reaction** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 29, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 17832 - 17840

2022 [01/20] / **CHN** - Yu, L. - Li, F. - Zhao, J. - Chen, Z. **Revisiting catalytic performance of supported metal dimers for oxygen reduction reaction via magnetic coupling from first principles** In: **Advanced Powder Materials**, 2022, Roč. 1, č. 3. - SCO, s. Art. No. 100031

2022 [01/20] / **CHE** - Wang, W. - Cai, M. - Wu, Y. - Ji, K. - Cheng, B. - Liu, X. - Lv, H. - Dai, S. **Defect Healing of MAPbI3 Perovskite Single Crystal Surface by Benzylamine** [elektronický dokument] In: **Symmetry**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 14, č. 6, [online]. ISSN (online) 2073-8994. - SCO, s. Art. No. 1099

2022 [01/20] / **DEU** - Zhou, Y. - Martin, A.J. - Dattila, F. - Xi, S. - Lopez, N. - Perez-Ramirez, J. - Yeo, B.S. **Long-chain hydrocarbons by CO2 electroreduction using polarized nickel catalysts** [elektronický dokument] In: **Nature Catalysis**. Berlín: Springer Nature, 2022, Roč. 5, č. 6. ISSN (online) 2520-1158. - SCO, s. 545 - 554

2022 [01/20] / **DEU** - Zhang, G. - Li, G. - Wang, J. - Tong, H. - Wang, J. - Du, Y. - Sun, S. - Dang, F. **2D SnSe Cathode Catalyst Featuring an Efficient Facet-Dependent Selective Li2O2 Growth/Decomposition for Li-Oxygen Batteries** [elektronický dokument] In: **Advanced Energy Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2022, Roč. 12, č. 21, [tlačená forma] [online]. ISSN 1614-6832. ISSN (online) 1614-6840. - SCO, s. Art. No. 2103910

2022 [01/20] / **USA** - Liu, P. - Liu, T. - Wang, Q. - Yang, Y. **Triggering the Direct C-C Coupling of Gaseous CO into C2Oxygenates by Synergizing Interfacial Interactions and Reversible Spatial Dynamic Confinement** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 20. - SCO, s. 8645 - 8654

2022 [01/20] / **USA** - Shubin, A.A. - Volodin, A.M. - Vedyagin, A.A. **Direct Electron Transfer between Aromatic Molecules inside and outside the ZSM-5 Zeolite Channels: An Identification of the EPR Spectra of 1,3,5-Trimethylbenzene Radical Cations** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 17. - SCO, s. 7421 - 7430

2022 [01/20] / **USA** - Tristant, D. - Cupo, A. - Vekhter, I. - Meunier, V. - Shelton, W.A. **Electronic and vibrational properties of bulk Cr2Ge2Te6 from first-principles calculations** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 105, č. 18, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 184420

2022 [01/20] / **CHE** - Meng, H. - Han, B. - Li, F. - Zhao, J. - Chen, Z. **Understanding the CH4 Conversion over Metal Dimers from First Principles** [elektronický dokument] In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 12, č. 9, [online]. ISSN (online) 2079-4991. - SCO, s. Art. No. 1518

2022 [01/20] / **NLD** - Wen, X. - Bai, P. - Liang, J. - Zheng, S. - Tian, Y. **Slab model studies of H2S adsorption/dissociation and diffusion on pristine FeS(001) surfaces and FeS(001) surfaces with pre-adsorbed X atoms (X = H, O, and S)** [elektronický dokument] In: **Journal of Materials Research and Technology**. Amsterdam: Elsevier, 2022, Roč. 18, [tlačená forma] [online]. ISSN 2238-7854. ISSN (online) 2214-0697. - SCO, s. 1124 - 1136

2022 [01/20] / **NLD** - Tan, S. - Wang, C. - Foucaud, Y. - Badawi, M. - Guo, H. - Sun, K. - Yang, G. - Mintova, S. **Ordered sodium zeolite-templated carbon with high first discharge capacity for sodium battery application** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 336, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 111853

2022 [01/20] / **NLD** - He, M. - Long, J. - Li, M. - Zheng, R. - Hu, A. - Du, D. - Yan, Y. - Ran, Z. - Ren, L. - Li, R. - Zhao, C. - Wen, X. - Xu, H. - Shu, C. **Synergy of cobalt vacancies and iron doping in cobalt selenide to promote oxygen electrode reactions in lithium-oxygen batteries** [elektronický dokument] In: **Journal of colloid and interface science**. Amsterdam: Elsevier, 2022, Roč. 612, [tlačená forma] [online]. ISSN 0021-9797. ISSN (online) 1095-7103. - SCO, s. 171 - 180

2022 [01/20] / **USA** - Chen, P. - Zhao, C. - Wang, H. - Li, Y. - Tan, G. - Shao, Z. - Nishiyama, Y. - Hu, T. - Wohlert, J. **Quantifying the Contribution of the Dispersion Interaction and Hydrogen Bonding to the Anisotropic Elastic Properties of Chitin and Chitosan** [elektronický dokument] In: **Biomacromolecules**. Washington: American Chemical Society, 2022, Roč. 23, č. 4, [tlačená forma] [online]. ISSN 1525-7797. ISSN (online) 1526-4602. - SCO, s. 1633 - 1642

2022 [01/20] / **GBR** - Yu, L. - Li, F. **Metal dimers embedded vertically in defect-graphene as gas sensors: a first-principles study** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 17, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 9842 - 9847

2022 [01/20] / **USA** - Pham, C.H. - Lindsey, R.K. - Fried, L.E. - Goldman, N. **High-Accuracy Semiempirical Quantum Models Based on a Minimal Training Set** In: **Journal of Physical Chemistry Letters**, 2022, Roč. 13, č. 13. - SCO, s. 2934 - 2942

2022 [01/20] / **CHE** - Gao, Y. - Xie, Y. - Wang, S. - Li, S. - Chen, L. - Zhang, J. **Electronic and Optical Properties of Twin T-Graphene Co-Doped with Boron and Phosphorus** In: **Materials**, 2022, Roč. 15, č. 8. - SCO, s. Art. No. 2876

2022 [01/20] / **NLD** - Xu, Y. - Zhu, X. - Cheng, Z. - Lu, Z. - He, W. - Zhang, G. **A novel ultra-low friction heterostructure: Aluminum substrate-honeycomb borophene/graphene heterojunction** [elektronický dokument] In: **Computational Materials Science**. Amsterdam: Elsevier, 2022, Roč. 205, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO, s. Art. No. 111236

2022 [01/20] / **NLD** - Nikmanesh, S. - Safaiee, R. - Sheikhi, M.H. **Enhanced methane-sensing performances of Pd (monomer or dimer) decorated or doped gamma-Graphyne: A DFT insight** [elektronický dokument] In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2022, Roč. 29, [online]. ISSN (online) 2468-0230. - SCO, s. Art. No. 101658

2022 [01/20] / **NLD** - Ren, M. - Zhang, M. **A novel tunable two dimensional ferroelectric material SbAs(CH2OCH3)2 with topological and valley polarized properties** In: **Physica E: Low-Dimensional Systems and Nanostructures**, 2022, Roč. 138. - SCO, s. Art. No. 115123

2022 [01/20] / **NLD** - Wang, X. - Wang, X. - Tian, W. - Meng, A. - Li, Z. - Li, S. - Wang, L. - Li, G. **High-energy ball-milling constructing P-doped g-C3N4/MoP heterojunction with Mo-N bond bridged interface and Schottky barrier for enhanced photocatalytic H2 evolution** In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2022, Roč. 303, [tlačená forma]. ISSN 0926-3373. - SCO, s. Art. No. 120933

2022 [01/20] / **NLD** - Liu, T. - Ju, X. - Hu, Z. - Xie, R. **Cobalt oxide confined in mesoporous SiO2 as effective catalyst for CO oxidation** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 333, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 111733

2022 [01/20] / **NLD** - Chen, J. - Ma, K. - Xiao, J. - Xu, L. - Dai, X. - Wang, Z. **Modulation of the electronic properties of blue phosphorene/stanene heterostructures by electric field and interlayer distance** [elektronický dokument] In: **Results in Physics**: The new online only, open access journal in Physics. Amsterdam: Elsevier, 2022, Roč. 34, [online]. ISSN (online) 2211-3797. - SCO, s. Art. No. 105252

2022 [01/20] / **NLD** - Li, A. - Peng, S. - Zhou, W. - Pan, J. - Zhang, B. - Ouyang, F. **Semiconductor-to-metal transitions in spin-valve-like van der Waals heterostructures based on buckled honeycombs** [elektronický dokument] In: **Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2022, Roč. 544, [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCO, s. Art. No. 168706

2022 [01/20] / **USA** - Liu, T.-W. - Gorky, F. - Carreon, M.L. - Gomez-Gualdron, D.A. **Energetics of Reaction Pathways Enabled by N and H Radicals during Catalytic, Plasma-Assisted NH3Synthesis** In: **ACS Sustainable Chemistry and Engineering**, 2022, Roč. 10, č. 6. - SCO, s. 2034 - 2051

2022 [01/20] / **USA** - Monteiro, M.C.O. - Dattila, F. - Lopez, N. - Koper, M.T.M. **The Role of Cation Acidity on the Competition between Hydrogen Evolution and CO2Reduction on Gold Electrodes** [elektronický dokument] In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2022, Roč. 144, č. 4, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 1589 - 1602

2022 [01/20] / **USA** - Sarangapani, P. - Charles, J. - Kubis, T. **Tuning Band Tails in Mono- and Multilayered Transition-Metal Dichalcogenides: A Detailed Assessment and a Quick-Reference Guide** [elektronický dokument] In: **Physical Review Applied**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 17, č. 2, [online]. ISSN (online) 2331-7019. - SCO, s. Art. No. A5

2022 [01/20] / **USA** - Gao, Q. - Li, Z. - Ma, M. - Tu, J. - Wang, R. - Liu, Q. - Chen, Z. - Zhang, Y. - Sun, Y. - Ning, J. - Yan,

P. - Yan, Y. - Lu, X. - Ruan, X. - He, L. - Xu, Y. **Isotropic spin polarization in Heusler Co2FeAl thin films** [elektronický dokument] In: **AIP Advances**. Melville: American Institute of Physics, 2022, Roč. 12, č. 2, [online]. ISSN (online) 2158-3226. - SCO, s. Art. No. 025005

2022 [01/20] / **CHE** - Fan, Q. - Zhang, W. - Qing, H. - Yang, J. **Exceptional Thermoelectric Properties of Bilayer GeSe: First Principles Calculation** In: **Materials**, 2022, Roč. 15, č. 3. - SCO, s. Art. No. 971

2022 [01/20] / **NLD** - Xu, C. - Hu, Y. - Wang, W. - Ma, J. **Adsorption of toxic gases on metal doped C3N monolayer: A theoretical study** [elektronický dokument] In: **Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2022, Roč. 1208, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCO, s. Art. No. 113559

2022 [01/20] / **GBR** - Qiu, J. - Chen, X. - Zhang, F. - Zhu, B. - Guo, H. - Liu, X. - Yu, J. - Bao, J. **Highly adjustable piezoelectric properties in two-dimensional LiAlTe2 by strain and stacking** [elektronický dokument] In: **Nanotechnology**. Bristol : Institute of Physics. IOP Publishing, 2022, Roč. 33, č. 5, [tlačená forma] [online]. ISSN 0957-4484. ISSN (online) 1361-6528. - SCO, s. Art. No. 055702

2022 [01/20] / **NLD** - Qin, X. - Zhao, J. - Wei, R. - Cao, Y. - He, M. **First-principles study on the thermodynamic and thermoelastic properties of pyrophyllite at high temperatures** In: **Physica B: Condensed Matter**, 2022, Roč. 625. - SCO, s. Art. No. 413513

2022 [01/20] / **NLD** - Xiong, W. - Wu, Y. - Sun, K.-Y. - Wu, X.S. - Zhou, Y.-H. - Cai, H.-L. - Zou, X. **Ultrathin niobium carbide alleviates colitis through absorbing ROS** In: **Materials and Design**. Amsterdam: Elsevier, 2022, Roč. 213. ISSN 0261-3069. - SCO, s. Art. No. 110351

2022 [01/20] / **NLD** - Powar, N.S. - Hiragond, C.B. - Bae, D. - In, S.-I. **Two-dimensional metal carbides for electro- and photocatalytic CO2 reduction: Review** [elektronický dokument] In: **Journal of CO_2 utilization**. Amsterdam: Elsevier, 2022, Roč. 55, [tlačená forma] [online]. ISSN 2212-9820. ISSN (online) 2212-9839. - SCO, s. Art. No. 101814

2022 [01/20] / **NLD** - Han, L. - Zou, Y. - Zeng, Q. - Guan, X. - Jia, B. - Gao, Y. - Liu, G. - Wu, L. **Strong interlayer interaction in two-dimensional layered PtTe2** [elektronický dokument] In: **Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2022, Roč. 305, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCO, s. Art. No. 122657

2021 [01/20] / **GBR** - Zhang, X. - Yang, B. - Guo, X. - Han, X. - Yan, Y. **Ferromagnetic barrier induced large enhancement of tunneling magnetoresistance in van der Waals perpendicular magnetic tunnel junctions** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 13, č. 47, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 19993 - 20001

2021 [01/20] / **NLD** - Barlocco, I. - Bellomi, S. - Delgado, J.J. - Chen, X. - Prati, L. - Dimitratos, N. - Roldan, A. - Villa, A. **Enhancing activity, selectivity and stability of palladium catalysts in formic acid decomposition: Effect of support functionalization** [elektronický dokument] In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2021, Roč. 382, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO, s. 61 - 70

2021 [01/20] / **GBR** - Lu, J. - Niu, G. - Ren, X. - Bao, D. - Chen, H. - Yang, H. - Lin, X. - Du, S. - Gao, H.-J. **Controllable fabrication and photocatalytic performance of nanoscale single-layer MoSe2islands with substantial edges on an Ag(111) substrate** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 13, č. 45, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 19165 - 19171

2021 [01/20] / **USA** - Yu, G. - Pan, A. - Chen, M. **Interface engineering of ferroelectricity in thin films of thiophosphate AB P2X6(A=Cu,Ag;B=In,Bi,Cr, V;X= S,Se)** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 104, č. 22, [tlačená forma] [online]. ISSN 2469-9950. ISSN

1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. A34

2021 [01/20] / **CHE** - Shakil, M. - Naz, A. - Zeba, I. - Gillani, S.S.A. - Rafique, M. - Ahmed, S. - Zafar, M. **Structural and Magnetic Behavior of MoS2 on Doping of Transition Metals: a DFT Study** [elektronický dokument] In: **Journal of Superconductivity and Novel Magnetism**. Cham: Springer Nature, 2021, Roč. 34, č. 12, [tlačená forma] [online]. ISSN 1557-1939. ISSN (online) 1557-1947. - SCO, s. 3441 - 3453

2021 [01/20] / **DEU** - Lee, Y.J. - Kim, H.-E. - Lee, E. - Lee, J. - Shin, S. - Yun, H. - Kim, E.J. - Jung, H. - Ham, H.C. - Kim, B.J. - Lee, H. **Ultra-Low Pt Loaded Porous Carbon Microparticles with Controlled Channel Structure for High-Performance Fuel Cell Catalysts** [elektronický dokument] In: **Advanced Energy Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2021, Roč. 11, č. 48, [tlačená forma] [online]. ISSN 1614-6832. ISSN (online) 1614-6840. - SCO, s. Art. No. 2102970

2021 [01/20] / **NLD** - Yuan, H. - Su, J. - Zhang, P. - Lin, Z. - Zhang, J. - Zhang, J. - Chang, J. - Hao, Y. **Tuning the intrinsic electric field of Janus-TMDs to realize high-performance -Ga2O3 device based on-Ga2O3/Janus-TMD heterostructures** [elektronický dokument] In: **Materials Today Physics**. Amsterdam: Elsevier. Elsevier Science, 2021, Roč. 21, [online]. ISSN (online) 2542-5293. - SCO, s. Art. No. 100549

2021 [01/20] / **USA** - Liang, K. - Huang, T. - Yang, K. - Si, Y. - Wu, H.-Y. - Lian, J.-C. - Huang, W.-Q. - Hu, W.-Y. - Huang, G.-F. **Dipole Engineering of Two-Dimensional van der Waals Heterostructures for Enhanced Power-Conversion Efficiency: The Case of Janus Ga2SeTe/In S** [elektronický dokument] In: **Physical Review Applied**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 16, č. 5, [online]. ISSN (online) 2331-7019. - SCO, s. Art. No. 054043

2021 [01/20] / **NLD** - Liao, W. - Xie, K. - Liu, L. - Wang, X. - Luo, Y. - Liang, S. - Liu, F. - Jiang, L. **Triggering in-plane defect cluster on MoS2 for accelerated dinitrogen electroreduction to ammonia** In: **Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2021, Roč. 62, [tlačená forma] [online]. ISSN 2095-4956. - SCO, s. 359 - 366

2021 [01/20] / **NLD** - Xu, L. - Liu, Y. - Hu, Z. - Yu, J.C. **Converting cellulose waste into a high-efficiency photocatalyst for Cr(VI) reduction via molecular oxygen activation** In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2021, Roč. 295, [tlačená forma]. ISSN 0926-3373. - SCO, s. Art. No. 120253

2021 [01/20] / **GBR** - Pastukh, S. - Laskowska, M. - Dulski, M. - Krzykawski, T. - Parlinski, K. - Piekarz, P. **Ab initio studies for characterization and identification of nanocrystalline copper pyrophosphate confined in mesoporous silica** [elektronický dokument] In: **Nanotechnology**. Bristol : Institute of Physics. IOP Publishing, 2021, Roč. 32, č. 41, [tlačená forma] [online]. ISSN 0957-4484. ISSN (online) 1361-6528. - SCO, s. Art. No. 415701

2021 [01/20] / **USA** - Barlocco, I. - Capelli, S. - Lu, X. - Bellomi, S. - Huang, X. - Wang, D. - Prati, L. - Dimitratos, N. - Roldan, A. - Villa, A. **Disclosing the Role of Gold on Palladium - Gold Alloyed Supported Catalysts in Formic Acid Decomposition** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2021, Roč. 13, č. 19, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 4210 - 4222

2021 [01/20] / **USA** - Wang, J. - Cai, L. - Chen, J. - Guo, X. - Liu, Y. - Ma, Z. - Xie, Z. - Huang, H. - Chan, M. - Zhu, Y. - Liao, L. - Shao, Q. - Chai, Y. **Transferred metal gate to 2D semiconductors for sub-1 V operation and near ideal subthreshold slope** [elektronický dokument] In: **Science advances**. Washington: American Association for the Advancement of Science, 2021, Roč. 7, č. 44, [online]. ISSN (online) 2375-2548. - SCO, s. Art. No. eabf8744

2021 [01/20] / **USA** - Pavesi, D. - Dattila, F. - Van de Poll, R.C.J. - Anastasiadou, D. - Garcia-Muelas, R. - Figueiredo, M. - Gruter, G.-J.M. - Lopez, N. - Koper, M.T.M. - Schouten, K.J.P. **Modulation of the selectivity of CO2 to CO electroreduction in palladium rich Palladium-Indium nanoparticles** [elektronický dokument] In: **Journal of Catalysis**.

San Diego: Elsevier. Academic Press, 2021, Roč. 402, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 229 - 237

2021 [01/20] / **USA** - Xie, C. - Sun, Y. - Zhu, B. - Guo, P. - Liu, J. **Insight into the dissociation mechanism of ethanol molecule over the nano-aluminum surface: a density functional theory study** In: **Journal of Materials Science**, 2021, Roč. 56, č. 30. ISSN 0022-2461, 1573-4803. - SCO, s. 17096 - 17111

2021 [01/20] / **NLD** - Xu, Y. - Zhu, X. - Lu, Z. - Zhang, G. **Effects of oxygen atoms and oxygen molecules on the electronic properties of modified black phosphorus** [elektronický dokument] In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2021, Roč. 550, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO, s. Art. No. 111285

2021 [01/20] / **USA** - Jana, S. - Myneni, H. - Smiga, S. - Constantin, L.A. - Samal, P. **Benchmark test of a dispersion corrected revised Tao-Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 155, č. 11, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 114102

2021 [01/20] / **CHE** - Jiang, C. - Lv, Z. - Lv, S. - Sai, L. - Wang, S. - Li, F. **Theoretical Design of Novel Boron-Based Nanowires via Inverse Sandwich Clusters** [elektronický dokument] In: **Frontiers in Chemistry**. Lausanne: Frontiers Media, 2021, Roč. 9, [online]. ISSN (online) 2296-2646. - SCO, s. Art. No. 753617

2021 [01/20] / **NLD** - Zeng, H. - Bao, Y. - Chen, Z. - Hu, Y. - Wang, J. - Fan, X. **High-temperature ferromagnetism in monolayers MnGaX3 (X = Te, Se)** [elektronický dokument] In: **Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2021, Roč. 534, [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCO, s. Art. No. 168041

2021 [01/20] / **GBR** - Randrianandraina, J. - Badawi, M. - Cardey, B. - Grivet, M. - Groetz, J.-E. - Ramseyer, C. - Anzola, F.T. - Chambelland, C. - Ducret, D. **Adsorption of water in Na-LTA zeolites: An ab initio molecular dynamics investigation** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 34, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 19032 - 19042

2021 [01/20] / **GBR** - Feng, Q. - Li, X. - Li, X. - Yang, J. **CrSbS3monolayer: A potential phase transition ferromagnetic semiconductor** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 13, č. 33, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 14067 - 14072

2021 [01/20] / **USA** - Samanian, M. - Ghatee, M.H. **Study of the molybdenum dichalcogenide crystals: recent developments and novelty of the P-MoS2 structure** [elektronický dokument] In: **Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2021, Roč. 27, č. 9, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCO, s. Art. No. 268

2021 [01/20] / **USA** - Tristant, D. - Vekhter, I. - Meunier, V. - Shelton, W.A. **Partial charge transfer and absence of induced magnetization in EuS(111)/Bi2Se3 heterostructures** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 104, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 075128

2021 [01/20] / **GBR** - Gorelik, T.E. - Habermehl, S. - Shubin, A.A. - Gruene, T. - Yoshida, K. - Oleynikov, P. - Kaiser, U. - Schmidt, M.U. **Crystal structure of copper perchlorophthalocyanine analysed by 3D electron diffraction** In: **Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials**. Chester: International Union of Crystallography, 2021, Roč. 77. ISSN 2052-5206. - SCO, s. 662 - 675

2021 [01/20] / **DEU** - Monteiro, M.C.O. - Dattila, F. - Hagedoorn, B. - Garcia-Muelas, R. - Lopez, N. - Koper, M.T.M. **Absence of CO2 electroreduction on copper, gold and silver electrodes without metal cations in solution** [elektronický dokument] In: **Nature Catalysis**. Berlín: Springer Nature, 2021, Roč. 4, č. 8. ISSN (online) 2520-1158. - SCO, s. 654 - 662

2021 [01/20] / **NLD** - Yang, F. - Zhuo, Z. - Han, J. - Cao, X. - Tao, Y. - Zhang, L. - Liu, W. - Zhu, Z. - Dai, Y. **Optical and tuning electronic properties of GeC/MoS2 van der Waals heterostructures by electric field and strain: A first-principles study** [elektronický dokument] In: **Superlattices and Microstructures**: a journal devoted to the science and technology of synthetic microstructures, microdevices, surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 156, [tlačená forma] [online]. ISSN 0749-6036. ISSN (online) 1096-3677. - SCO, s. Art. No. 106935

2021 [01/20] / **NLD** - Feng, L. - Lu, J. - Zhang, X. - Xiang, G. **Tuning electronic structure and optical properties of monolayer GeAs and GeAs2 by alloying with nitrogen and phosphorus elements** In: **Physica B: Condensed Matter**, 2021, Roč. 614. - SCO, s. Art. No. 413033

2021 [01/20] / **USA** - Lu, X. - Roldan, A. **Are Carbon-Based Materials Good Supports for the Catalytic Reforming of Ammonia?** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 29. - SCO, s. 15950 - 15958

2021 [01/20] / **DEU** - Zhou, S. - Jin, K. - Buehler, M.J. **Understanding Plant Biomass via Computational Modeling** [elektronický dokument] In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2021, Roč. 33, č. 28, [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO, s. Art. No. 2003206

2021 [01/20] / **CHE** - Xiong, L. - Wang, H. - Yu, S. - Xiong, W. - Ouyang, C. **First-principles calculation identification of ultrahigh hydrogen storage capacity in g-Mg3N2** [elektronický dokument] In: **Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2021, Roč. 867, [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCO, s. Art. No. 158744

2021 [01/20] / **GBR** - Dong, Y. - Xu, B. - Hu, H. - Yang, J. - Li, F. - Gong, J. - Chen, Z. **C9N4and C2N6S3monolayers as promising anchoring materials for lithium-sulfur batteries: Weakening the shuttle effect: Via optimizing lithium bonds** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 23, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 12958 - 12967

2021 [01/20] / **GBR** - Wang, B.-H. - Gao, B. - Zhang, J.-R. - Chen, L. - Junkang, G. - Shen, S. - Au, C.-T. - Li, K. - Cai, M.-Q. - Yin, S.-F. **Thickness-induced band-gap engineering in lead-free double perovskite Cs2AgBiBr6for highly efficient photocatalysis** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 21, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 12439 - 12448

2021 [01/20] / **NLD** - Dong, Y. - Lv, X. - Yu, L. - Li, F. - Gong, J. **Two-dimensional phosphorus-based binary nanosheets for photocatalyzing water splitting: A first-principles study** [elektronický dokument] In: **Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2021, Roč. 772, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCO, s. Art. No. 138594

2021 [01/20] / **USA** - Xu, Y. - Cheng, Z. - Zhu, X. - Lu, Z. - Zhang, G. **Ultra-Low Friction of Graphene/Honeycomb Borophene Heterojunction** In: **Tribology Letters**, 2021, Roč. 69, č. 2. - SCO, s. Art. No. 44

2021 [01/20] / **NLD** - Zhang, C. - Zhou, B. - Wang, X. **Structure distortion related magnetic anisotropy in 5d transition-metal dimer adsorbed g-C3N4 monolayers** In: **Physica E: Low-Dimensional Systems and Nanostructures**, 2021, Roč. 130. - SCO, s. Art. No. 114697

2021 [01/20] / **GBR** - Peng, B. - Xu, L. - Zeng, J. - Qi, X. - Yang, Y. - Ma, Z. - Huang, X. - Wang, L.-L. - Shuai, C. **Layer-**

dependent photocatalysts of GaN/SiC-based multilayer van der Waals heterojunctions for hydrogen evolution [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 9, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 3059 - 3069

2021 [01/20] / **NLD** - Xu, L. - Zeng, J. - Li, Q. - Xia, L. - Luo, X. - Ma, Z. - Peng, B. - Xiong, S.X. - Li, Z. - Wang, L.-L. - Lei, Y. **Defect-engineered 2D/2D hBN/g-C3N4 Z-scheme heterojunctions with full visible-light absorption: Efficient metal-free photocatalysts for hydrogen evolution** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 547, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 149207

2021 [01/20] / **NLD** - Vacacela Gomez, C. - Guevara, M. - Tene, T. - Villamagua, L. - Usca, G.T. - Maldonado, F. - Tapia, C. - Cataldo, A. - Bellucci, S. - Caputi, L.S. **The liquid exfoliation of graphene in polar solvents** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 546, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 149046

2021 [01/20] / **NLD** - Liu, P. - Yang, Y. - Wang, Q. **Mechanism insights into direct conversion of syngas into C2 oxygenates via key intermediate C2O2 over Ni-Supported graphene** In: **Carbon**, 2021, Roč. 175. - SCO, s. 322 - 333

2021 [01/20] / **GBR** - Hofmann, O.T. - Zojer, E. - Hormann, L. - Jeindl, A. - Maurer, R.J. **First-principles calculations of hybrid inorganic-organic interfaces: From state-of-the-art to best practice** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 8132 - 8180

2021 [01/20] / **NLD** - Li, A. - Zhou, W. - Peng, S. - Wang, Y. - Long, M. - Ouyang, F. **Half-metallicity and enhanced magnetism in monolayer T-CrTe2 by lithium adsorption** In: **Physics Letters, Section A: General, Atomic and Solid State Physics**, 2021, Roč. 394. - SCO, s. Art. No. 127195

2021 [01/20] / **NLD** - Yu, B.-Y. - Xie, Y. - Wu, X. - Gao, Y. - Wang, S.-F. - Zhang, J.-M. **Structural and electronic properties of AlY (Y[dbnd]B, N, O) dual-doped twin graphene: A density functional theory study** In: **Physica E: Low-Dimensional Systems and Nanostructures**, 2021, Roč. 128. - SCO, s. Art. No. 114619

2021 [01/20] / **NLD** - Xie, Q.-X. - Zhao, Y. **The stability analysis of the monolayer triangular borophene adsorbed on substrates: First-principles simulation** [elektronický dokument] In: **Computational Materials Science**. Amsterdam: Elsevier, 2021, Roč. 190, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO, s. Art. No. 110271

2021 [01/20] / **NLD** - Tunega, D. - Zaoui, A. **Adsorption of polycyclic aromatic hydrocarbons on FeOOH polymorphs: A theoretical study** [elektronický dokument] In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2021, Roč. 706, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO, s. Art. No. 121795

2021 [01/20] / **GBR** - Lu, X. - Zhang, J. - Chen, W.-K. - Roldan, A. **Kinetic and mechanistic analysis of NH3decomposition on Ru(0001), Ru(111) and Ir(111) surfaces** [elektronický dokument] In: **Nanoscale Advances**. Londýn: The Royal Society of Chemistry, 2021, Roč. 3, č. 6, [online]. ISSN (online) 2516-0230. - SCO, s. 1624 - 1632

2021 [01/20] / **GBR** - Lv, X. - Yu, L. - Li, F. - Gong, J. - He, Y. - Chen, Z. **Penta-MS2(M = Mn, Ni, Cu/Ag and Zn/Cd) monolayers with negative Poisson's ratios and tunable bandgaps as water-splitting photocatalysts** [elektronický dokument] In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2021, Roč. 9, č. 11, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 6993 - 7004

2021 [01/20] / **USA** - Lei, C. - Chittari, B.L. - Nomura, K. - Banerjee, N. - Jung, J. - Macdonald, A.H. **Magnetoelectric Response of Antiferromagnetic CrI3Bilayers** [elektronický dokument] In: **Nano letters**. Washington: American Chemical

Society, 2021, Roč. 21, č. 5, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCO, s. 1948 - 1954

2021 [01/20] / **GBR** - Dong, Y. - Wang, S. - Yu, C. - Li, F. - Gong, J. - Zhao, J. **First-principles explorations on P8and N2assembled nanowire and nanosheet** [elektronický dokument] In: **NANO EXPRESS**. Bristol: Institute of Physics. IOP Publishing, 2021, Roč. 2, č. 1, [online]. ISSN (online) 2632-959X. - SCO, s. Art. No. 010004

2021 [01/20] / **GBR** - Behatha, A. - Sharma, V.K. - Gummula, S. - Venkatakrishnan, K. **A quasi two dimensional metallic state of CaHCl driven by La doping studied from first principles theory** In: **Materials Today Communications**, 2021, Roč. 26. - SCO, s. Art. No. 101830

2021 [01/20] / **GBR** - Xie, C. - Sun, Y. - Zhu, B. - Song, W. - Xu, M. **Adsorption mechanism of NH3, NO, and O2molecules over the FexOy/AC catalyst surface: a DFT-D3 study** [elektronický dokument] In: **New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2021, Roč. 45, č. 6, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCO, s. 3169 - 3180

2021 [01/20] / **USA** - Chizallet, C. - Schlaup, C. - Fonda, E. - Carrier, X. **Surface orientation dependent interaction of cobalt (II) precursors with alpha-alumina** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 394, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 157 - 166

2021 [01/20] / **NLD** - Wang, S.-F. - Wang, B.-T. - Bo, T. - Zhang, J.-R. - Wang, F.-W. **Theoretical investigation of Ti2B monolayer as powerful anode material for Li/Na batteries with high storage capacity** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 538, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 148048

2021 [01/20] / **USA** - Karna, S.K. - Tristant, D. - Hebert, J.K. - Cao, G. - Chapai, R. - Phelan, W.A. - Zhang, Q. - Wu, Y. - Dhital, C. - Li, Y. - Cao, H.B. - Tian, W. - Dela Cruz, C.R. - Aczel, A.A. - Zaharko, O. - Khasanov, A. - McGuire, M.A. - Roy, A. - Xie, W. - Browne, D.A. - Vekhter, I. - Meunier, V. - Shelton, W.A. - Adams, P.W. - Sprunger, P.T. - Young, D.P. - Jin, R. - Ditusa, J.F. **Helical magnetic order and Fermi surface nesting in noncentrosymmetric ScFeGe** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 103, č. 1, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 014443

2021 [01/20] / **GBR** - Shubin, A.A. - Zilberberg, I.L. **Entropy driven preference for alkene adsorption at the pore mouth as the origin of pore-mouth catalysis for alkane hydroisomerization in 1D zeolites** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 2, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 563 - 574

2021 [01/20] / **GBR** - Meng, L. - Lu, J. - Bai, Y. - Liu, L. - Tang, J. - Zhang, X. **Graphene adlayer growth between nonepitaxial graphene and the Ni(111) substrate: a theoretical study** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 3, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 2222 - 2228

2021 [01/20] / **GBR** - Li, S. - Ceccato, M. - Lu, X. - Frank, S. - Lock, N. - Roldan, A. - Hu, X.-M. - Skrydstrup, T. - Daasbjerg, K. **Incorporation of nickel single atoms into carbon paper as self-standing electrocatalyst for CO2reduction** [elektronický dokument] In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2021, Roč. 9, č. 3, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 1583 - 1592

2021 [01/20] / **USA** - An, J. - Wanaguru, P. - Tan, Z. - Peng, Y. - Zhang, Q. **Curvature-induced bandgap reduction in TiO2double-walled nanotubes** [elektronický dokument] In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2021, Roč. 129, č. 2, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO, s. Art. No. 024303

2021 [01/20] / **GBR** - Huang, J. - Wang, Q. - Liu, P. - Chen, G.-H. - Yang, Y. **Tuning adlayer-substrate interactions of graphene/h-BN heterostructures on Cu(111)-Ni and Ni(111)-Cu surface alloys** [elektronický dokument] In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 4, [online]. ISSN (online) 2046-2069. - SCO, s. 1916 - 1927

2021 [01/20] / **NLD** - Nishiyama, Y. **Combining computational and experimental studies for a better understanding of cellulose and its analogs** In: **Advances in Carbohydrate Chemistry and Biochemistry**. Amsterdam: Elsevier, 2021. - SCO, s. 1 - 14

2021 [01/20] / **USA** - Hu, Y. - Jin, S. - Luo, Z.F. - Zeng, H.H. - Wang, J.H. - Fan, X.L. **Conversation from antiferromagnetic MnBr2 to ferromagnetic Mn3Br8 monolayer with large MAE** [elektronický dokument] In: **Nanoscale research letters**. New York: Springer Nature, 2021, Roč. 16, č. 1, [tlačená forma] [online]. ISSN 1931-7573. ISSN (online) 1556-276X. - SCO, s. Art. No. 72

2021 [01/20] / **NLD** - Ding, L.-J. - Li, G.-G. - Zhang, C.-W. - Li, P. - Wang, P.-J. **Novel two-dimensional KAB (A = Cu, Au, B = S, Se) photoelectric materials with Prominent carrier mobility and optical properties** [elektronický dokument] In: **Superlattices and Microstructures**: a journal devoted to the science and technology of synthetic microstructures, microdevices, surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 149, [tlačená forma] [online]. ISSN 0749-6036. ISSN (online) 1096-3677. - SCO, s. Art. No. 106773

2021 [01/20] / **DEU** - Nikmanesh, S. - Safaiee, R. - Sheikhi, M.H. **A novel high-performance methane sensor based on Ti-Decorated 2D -graphyne: A dispersion-corrected DFT insight** [elektronický dokument] In: **Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2021, Roč. 257, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCO, s. Art. No. 123808

2020 [01/12] / **NLD** - Berro, Y. - Badawi, M. - El Haj Hassan, F. - Kassir, M. - Tielens, F. **Water-silanol interactions on the amorphous silica surface: A dispersion-corrected DFT investigation** [elektronický dokument] In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2020, Roč. 320, [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. Art. No. 114496

2020 [01/12] / **USA** - Raynor, S. - Song, H.H. **Development of a Cyclic Periodic Wave Function Approach for the Study of Infinitely Periodic Solid-State Systems** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 48, [online]. ISSN (online) 2470-1343. - SCO, s. 31060 - 31068

2020 [01/12] / **USA** - Jana, S. - Patra, A. - Asmiga, S. - Constantin, L.A. - Samal, P. **Insights from the density functional performance of water and water-solid interactions: SCAN in relation to other meta-GGAs** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 21, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 214116

2020 [01/12] / **RUS** - Troitskaya, E.P. - Pilipenko, E.A. - Gorbenko, I.I. **Specific Heat Capacity and the Debye Temperature of a Compressed Crystalline Neon in the Model of Deformable Atoms** [elektronický dokument] In: **Physics of the Solid State**. Moskva: Nauka Publishers. MAIK Nauka/Interperiodica. Pleiades Publishing, 2020, Roč. 62, č. 12, [tlačená forma]. ISSN 1063-7834. ISSN (online) 1090-6460. - SCO, s. 2393 - 2399

2020 [01/12] / **DEU** - Bafekry, A. - Stampfl, C. - Peeters, F.M. **Dirac half-metallicity of Thin PdCl3 Nanosheets: Investigation of the Effects of External Fields, Surface Adsorption and Defect Engineering on the Electronic and Magnetic Properties** In: **Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2020, Roč. 10, č. 1, [tlačená forma]. ISSN 1437-7624. - SCO, s. Art. No. 213

2020 [01/12] / **CHE** - Li, X. - Paier, W. - Paier, J. **Machine Learning in Computational Surface Science and Catalysis: Case Studies on Water and Metal-Oxide Interfaces** [elektronický dokument] In: **Frontiers in Chemistry**. Lausanne: Frontiers Media, 2020, Roč. 8, [online]. ISSN (online) 2296-2646. - SCO, s. Art. No. 601029

2020 [01/12] / **GBR** - Park, H. - Han, D.-H. - Lim, H.T. - Yoon, E. - Lee, G.-D. **Thermodynamic insights into interfacial interactions in TiN/amorphous Al2O3heterostructures:: Ab initio molecular dynamics and first principles investigation** [elektronický dokument] In: **Inorganic Chemistry Frontiers**. London: The Royal Society of Chemistry, 2020, Roč. 7, č. 22, [tlačená forma] [online]. ISSN 2052-1545. ISSN (online) 2052-1553. - SCO, s. 4347 - 4356

2020 [01/12] / **GBR** - Pham, K.D. - Ly, T.H. - Vu, T.V. - Hai, L.L. - Nguyen, H.T.T. - Le, P.T.T. - Khyzhun, O.Y. **Gas adsorption properties (N2, H2, O2, NO, NO2, CO, CO2, and SO2) on a Sc2CO2monolayer: A first-principles study** [elektronický dokument] In: **New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2020, Roč. 44, č. 43, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCO, s. 18763 - 18769

2020 [01/12] / **GBR** - Bafekry, A. - Stampfl, C. - Nguyen, C. - Ghergherehchi, M. - Mortazavi, B. **Tunable electronic properties of the dynamically stable layered mineral Pt2HgSe3(Jacutingaite)** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 42, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 24471 - 24479

2020 [01/12] / **NLD** - Zhong, Y. - Hu, Z. - Sun, T. - Wang, W. - Kong, Y. - Xu, J. **Pauling's rules guided Monte Carlo search (PAMCARS): A shortcut of predicting inorganic crystal structures** [elektronický dokument] In: **Computer Physics Communications**: An International Journal and Program Library for Computational Physics and Physical Chemistry. Amsterdam: Elsevier, 2020, Roč. 256, [tlačená forma] [online]. ISSN 0010-4655. ISSN (online) 1879-2944. - SCIE ; SCO ; WOS CC, s. Art. No. 107486

2020 [01/12] / **USA** - Raynor, S. - Song, H.H. **A cyclic periodic wave function approach for the study of infinitely periodic solid-state systems. I. Application to the C−H···pí(C≡C) hydrogen bonding systems** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 42, [online]. ISSN (online) 2470-1343. - SCO, s. 27546 - 27555

2020 [01/12] / **USA** - Chabungbam, S. - Dutta, S. - Mohakud, S. **Magnetoelasticity in CrxTe3 (X = C, Si) van der Waals heterobilayers** [elektronický dokument] In: **ACS Applied Electronic Materials**. Washington: American Chemical Society, 2020, Roč. 2, č. 10, [online]. ISSN (online) 2637-6113. - SCO, s. 3171 - 3177

2020 [01/12] / **USA** - Song, H.H. - Raynor, S. **A cyclic periodic wave function approach for the study of infinitely periodic solid-state systems: II. Application to helical polysaccharides** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 42, [online]. ISSN (online) 2470-1343. - SCO, s. 27556 - 27565

2020 [01/12] / **USA** - Liu, H.-Y. - Lin, S.-Y. - Wu, J.-Y. - Wu, J.-Y. **Stacking-configuration-enriched essential properties of bilayer graphenes and silicenes** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 15, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 0024421

2020 [01/12] / **NLD** - Gao, Z. - Li, L. - Huang, H. - Xu, S. - Yan, G. - Zhao, M. - Ding, Z. **Adsorption characteristics of acid gases (NO, NO2, SO2 and SO3) on different single-atom nickel adsorbent: A first-principles study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 527, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 146939

2020 [01/12] / **CHN** - Li, A. - Zhou, W. - Pan, J. - Xia, Q. - Long, M. - Ouyang, F. **Coupling Stacking Orders with Interlayer Magnetism in Bilayer H-VSe2** [elektronický dokument] In: **Chinese Physics Letters**. Peking: Chinese Physical Society, 2020, Roč. 37, č. 10, [tlačená forma] [online]. ISSN 0256-307X. ISSN (online) 1741-3540. - SCO, s. Art. No. 107101

2020 [01/12] / **NLD** - Pohls, J.-H. - Heyberger, M. - Mar, A. **Comparison of computational and experimental inorganic crystal structures** [elektronický dokument] In: **Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2020, Roč. 290, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCO, s. Art. No. 121557

2020 [01/12] / **NLD** - Liu, W.-H. - Zeng, W. - Qin, H. - Gan, Y.-D. - Liu, F.-S. - Tang, B. - Liu, Q.-J. **Theoretical study on the effect of different surfaces on structure, excess energy, electronic structure and impact sensitivity in 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane** [elektronický dokument] In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2020, Roč. 700, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO, s. Art. No. 121650

2020 [01/12] / **USA** - Guo, H. - Zhang, X. - Lu, G. **Shedding light on moire excitons: A first-principles perspective** [elektronický dokument] In: **Science advances**. Washington: American Association for the Advancement of Science, 2020, Roč. 6, č. 42, [online]. ISSN (online) 2375-2548. - SCO, s. Art. No. eabc5638

2020 [01/12] / **NLD** - Tsyshevsky, R. - Head, A.R. - Trotochaud, L. - Bluhm, H. - Kuklja, M.M. **Mechanisms of Degradation of Toxic Nerve Agents: Quantum-chemical Insight into Interactions of Sarin and Soman with Molybdenum Dioxide** [elektronický dokument] In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2020, Roč. 700, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO, s. Art. No. 121639

2020 [01/12] / **USA** - Jafari, A. - Klobes, B. - Sergueev, I. - Moseley, D.H. - Manley, M.E. - Dronskowski, R. - Deringer, V.L. - Stoffel, R.P. - Bessas, D. - Chumakov, A.I. - Ruffer, R. - Mahmoud, A. - Bridges, C.A. - Daemen, L.L. - Cheng, Y. - Ramirez-Cuesta, A.J. - Hermann, R.P. **Phonon Spectroscopy in Antimony and Tellurium Oxides** In: **Journal of Physical Chemistry A**, 2020, Roč. 124, č. 39. - SCO, s. 7869 - 7880

2020 [01/12] / **USA** - Hernangomez-Perez, D. - Schlor, J. - Egger, D.A. - Patera, L.L. - Repp, J. - Evers, F. **Reorganization energy and polaronic effects of pentacene on NaCl films** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 11, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 115419

2020 [01/12] / **GBR** - Yang, F. - Han, J. - Zhang, L. - Tang, X. - Zhuo, Z. - Tao, Y. - Cao, X. - Dai, Y. **Adjustable electronic and optical properties of BlueP/MoS2van der Waals heterostructure by external strain: A first-principles study** [elektronický dokument] In: **Nanotechnology**. Bristol : Institute of Physics. IOP Publishing, 2020, Roč. 31, č. 37, [tlačená forma] [online]. ISSN 0957-4484. ISSN (online) 1361-6528. - SCO, s. Art. No. 375706

2020 [01/12] / **CHE** - Yan, W.J. - Zheng, Y.F. - Zhou, T.W. - Wang, G.Z. - Wang, D.D. - Yuan, H.K. **Formation of a Key Intermediate Complex Species in Catalytic Hydrolysis of NH3BH3 by Bimetal Clusters: Metal-Dihydride and Boron-Multihydroxy** [elektronický dokument] In: **Frontiers in Chemistry**. Lausanne: Frontiers Media, 2020, Roč. 8, [online]. ISSN (online) 2296-2646. - SCO, s. Art. No. 604

2020 [01/12] / **USA** - Zhou, Y. - Sethi, G. - Zhang, C. - Ni, X. - Liu, F. **Giant intrinsic circular dichroism of enantiomorphic flat Chern bands and flatband devices** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 12, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 125115

2020 [01/12] / **GBR** - Zhang, C. - Wang, X. - Mi, W. **5d transition-metal atom/5d-3d dimer adsorption tailored electronic structure and magnetic anisotropy of two-dimensional WSe2monolayers** [elektronický dokument] In:

Journal of Materials Chemistry C: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2020, Roč. 8, č. 33, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO, s. 11417 - 11425

2020 [01/12] / **CHE** - Qin, X. - Zhao, J. - Wang, J. - He, M. **Atomic structure, electronic, and mechanical properties of pyrophyllite under pressure: A first-principles study** [elektronický dokument] In: **Minerals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 10, č. 9, [online]. ISSN (online) 2075-163X. - SCO, s. Art. No. 778

2020 [01/12] / **CHE** - Han, B. - Meng, H. - Li, F. - Zhao, J. **Fe3 cluster anchored on the C2N monolayer for efficient electrochemical nitrogen fixation** In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 10, č. 9, [online]. ISSN 2073-4344. - SCO, s. Art. No. 974

2020 [01/12] / **USA** - Takagi, M. - Maeda, S. **Global Search for Crystal Structures of Carbon under High Pressure** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 29, [online]. ISSN (online) 2470-1343. - SCO, s. 18142 - 18147

2020 [01/12] / **GBR** - Bafekry, A. - Obeid, M.M. - Nguyen, C.V. - Ghergherehchi, M. - Bagheri, Tagani M. **Graphene hetero-multilayer on layered platinum mineral jacutingaite (Pt2HgSe3): Van der Waals heterostructures with novel optoelectronic and thermoelectric performances** [elektronický dokument] In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2020, Roč. 8, č. 26, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 13248 - 13260

2020 [01/12] / **GBR** - Bafekry, A. - Nguyen, C.V. - Goudarzi, A. - Ghergherehchi, M. - Shafieirad, M. **Investigation of strain and doping on the electronic properties of single layers of C6N6and C6N8: A first principles study** [elektronický dokument] In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 10, č. 46, [online]. ISSN (online) 2046-2069. - SCO, s. 27743 - 27751

2020 [01/12] / **USA** - Gao, Y. - Nolan, A.M. - Du, P. - Wu, Y. - Yang, C. - Chen, Q. - Mo, Y. - Bo, S.-H. **Classical and Emerging Characterization Techniques for Investigation of Ion Transport Mechanisms in Crystalline Fast Ionic Conductors** [elektronický dokument] In: **Chemical Reviews**. Washington: American Chemical Society, 2020, Roč. 120, č. 13, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO, s. 5954 - 6008

2020 [01/12] / **USA** - Morales-Garcia, A. - Illas, F. **Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 7, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 73601

2020 [01/12] / **GBR** - Cakiroglu, O. - Mehmood, N. - Cicek, M.M. - Aikebaier, A. - Rasouli, H.R. - Durgun, E. - Kasirga, T.S. **Thermal conductivity measurements in nanosheets via bolometric effect** [elektronický dokument] In: **2d materials**. Bristol: Institute of Physics. IOP Publishing, 2020, Roč. 7, č. 3, [online]. ISSN (online) 20531583. - SCO, s. Art. No. 035003

2020 [01/12] / **GBR** - Wang, S. - Gu, J. - Dong, Y. - Sai, L. - Li, F. **A super stable assembled P nanowire with variant structural and magnetic/electronic properties: Via transition metal adsorption** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 12, č. 23, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 12454 - 12461

2020 [01/12] / **GBR** - Zhang, D.-X. - Yin, H. - Zhong, H.-F. - Gan, L.-Y. - Wang, P. **Linear scaling relations for N2H4 decomposition over transition metal catalysts** [elektronický dokument] In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2020, Roč. 45, č. 32, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO, s. 16114 - 16121

2020 [01/12] / Bafekry, A. - Stampfl, C. - Peeters, F.M. **The Electronic, Optical, and Thermoelectric Properties of Monolayer PbTe and the Tunability of the Electronic Structure by External Fields and Defects** In: **Physica Status Solidi (B) Basic Research**, 2020, Roč. 257, č. 6. - SCO, s. Art. No. 2000182

2020 [01/12] / Chen, Z. - Fan, X. - Shen, Z. - Luo, Z. - Yang, D. - Ma, S. **Two-dimensional intrinsic ferromagnetic half-metals: monolayers Mn3X4 (X = Te, Se, S)** In: **Journal of Materials Science**, 2020, Roč. 55, č. 18. ISSN 0022-2461, 1573-4803. - SCO, s. 7680 - 7690

2020 [01/12] / **USA** - Sattari Baboukani, B. - Ye, Z. -, G. Reyes K. - Nalam, P.C. **Prediction of Nanoscale Friction for Two-Dimensional Materials Using a Machine Learning Approach** In: **Tribology Letters**, 2020, Roč. 68, č. 2. - SCO, s. Art. No. 57

2020 [01/12] / Huang, H. - Zhou, J. - Xie, M. - Liu, H. **Mechanistic Study on Graphene Oxidation by KMnO4in Solution Phase and Resultant Carbon-Carbon Unzipping** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 20. - SCO, s. 11165 - 11173

2020 [01/12] / **GBR** - Komaty, S. - Daouli, A. - Badawi, M. - Anfray, C. - Zaarour, M. - Valable, S. - Mintova, S. **Incorporation of trivalent cations in NaX zeolite nanocrystals for the adsorption of O2in the presence of CO2** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 18, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 9934 - 9942

2020 [01/12] / Granet, J. - Sicot, M. - Gerber, I.C. - Kremer, G. - Pierron, T. - Kierren, B. - Moreau, L. - Fagot-Revurat, Y. - Lamare, S. - Cherioux, F. - Malterre, D. **Adsorption-Induced Kondo Effect in Metal-Free Phthalocyanine on Ag(111)** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 19. - SCO, s. 10441 - 10452

2020 [01/12] / Cai, L. - Zhang, N. - Qiu, B. - Chai, Y. **Computational Design of Transition Metal Single-Atom Electrocatalysts on PtS2 for Efficient Nitrogen Reduction** In: **ACS Applied Materials and Interfaces**, 2020, Roč. 12, č. 18. - SCO, s. 20448 - 20455

2020 [01/12] / **DEU** - Teitz, L. - Caspary, Toroker M. **Theoretical Investigation of Dielectric Materials for Two-Dimensional Field-Effect Transistors** [elektronický dokument] In: **Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2020, Roč. 30, č. 18, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCO, s. Art. No. 1808544

2020 [01/12] / **NLD** - Ma, Y. - Wang, M. - Zhou, X. **First-principles investigation of beta-Ge3N4 loaded with RuO2 cocatalyst for photocatalytic overall water splitting** In: **Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 44, [tlačená forma] [online]. ISSN 2095-4956. - SCO, s. 24 - 32

2020 [01/12] / **NLD** - Beheshti, A. - Panahi, F. - Soleymani-Babadi, S. - Mayer, P. - Lipkowski, J. - Motamedi, H. - Samiee, S. **Rational synthesis, structural characterization, theoretical studies, antibacterial activity and selective dye absorption of new silver coordination polymers generated from a flexible bis (imidazole-2-thione) ligand** [elektronický dokument] In: **Inorganica Chimica Acta**: a Monthly Journal with an International Panel of Referees: the International Inorganic Chemistry Journal. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 504, [tlačená forma] [online]. ISSN 0020-1693. ISSN (online) 1873-3255. - SCO, s. Art. No. 119406

2020 [01/12] / Bhandari, A. - Bhattacharya, J. - Pala, R.G.S. **Adsorption Preference of HF over Ethylene Carbonate Leads to Dominant Presence of Fluoride Products in LiFePO4 Cathode-Electrolyte Interface in Li-Ion Batteries** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 17. - SCO, s. 9170 - 9177

2020 [01/12] / **USA** - Shi, Q. - Zhang, D.-X. - Yin, H. - Qiu, Y.-P. - Zhou, L.-L. - Chen, C. - Wu, H. - Wang, P. **Noble-Metal-Free Ni-W-O-Derived Catalysts for High-Capacity Hydrogen Production from Hydrazine Monohydrate** In:

ACS Sustainable Chemistry and Engineering, 2020, Roč. 8, č. 14. - SCO, s. 5595 - 5603

2020 [01/12] / **NLD** - Bafekry, A. **Graphene-like BC6N single-layer: Tunable electronic and magnetic properties via thickness, gating, topological defects, and adatom/molecule** In: **Physica E: Low-Dimensional Systems and Nanostructures**, 2020, Roč. 118. - SCO, s. Art. No. 113850

2020 [01/12] / **GBR** - Cai, X. - Jia, X. - Liu, Y. - Zhang, L. - Yu, W. - Wang, B. - Yang, X. - Wang, Q. - Jia, Y. **Enhanced carrier mobility and tunable electronic properties in alfa-tellurene monolayer: Via an alfa-tellurene and h-BN heterostructure** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 11, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 6434 - 6440

2020 [01/12] / **USA** - Li, X. - Paier, J. **Vibrational properties of CO2 adsorbed on the Fe3O4 (111) surface: Insights gained from DFT** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 152, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 104702

2020 [01/12] / **NLD** - Saidi, M.Z. - Pasc, A. - El Moujahid, C. - Canilho, N. - Badawi, M. - Delgado-Sanchez, C. - Celzard, A. - Fierro, V. - Peignier, R. - Kouitat-Njiwa, R. - Akram, H. - Chafik, T. **Improved tribological properties, thermal and colloidal stability of poly-alfa-olefins based lubricants with hydrophobic MoS2 submicron additives** [elektronický dokument] In: **Journal of colloid and interface science**. Amsterdam: Elsevier, 2020, Roč. 562, [tlačená forma] [online]. ISSN 0021-9797. ISSN (online) 1095-7103. - SCO, s. 91 - 101

2020 [01/12] / **GBR** - Zheng, F.-B. - Zhang, L. - Zhang, J. - Wang, P.-J. - Zhang, C.-W. **Germanene/GaGeTe heterostructure: A promising electric-field induced data storage device with high carrier mobility** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 9, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 5163 - 5169

2020 [01/12] / Wu, J. - Meng, L. - Yu, J. - Li, Y. **A First-Principles Study of Electronic Properties of Twisted MoTe2** In: **Physica Status Solidi (B) Basic Research**, 2020, Roč. 257, č. 3. - SCO, s. Art. No. 1900412

2020 [01/12] / **USA** - Pitussi, I. - Schechter, A. - Teller, H. - Natan, A. - Kornweitz, H. **Tailored Pt Coatings on Metallic Tin - An Effective Catalyst for Fuel Cells Anodes** [elektronický dokument] In: **Journal of the Electrochemical Society**. Pennington: The Electrochemical Society, 2020, Roč. 167, č. 4, [tlačená forma] [online]. ISSN 0013-4651. ISSN (online) 1945-7111. - SCO, s. Art. No. 044512

2020 [01/12] / **GBR** - Liu, N. - Luo, X. - Yuan, X. - Luo, K. - He, J. - Yu, D. - Zhao, Y. **Effect of the bond polarity on interlayer interactions in B-C-N layered materials: A dispersion-corrected density functional study** In: **Materials Today Communications**, 2020, Roč. 22. - SCO, s. Art. No. 100781

2020 [01/12] / **NLD** - Bafekry, A. - Akgenc, B. - Shayesteh, S.F. - Mortazavi, B. **Tunable electronic and magnetic properties of graphene/carbon-nitride van der Waals heterostructures** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 505, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 144450

2020 [01/12] / Sethio, D. - Martins, J.B.L. - Lawson Daku, L.M. - Hagemann, H. - Kraka, E. **Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr, Ba, Pb and X = Cl, Br, I)** In: **Journal of Physical Chemistry A**, 2020, Roč. 124, č. 8. - SCO, s. 1619 - 1633

2020 [01/12] / **USA** - Hua, Q. - Zhou, X. - Zhang, B. - Wang, M. - Liu, J. - Wang, Y. - Jiang, L. **Band Modulation and Interfacial Engineering to Generate Efficient Visible-Light-Induced Bifunctional Photocatalysts** In: **ACS Sustainable Chemistry and Engineering**, 2020, Roč. 8, č. 7. - SCO, s. 2919 - 2930

2020 [01/12] / **GBR** - Lu, X. - Francis, S. - Motta, D. - Dimitratos, N. - Roldan, A. **Mechanistic study of hydrazine decomposition on Ir(111)** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 7, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 3883 - 3896

2020 [01/12] / **GBR** - Xu, B. - Li, S. - Jiao, H. - Yin, J. - Liu, Z. - Zhong, W. **A two-dimensional quinazoline based covalent organic framework with a suitable direct gap and superior optical absorption for photovoltaic applications** [elektronický dokument] In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2020, Roč. 8, č. 7, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 3865 - 3871

2020 [01/12] / **USA** - Bafekry, A. - Neek-Amal, M. **Tuning the electronic properties of graphene-graphitic carbon nitride heterostructures and heterojunctions by using an electric field** [elektronický dokument]. DOI 10.1103/PhysRevB.101.085417 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 101, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. Art. No. 085417

2020 [01/12] / **USA** - Jana, S. - Patra, A. - Constantin, L.A. - Samal, P. **Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 152, č. 4, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 044111

2020 [01/12] / **USA** - Shahrokhi, M. **Role of Intermediate Dynamics in Controlling Hydrogenation Selectivity by Heterogeneous Catalysis** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 2, [online]. ISSN (online) 2470-1343. - SCO, s. 1270 - 1276

2020 [01/12] / **USA** - Ouyang, W. - Azuri, I. - Mandelli, D. - Tkatchenko, A. - Kronik, L. - Urbakh, M. - Hod, O. **Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 1, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 666 - 676

2020 [01/12] / **GBR** - Yang, J. - Yuan, Y. - Chen, G. **First-principles study of potassium adsorption and diffusion on graphene** [elektronický dokument] In: **Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2020, Roč. 118, č. 1, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCO, s. Art. No. e1581291

2020 [01/12] / **CHN** - Cao, H.-L. - Cheng, X.-L. - Zhang, H. **Beryllium carbide as diffusion barrier against Cu: First-principles study** [elektronický dokument] In: **Chinese Physics B**. Peking: Chinese Physical Society, 2020, Roč. 29, č. 1, [tlačená forma] [online]. ISSN 1674-1056. ISSN (online) 2058-3834. - SCO, s. Art. No. 016601

2020 [01/12] / **NLD** - Li, B. - Zhang, S.-F. - Ji, W.-X. - Zhang, C.-W. - Li, P. - Wang, P.-J. **The electric-field and strain inducing electronic and optical properties of the blue phosphorene/ZnO heterostructures** In: **Physica E: Low-Dimensional Systems and Nanostructures**, 2020, Roč. 115. - SCO, s. Art. No. 113650

2020 [01/12] / **GBR** - Lin, X. - Wen, H. - Zhang, D.-X. - Cao, G.-X. - Wang, P. **Highly dispersed nickel nitride nanoparticles on nickel nanosheets as an active catalyst for hydrazine electrooxidation** [elektronický dokument] In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2020, Roč. 8, č. 2, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 632 - 638

2020 [01/12] / **GBR** - Dang, D.T.-X. - Nguyen, H.T.-D. - Thoai, N. - Kuo, J.-L. - Nguyen, N.T.T. - Nguyen-Manh, D. **Mechano-chemical stability and water effect on gas selectivity in mixed-metal zeolitic imidazolate frameworks: A systematic investigation from van der Waals corrected density functional theory** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 3, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 1598 - 1610

2020 [01/12] / Evarestov, R.A. **Binary oxides of transition metals: V2O5** In: **NanoScience and Technology**. Cham: Springer, 2020. - SCO, s. 453 - 518

2020 [01/12] / **GBR** - Li, F.Y. - Lv, X.D. - Gu, J.X. - Tu, K.X. - Gong, J. - Jin, P. - Chen, Z.F. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 12, č. 1, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 85 - 92

2020 [01/12] / Deng, X.Z. - Zhang, J.R. - Zhao, Y.Q. - Yu, Z.L. - Yang, J.L. - Cai, M.Q. **In: Journal of Physics-Condensed Matter**, 2020, Roč. 32, č. 6. - SCIE ; WOS CC, s. Art. No. 065004

2020 [01/12] / Bafekry, A. - Stampfl, C. - Ghergherehchi, M. - Shayesteh, S.F. **In: Carbon**, 2020, Roč. 157. - SCIE ; WOS CC, s. 371 - 384

2020 [01/12] / Shen, Z.H. - Fan, X.L. - Yang, D.X. - Gong, Y.H. - Ma, S.G. - Guo, N.J. - Hu, Y. - Benassi, E. - Lau, W. **In: Journal of Physics-Condensed Matter**, 2020, Roč. 32, č. 8. - SCIE ; WOS CC, s. Art. No. 085801

2020 [01/12] / Zhu, X.H. - Liu, K. - Lu, Z.B. - Xu, Y.P. - Qi, S.S. - Zhang, G.G. **In: Physica E-Low-Dimensional Systems & Nanostructures**, 2020, Roč. 117. - SCIE ; WOS CC, s. Art. No. 113827

2019 [01/12] / Jiao, Y. - Hong, W.Z. - Li, P.Y. - Wang, L.X. - Chen, G. **In: Applied Catalysis B-environmental**, 2019, Roč. 244. - SCIE ; WOS CC, s. 732 - 739

2019 [01/12] / **NLD** - Zhang, W.Y. - Zhang, Y. - Su, H.S. - Zhu, X.R. - Wang, L. - Zhang, J.L. **In: Journal of luminescence**: an interdisciplinary journal of research on excited state processes in condensed matter. Amsterdam: Elsevier, 2019, Roč. 205, [tlačená forma] [online]. ISSN 0022-2313. ISSN (online) 1872-7883. - SCIE ; WOS CC, s. 7 - 13

2019 [01/12] / **GBR** - Shwetha, G. - Aparajita, A.N.A. - Chandra, S. - Shekar, N.V.C. - Kalavathi, S. **In: Materials Research Express**. Bristol: Institute of Physics. IOP Publishing, 2019, Roč. 6, č. 2, [online]. ISSN (online) 2053-1591. - SCIE ; WOS CC, s. Art. No. 026531

2019 [01/12] / Ren, M.J. - Li, M.M. - Yuan, M. - Li, P. - Chen, X.L. **In: Physica E-Low-Dimensional Systems & Nanostructures**, 2019, Roč. 106. - SCIE ; WOS CC, s. 73 - 77

2019 [01/12] / **NLD** - Ranea, V.A. - Quina, P.L.D. - Yalet, N.M. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2019, Roč. 679, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 110 - 116

2019 [01/12] / **DEU** - Qian, C.X. - Sun, W. - Hung, D.L.H. - Qiu, C.Y. - Makaremi, M. - Kumar, S.G.H. - Wan, L.L. - Ghoussoub, M. - Wood, T.E. - Xia, M.K. - Tountas, A.A. - Li, Y.F. - Wang, L. - Dong, Y.C. - Gourevich, I. - Singh, C.V. - Ozin, G.A. **In: Nature Catalysis**. Berlín: Springer Nature, 2019, Roč. 2, č. 1. ISSN (online) 2520-1158. - SCIE ; WOS CC, s. 46 - 54

2019 [01/12] / **GBR** - Li, B. - Ren, C.C. - Zhang, S.F. - Ji, W.X. - Zhang, C.W. - Li, P. - Wang, P.J. **In: Journal of Nanomaterials**. Londýn: Hindawi Publishing Corporation, 2019, Roč. 2019, [tlačená forma] [online]. ISSN 1687-4110. ISSN (online) 1687-4129. - SCIE ; WOS CC, s. Art. No. 4020762

2019 [01/12] / **CHE** - Destefanis, M. - Ravoux, C. - Cossard, A. - Erba, A. **In: Minerals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 1, [online]. ISSN (online) 2075-163X. - SCIE ; WOS CC, s. Art. No. 16

2019 [01/12] / **USA** - Albani, D. - Karajovic, K. - Tata, B. - Li, Q. - Mitchell, S. - Lopez, N. - Perez-Ramirez, J. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 457 - 464

2019 [01/12] / **USA** - Liu, T.T. - Luo, W.J. - Cole, D.R. - Asthagiri, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 150, č. 4, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 044703

2019 [01/12] / **DEU** - Shahbaz, M. - Szalewicz, K. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2019, Roč. 138, č. 2, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 25

2019 [01/12] / Beltran, A. - Gracia, L. - Andres, J. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 5. - SCIE ; WOS CC, s. 3239 - 3253

2019 [01/12] / **NLD** - Zhang, J.R. - Zhao, Y.Q. - Chen, L. - Yin, S.F. - Cai, M.Q. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 469, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 27 - 33

2019 [01/12] / **NLD** - Kodaya, Y. - Oki, T. - Yamakado, H. - Tokoyama, H. - Ohno, K. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2019, Roč. 718, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 32 - 37

2019 [01/12] / **NLD** - Souissi, M. - Sahara, R. - Darvishi, S. - Ahadian, S. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2019, Roč. 300, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 145 - 149

2019 [01/12] / Bai, Y.J. - Deng, K.M. - Kan, E.J. **In: Physica E-Low-Dimensional Systems & Nanostructures**, 2019, Roč. 108. - SCIE ; WOS CC, s. 44 - 52

2019 [01/12] / **CHE** - Kouarta, H. - Zanat, K. - Belkhir, H. **In: Journal of Superconductivity and Novel Magnetism**. Cham: Springer Nature, 2019, Roč. 32, č. 4, [tlačená forma] [online]. ISSN 1557-1939. ISSN (online) 1557-1947. - SCIE ; WOS CC, s. 805 - 819

2019 [01/12] / Li, X.K. - Paier, J. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 13. - SCIE ; WOS CC, s. 8429 - 8438

2019 [01/12] / **GBR** - Xiong, L.X. - Hu, J.P. - Yu, S.C. - Wu, M.S. - Xu, B. - Ouyang, C.Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 13, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 7053 - 7060

2019 [01/12] / **CHE** - Li, W.L. - Zhang, Y. - Long, X. - Cao, J.X. - Xin, X. - Guan, X.X. - Peng, J.F. - Zheng, X.J. **In: Sensors**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 19, č. 9, [tlačená forma] [online]. ISSN 1424-3210. ISSN (online) 1424-8220. - SCIE ; WOS CC, s. Art. No. 2123

2019 [01/12] / Chen, F. - Fan, L. - Hou, X. - Li, C.M. - Chen, Z.Q. **In: materials**, 2019, Roč. 12, č. 10. - SCIE ; WOS CC, s.

Art. No. 1601

2019 [01/12] / Bafekry, A. - Shayesteh, S.F. - Peeters, F.M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 19. - SCIE ; WOS CC, s. 12485 - 12499

2019 [01/12] / Barzaga, R. - Martinez, J.A. - Farias, M.H. - Hernandez, M.P. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 19. - SCIE ; WOS CC, s. 12183 - 12194

2019 [01/12] / Wang, Y.L. - Jiang, Y. - Hu, S.L. - Peng, S. - Xu, C.H. - Lu, A.X. **In: Journal of the American Ceramic Society**, 2019, Roč. 102, č. 6. ISSN 0002-7220. - SCIE ; WOS CC, s. 3663 - 3672

2019 [01/12] / **USA** - Tran, F. - Kalantari, L. - Traore, B. - Rocquefelte, X. - Blaha, P. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 6, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / **NLD** - Long, X. - Li, X. - Wei, X.L. - Can, J.X. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2019, Roč. 725, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 75 - 79

2019 [01/12] / **NLD** - Wang, Q. - Liu, P.F. - Bian, X. - Huang, J.M. - Li, W.Q. - Chen, G.H. - Yang, Y.H. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 480, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 154 - 161

2019 [01/12] / Yang, D.X. - Fang, X.L. - Zhao, D.X. - An, Y.R. - Hu, Y. - Luo, Z.F. **In: Physica E-Low-Dimensional Systems & Nanostructures**, 2019, Roč. 111. - SCIE ; WOS CC, s. 84 - 90

2019 [01/12] / **GBR** - Wang, L.J. - Wang, J. - Zhang, Z.Z. - Wang, L.X. - Wang, W.H. - Liu, J.Y. - Hong, Z.L. - Cho, K. - Wang, W.C. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2019, Roč. 7, č. 27, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 16231 - 16238

2019 [01/12] / **MEX** - Cornejo, M. - Baykara, H. - Vidal, A.B. - Arroyo, D. - Zambrano, D. - Iza, P. - Samaniego, S. - Martiz, A. - Ludena, E.V. **In: Revista Mexicana de Ingenieria Quimica**. Mexico: UAM Unidad Iztapalapa División de Ciencias Básicas e Ingeniería, 2019, Roč. 18, č. 2. ISSN 1665-2738. ISSN (online) 2395-8472. - SCIE ; WOS CC, s. 463 - 476

2019 [01/12] / **CHE** - Hessou, E.P. - Ponce-Vargas, M. - Mensah, J.B. - Tielens, F. - Santos, J.C. - Badawi, M. **In: Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 5, [online]. ISSN (online) 2079-4991. - SCIE ; WOS CC, s. Art. No. 715

2019 [01/12] / **GBR** - Lin, K. - Zhao, Y.P. **In: Extreme Mechanics Letters**. Oxford: Elsevier, 2019, Roč. 30, [online]. ISSN (online) 2352-4316. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / **CHE** - Ananthaneni, S. - Smith, Z. - Rankin, R.B. **In: Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 7, [online]. ISSN 2073-4344. - SCIE ; WOS CC, s. Art. No. 604

2019 [01/12] / Xu, L. - Li, Q. - Li, X.F. - Long, M.Q. - Chen, T. - Peng, B.J. - Wang, L.L. - Yang, Y.W. - Shuai, C.J. **In: Catalysis Science & Technology**, 2019, Roč. 9, č. 15. - SCIE ; WOS CC, s. 3896 - 3906

2019 [01/12] / **CHE** - Lazic, P. - Milat, O. - Gumhalter, B. - Tomic, S. **In: Crystals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 7, [online]. ISSN (online) 2073-4352. - SCIE ; WOS CC, s. Art. No. 348

2019 [01/12] / **USA** - Duim, H. - Fang, H.H. - Adjokatse, S. - ten Brink, G.H. - Marques, M.A.L. - Kooi, B.J. - Blake, G.R. - Botti, S. - Loi, M.A. **In: Applied Physics Reviews**. Melville: American Institute of Physics, 2019, Roč. 6, č. 3, [online]. ISSN (online) 1931-9401. - SCIE ; WOS CC, s. Art. No. 031401

2019 [01/12] / **USA** - Padial, N.M. - Castells-Gil, J. - Almora-Barrios, N. - Romero-Angel, M. - da Silva, I. - Barawi, M. - Garcia-Sanchez, A. - O'Shea, V.A.D. - Marti-Gastaldo, C. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2019, Roč. 141, č. 33, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 13124 - 13133

2019 [01/12] / **GBR** - Xiong, L.X. - Wang, H.W. - Xiong, W. - Yu, S.C. - Ouyang, C.Y. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 47, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 27378 - 27385

2019 [01/12] / **CHN** - Yu, W.Q. - Xiao, H.J. - Wang, G.M. **In: Chinese Physics B**. Peking: Chinese Physical Society, 2019, Roč. 28, č. 10, [tlačená forma] [online]. ISSN 1674-1056. ISSN (online) 2058-3834. - SCIE ; WOS CC, s. Art. No. 103101

2019 [01/12] / Zhang, J.R. - Deng, X.Z. - Gao, B. - Chen, L. - Au, C.T. - Li, K.L. - Yin, S.F. - Cai, M.Q. **In: Catalysis Science & Technology**, 2019, Roč. 9, č. 17. - SCIE ; WOS CC, s. 4659 - 4667

2019 [01/12] / **GBR** - Janatipour, N. - Mandavifar, Z. - Noorizadeh, S. - Shojaei, F. **In: New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2019, Roč. 43, č. 33, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCIE ; WOS CC, s. 13122 - 13133

2019 [01/12] / **CHN** - Ai, W. - Hu, X.H. - Pan, L. - Chen, C.C. - Wang, Y.F. - Shen, X.D. **In: Acta Physica Sinica**. [s.l.]: Chinese Physical Society, 2019, Roč. 68, č. 19, [tlačená forma] [online]. ISSN 1000-3290. - SCIE ; WOS CC, s. Art. No. 197101

2019 [01/12] / Salazar, J.M. - Badawi, M. - Radola, B. - Macaud, M. - Simon, J.M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 38. - SCIE ; WOS CC, s. 23455 - 23463

2019 [01/12] / **GBR** - Bafekry, A. - Shayesteh, S.F. - Peeters, F.M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 21070 - 21083

2019 [01/12] / **GBR** - Wei, H.L. - Sun, J.P. - Hu, Y.F. - Li, Z. - Ai, M. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 56, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 32608 - 32619

2019 [01/12] / **USA** - Bafekry, A. - Shayesteh, S.F. - Ghergherehchi, M. - Peeters, F.M. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2019, Roč. 126, č. 14, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 144304

2019 [01/12] / **NLD** - Gao, B. - Zhang, J.R. - Chen, L. - Guo, J.K. - Shen, S. - Au, C.T. - Yin, S.F. - Cai, M.Q. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 492, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 157 - 165

2019 [01/12] / Tsyshevsky, R. - Holdren, S. - Eichhorn, B.W. - Zachariah, M.R. - Kuklja, M.M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 43. - SCIE ; WOS CC, s. 26432 - 26441

2019 [01/12] / Ngassam, F. - Urbain, E. - Joly, L. - Boukari, S. - Arabski, J. - Bertran, F. - Le Fevre, P. - Garreau, G. - Wetzel, P. - Alouani, M. - Bowen, M. - Weber, W. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 43. - SCIE ;

WOS CC, s. 26475 - 26480

2019 [01/12] / **NLD** - Nie, K. - Wang, X.C. - Mi, W.B. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 493, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 404 - 410

2019 [01/12] / **USA** - Zheng, Y.S. - Jiang, X.X. - Xue, X.X. - Dai, J.Y. - Feng, Y.X. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 17, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 174102

2019 [01/12] / Ai, W. - Kou, L.Z. - Hu, X.H. - Wang, Y.F. - Krasheninnikov, A.V. - Sun, L.T. - Shen, X.D. **In: Journal of Physics-Condensed Matter**, 2019, Roč. 31, č. 44. - SCIE ; WOS CC, s. Art. No. 445301

2019 [01/12] / **USA** - Ikeda, Y. - Tanaka, I. - Neugebauer, J. - Kormann, F. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 11, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 113603

2019 [01/12] / **GBR** - Yu, S.C. - Wang, Z.Q. - Xiong, L.X. - Xiong, W. - Ouyang, C.Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 42, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 23485 - 23491

2019 [01/12] / Fang, L.M. - Liang, W.Z. - Feng, Q.G. - Luo, S.N. **In: Journal of Physics-Condensed Matter**, 2019, Roč. 31, č. 45. - SCIE ; WOS CC, s. Art. No. 455001

2019 [01/12] / **USA** - Li, X.Y. - Chiong, R. - Hu, Z.Y. - Cornforth, D. - Page, M.J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2019, Roč. 15, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 6882 - 6894

2019 [01/12] / **NLD** - Bafekry, A. - Mortazavic, B. - Shayesteh, S.F. **In: Journal of Magnetism and Magnetic Materials**. Amsterdam: Elsevier, 2019, Roč. 491, [tlačená forma] [online]. ISSN 0304-8853. ISSN (online) 1873-4766. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / **USA** - Liu, W.H. - Zeng, W. - Qin, H. - Jiang, C.L. - Liu, F.S. - Tang, B. - Lei, Y.X. - Liu, Q.J. **In: Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2019, Roč. 25, č. 12, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCIE ; WOS CC, s. Art. No. 356

2019 [01/12] / Wang, Y.F. - Zhu, X.H. - Lu, Z.B. - Lin, B. - Zhang, G.G. **In: Physica B-Condensed Matter**, 2019, Roč. 575. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / **USA** - Terentjev, A.V. - Constantin, L.A. - Artacho, E. - Pitarke, J.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235439

2018 [01/12] / **USA** - Koch, D. - Manzhos, S. **In: MRS Advances**. New York: Springer Nature, 2018, Roč. 3, č. 60, [tlačená forma] [online]. ISSN 2731-5894. ISSN (online) 2059-8521. - SCIE ; WOS CC, s. 3507 - 3512

2018 [01/12] / **NLD** - Hu, Y.W. - Long, L.B. - Mao, Y.L. - Zhong, J.X. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 442, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 390 - 397

2018 [01/12] / **USA** - Srour, J. - Badawi, M. - Hassan, F.E. - Postnikov, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 054106

2018 [01/12] / **GBR** - Tada, K. - Maeda, Y. - Ozaki, H. - Tanaka, S. - Yamazaki, S. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 30, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 20235 - 20246

2018 [01/12] / **GBR** - Cheng, H.X. - Zhou, J. - Yang, M. - Shen, L. - Linghu, J.J. - Wu, Q.Y. - Qian, P. - Feng, Y.P. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2018, Roč. 6, č. 31, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 8435 - 8443

2018 [01/12] / Cabral, L. - Sabino, F.P. - Lima, M.P. - Marques, G.E. - Lopez-Richard, V. - Da Silva, J.L.F. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 33. - SCIE ; WOS CC, s. 18895 - 18901

2018 [01/12] / **GBR** - Singh, Y. - Back, S. - Jung, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 32, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 21095 - 21104

2018 [01/12] / Tuerhong, R. - Ngassam, F. - Watanabe, S. - Onoe, J. - Alouani, M. - Bucher, J.P. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 34. - SCIE ; WOS CC, s. 20046 - 20054

2018 [01/12] / **DEU** - Li, Q. - Xu, L. - Luo, K.W. - Wang, L.L. - Li, X.F. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2018, Roč. 216, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 64 - 71

2018 [01/12] / **GBR** - Wen, Y.P. - Zhang, W.Y. - Zhu, X.R. - Zhang, J.L. - Wang, L. **In: Energy**: the International Journal. Londýn: Elsevier, 2018, Roč. 158, [tlačená forma] [online]. ISSN 0360-5442. ISSN (online) 1873-6785. - SCIE ; WOS CC, s. 537 - 545

2018 [01/12] / **USA** - Fronzi, M. - Assadi, M.H.N. - Ford, M.J. **In: ACS Omega**. Washington: American Chemical Society, 2018, Roč. 3, č. 9, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 12215 - 12228

2018 [01/12] / Huang, P.C. - Liu, W. - He, Z.H. - Xiao, C. - Yao, T. - Zou, Y.M. - Wang, C.M. - Qi, Z.M. - Tong, W. - Pan, B.C. - Wei, S.Q. - Xie, Y. **In: Science China-Chemistry**, 2018, Roč. 61, č. 9. - SCIE ; WOS CC, s. 1187 - 1196

2018 [01/12] / **GBR** - Wang, X.S. - Wang, Z.W. - Zhang, J.D. - Wang, X. - Zhang, Z.P. - Wang, J.L. - Zhu, Z.H. - Li, Z.Y. - Liu, Y. - Hu, X.F. - Qiu, J.W. - Hu, G.H. - Chen, B. - Wang, N. - He, Q.Y. - Chen, J.Z. - Yan, J.X. - Zhang, W. - Hasan, T. - Li, S.Z. - Li, H. - Zhang, H. - Wang, Q. - Huang, X. - Huang, W. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2018, Roč. 9, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 3611

2018 [01/12] / **NLD** - Wei, Z.D. - Zhao, Y. - Fan, F.T. - Li, C. **In: Computational Materials Science**. Amsterdam: Elsevier, 2018, Roč. 153, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 28 - 35

2018 [01/12] / **CHE** - Liu, J. - Tian, L.Q. - Mou, Y. - Jia, W.L. - Zhang, L. - Liu, R.J. **In: Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2018, Roč. 764, [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCIE ; WOS CC, s. 674 - 678

2018 [01/12] / **DEU** - Ding, R. - Wang, X.P. - Feng, J. - Li, X.B. - Dong, F.X. - Tian, W.Q. - Du, J.R. - Fang, H.H. - Wang, H.Y. - Yamao, T. - Hotta, S. - Sun, H.B. **In: Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2018, Roč. 30, č. 43, [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCIE ; WOS CC, s. Art. No. 1801078

2018 [01/12] / **GBR** - Shackery, I. - Pezeshki, A. - Park, J.Y. - Palanivel, U. - Kwon, H.J. - Yoon, H.S. - Im, S. - Cho, J.S. - Jun, S.C. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2018, Roč. 6, č. 40, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 10714 - 10722

2018 [01/12] / **DEU** - Rerat, M. - Pascale, F. - Noel, Y. - Carbonniere, P. - Dovesi, R. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2018, Roč. 137, č. 11, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 150

2018 [01/12] / Li, C.Y. - Debnath, B. - Tan, X.J. - Su, S.S. - Xu, K. - Ge, S.P. - Neupane, M.R. - Lake, R.K. **In: Carbon**, 2018, Roč. 138. - SCIE ; WOS CC, s. 451 - 457

2018 [01/12] / **NLD** - Ghanbari, R. - Safaiee, R. - Golshan, M.M. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 457, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 303 - 314

2018 [01/12] / **USA** - Aoyama, S. - Kaiwa, J. - Chantngarm, P. - Tanibayashi, S. - Saito, H. - Hasegawa, M. - Nishidate, K. **In: AIP Advances**. Melville: American Institute of Physics, 2018, Roč. 8, č. 11, [online]. ISSN (online) 2158-3226. - SCIE ; WOS CC, s. Art. No. 115113

2018 [01/12] / **USA** - Najafi, L. - Taheri, B. - Martin-Garcia, B. - Bellani, S. - Di Girolamo, D. - Agresti, A. - Oropesa-Nunez, R. - Pescetelli, S. - Vesce, L. - Calabro, E. - Prato, M. - Castillo, A.E.D. - Di Carlo, A. - Bonaccorso, F. **In: ACS Nano**. Washington: American Chemical Society, 2018, Roč. 12, č. 11, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 10736 - 10754

2018 [01/12] / **CHE** - Xu, W.W. - Xia, F.F. - Chen, L.J. - Wu, M. - Gang, T.Q. - Huang, Y.F. **In: Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2018, Roč. 768, [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCIE ; WOS CC, s. 722 - 732

2018 [01/12] / **USA** - Mosyagin, I. - Gambino, D. - Sangiovanni, D.G. - Abrikosov, I.A. - Caffrey, N.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 17, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 174103

2018 [01/12] / Zhang, W.Y. - Heng, P.P. - Su, H.S. - Ren, T.G. - Wang, L. - Zhang, J.L. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 44. - SCIE ; WOS CC, s. 25219 - 25228

2018 [01/12] / Lei, J. - Xu, M.C. - Hu, S.J. **In: Sensors and Actuators B-Chemical**, 2018, Roč. 273. - SCIE ; WOS CC, s. 448 - 454

2018 [01/12] / **USA** - Meneses-Gustin, D. - Cabral, L. - Lima, M.P. - Da Silva, J.L.F. - Margapoti, E. - Ulloa, S.E. - Marques, G.E. - Lopez-Richard, V. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 241403

2018 [01/12] / **GBR** - Onen, A. - Kecik, D. - Durgun, E. - Ciraci, S. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 10, č. 46, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s.

21842 - 21850

2018 [01/12] / **USA** - Terentjev, A.V. - Constantin, L.A. - Pitarke, J.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 214108

2018 [01/12] / **GBR** - Hou, P.G. - Lian, L.L. - Cai, Y.M. - Liu, B. - Wang, B. - Wei, S.L. - Li, D. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 8, č. 8, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 4314 - 4320

2018 [01/12] / Zhou, L.Q. - Guo, Y. - Zhao, J.J. **In: Physica E-Low-Dimensional Systems & Nanostructures**, 2018, Roč. 95. - SCIE ; WOS CC, s. 149 - 153

2018 [01/12] / **GBR** - Hu, H. - Loh, S.M. - Leung, T.C. - Lin, M.C. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 8, č. 40, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 22625 - 22634

2018 [01/12] / **USA** - McCrum, I.T. - Hickner, M.A. - Janik, M.J. **In: Journal of the Electrochemical Society**. Pennington: The Electrochemical Society, 2018, Roč. 165, č. 2, 114- [tlačená forma] [online]. ISSN 0013-4651. ISSN (online) 1945-7111. - SCIE ; WOS CC, s.

2018 [01/12] / Rasander, M. - Hugosson, H.W. - Delin, A. **In: Journal of Physics-Condensed Matter**, 2018, Roč. 30, č. 1. - SCIE ; WOS CC, s. Art. No. 015702

2018 [01/12] / **USA** - Ji, L.P. - Shi, J. - Zhang, Z.Y. - Wang, J. - Zhang, J.C. - Tao, C.L. - Cao, H.N. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 148, č. 1, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 014704

2018 [01/12] / Freire, R.L.H. - Guedes-Sobrinho, D. - Kiejna, A. - Da Silva, J.L.F. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 3. - SCIE ; WOS CC, s. 1577 - 1588

2018 [01/12] / **NLD** - Aydin, H. - Bacaksiz, C. - Yagmurcukardes, N. - Karakaya, C. - Mermer, O. - Can, M. - Senger, R.T. - Sahin, H. - Selamet, Y. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 428, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 1010 - 1017

2018 [01/12] / **GBR** - Li, Q. - Garcia-Muelas, R. - Lopez, N. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2018, Roč. 9, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 526

2018 [01/12] / Levita, G. - Kajita, S. - Righi, M.C. **In: Carbon**, 2018, Roč. 127. - SCIE ; WOS CC, s. 533 - 540

2018 [01/12] / **GBR** - Yuan, M. - Ji, W.X. - Ren, M.J. - Li, P. - Li, F. - Zhang, S.F. - Zhang, C.W. - Wang, P.J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 6, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 4308 - 4316

2018 [01/12] / **NLD** - Zhang, R.H. - Zhao, J. - Yang, Y.C. - Shi, W. - Lu, Z.B. - Wang, J.J. **In: Current Applied Physics**. Amsterdam: Elsevier. Elsevier Science, 2018, Roč. 18, č. 3, [tlačená forma] [online]. ISSN 1567-1739. ISSN (online) 1878-1675. - SCIE ; WOS CC, s. 317 - 323

2018 [01/12] / Nishiyama, Y. **In: Philosophical Transactions of the Royal Society A-Mathematical Physical and Engineering Sciences**, 2018, Roč. 376, č. 2112. - SCIE ; WOS CC, s. Art. No. 20170047

2018 [01/12] / **GBR** - Zhou, C. - Li, X.X. - Gong, Z.L. - Jia, C.C. - Lin, Y.W. - Gu, C.H. - He, G. - Zhong, Y.W. - Yang, J.L. - Guo, X.F. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2018, Roč. 9, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 807

2018 [01/12] / **NLD** - Xie, Z.J. - Hui, L.L. - Wang, J.H. - Zhu, G.A. - Chen, Z.Q. - Li, C.M. **In: Computational Materials Science**. Amsterdam: Elsevier, 2018, Roč. 144, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 304 - 314

2018 [01/12] / **CHE** - Terentjev, A.V. - Cortona, P. - Constantin, L.A. - Pitarke, J.M. - Della Sala, F. - Fabiano, E. **In: Computation**. Basel: Multidisciplinary Digital Publishing Institute, 2018, Roč. 6, č. 1, [online]. ISSN (online) 2079-3197. - SCIE ; WOS CC, s. Art. No. 7

2018 [01/12] / **GBR** - Gul, A. - Bacaksiz, C. - Unsal, E. - Akbali, B. - Tomak, A. - Zareie, H.M. - Sahin, H. **In: Materials Research Express**. Bristol: Institute of Physics. IOP Publishing, 2018, Roč. 5, č. 3, [online]. ISSN (online) 2053-1591. - SCIE ; WOS CC, s. Art. No. 036415

2018 [01/12] / **NLD** - Makaremi, M. - Mortazavi, B. - Singh, C.V. **In: Applied Materials Today**. Amsterdam: Elsevier, 2018, Roč. 10, [tlačená forma] [online]. ISSN 2352-9407. ISSN (online) 2352-9415. - SCIE ; WOS CC, s. 115 - 121

2018 [01/12] / Wang, V. - Wu, Z.Q. - Kawazoe, Y. - Geng, W.T. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 12. - SCIE ; WOS CC, s. 6930 - 6942

2018 [01/12] / **NLD** - Liu, B. - Zhao, Y.Q. - Yu, Z.L. - Wang, L.Z. - Cai, M.Q. **In: Journal of colloid and interface science**. Amsterdam: Elsevier, 2018, Roč. 513, [tlačená forma] [online]. ISSN 0021-9797. ISSN (online) 1095-7103. - SCIE ; WOS CC, s. 677 - 683

2018 [01/12] / **USA** - Li, Z.Q. - He, C.Y. - Ouyang, T. - Zhang, C.X. - Tang, C. - Romer, R.A. - Zhong, J.X. **In: Physical Review Applied**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 9, č. 4, [online]. ISSN (online) 2331-7019. - SCIE ; WOS CC, s. Art. No. 044032

2018 [01/12] / **NLD** - Tada, K. - Koga, H. - Okumura, M. - Tanaka, S. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2018, Roč. 670, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 23 - 32

2018 [01/12] / **USA** - Domingo, M. - Shahrokhi, M. - Remediakis, I.N. - Lopez, N. **In: Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2018, Roč. 61, č. 5-6, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCIE ; WOS CC, s. 412 - 418

2018 [01/12] / Penschke, C. - Paier, J. - Sauer, J. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 16. - SCIE ; WOS CC, s. 9101 - 9110

2018 [01/12] / **NLD** - Li, L.L. - Zhang, H. - Cheng, X.L. - Miyamoto, Y. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 441, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 647 - 653

2018 [01/12] / **USA** - Li, Q. - Lopez, N. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 5, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 4230 - 4240

2018 [01/12] / **GBR** - Hu, X.H. - Wang, Y.F. - Shen, X.D. - Krasheninnikov, A.V. - Sun, L.T. - Chen, Z.F. **In: 2d materials**. Bristol: Institute of Physics. IOP Publishing, 2018, Roč. 5, č. 3, [online]. ISSN (online) 20531583. - SCIE ; WOS CC, s. Art. No. 031012

2018 [01/12] / **GBR** - Makaremi, M. - Mortazavi, B. - Singh, C.V. **In: Materials Today Energy**. London: Elsevier, 2018, Roč. 8, [online]. ISSN (online) 2468-6069. - SCIE ; WOS CC, s. 22 - 28

2018 [01/12] / **DEU** - Urbain, E. - Ibrahim, F. - Studniarek, M. - Nyakam, F.N. - Joly, L. - Arabski, J. - Scheurer, F. - Bertran, F. - Le Fevre, P. - Garreau, G. - Denys, E. - Wetzel, P. - Alouani, M. - Beaurepaire, E. - Boukari, S. - Bowen, M. - Weber, W. **In: Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2018, Roč. 28, č. 29, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCIE ; WOS CC, s. Art. No. 1707123

2018 [01/12] / **GBR** - Albani, D. - Shahrokhi, M. - Chen, Z.P. - Mitchell, S. - Hauert, R. - Lopez, N. - Perez-Ramirez, J. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2018, Roč. 9, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 2634

2018 [01/12] / **GBR** - Shang, J.M. - Pan, L.F. - Wang, X.T. - Li, J.B. - Deng, H.X. - Wei, Z.M. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2018, Roč. 6, č. 27, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 7201 - 7206

2018 [01/12] / **GBR** - Yuan, Z.H. - Li, S.C. - Liu, J.C. - Kong, X.G. - Gao, T. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2018, Roč. 43, č. 29, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 13639 - 13648

2018 [01/12] / **NLD** - Mao, Y.L. - Long, L.B. - Yuan, J.M. - Zhong, J.X. - Zhao, H.Q. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2018, Roč. 706, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 501 - 508

2018 [01/12] / **GBR** - Caffrey, N.M. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 10, č. 28, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 13520 - 13530

2017 [01/12] / **NLD** - Alves, A.P.P. - Koizumi, R. - Samanta, A. - Machado, L.D. - Singh, A.K. - Galvao, D.S. - Silva, G.G. - Tiwary, C.S. - Ajayan, P.M. **In: Nano Energy**. Amsterdam: Elsevier, 2017, Roč. 31, [tlačená forma] [online]. ISSN 2211-2855. ISSN (online) 2211-3282. - SCIE ; WOS CC, s. 225 - 232

2017 [01/12] / **GBR** - Yang, Y. - Zhang, Z.H. - Penev, E.S. - Yakobson, B.I. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2017, Roč. 9, č. 5, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 1805 - 1810

2017 [01/12] / Besse, R. - Da Silva, J.L.F. **In: Journal of Physics-Condensed Matter**, 2017, Roč. 29, č. 3. - SCIE ; WOS CC, s. Art. No. 035402

2017 [01/12] / **USA** - Lu, J.C. - Bao, D.L. - Qian, K. - Zhang, S. - Chen, H. - Lin, X. - Du, S.X. - Gao, H.J. **In: ACS Nano**. Washington: American Chemical Society, 2017, Roč. 11, č. 2, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 1689 - 1695

2017 [01/12] / **GBR** - Luo, Z.F. - Fan, X.L. - Pan, R. - An, Y.R. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2017, Roč. 42, č. 5, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 3106 - 3113

2017 [01/12] / Guan, Z.Y. - Lian, C.S. - Hu, S.L. - Ni, S. - Li, J. - Duan, W.H. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 6. - SCIE ; WOS CC, s. 3654 - 3660

2017 [01/12] / **USA** - Bacaksiz, C. - Dominguez, A. - Rubio, A. - Senger, R.T. - Sahin, H. **In: Physical Review B**. College

Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075423

2017 [01/12] / Vela, S. - Reardon, M.B. - Jakobsche, C.E. - Turnbull, M.M. - Ribas-Arino, J. - Novoa, J.J. **In: Chemistry-A European Journal**, 2017, Roč. 23, č. 14. - SCIE ; WOS CC, s. 3479 - 3489

2017 [01/12] / Liu, Y.C. - Wang, V. - Xia, M.G. - Zhang, S.L. **In: Journal of Physics-Condensed Matter**, 2017, Roč. 29, č. 9. - SCIE ; WOS CC, s. Art. No. 095702

2017 [01/12] / Lu, Z.P. - Xue, X.G. - Meng, L.Y. - Zeng, Q. - Chi, Y. - Fan, G.J. - Li, H.Z. - Zhang, Z.M. - Nie, F.D. - Zhang, C.Y. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 15. - SCIE ; WOS CC, s. 8262 - 8271

2017 [01/12] / **USA** - Onen, A. - Kecik, D. - Durgun, E. - Ciraci, S. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 15, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 155435

2017 [01/12] / Madhuri, K.P. - Kaur, P. - Ali, M.E. - John, N.S. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 17. - SCIE ; WOS CC, s. 9249 - 9259

2017 [01/12] / Wang, V. - Geng, W.T. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 18. - SCIE ; WOS CC, s. 10224 - 10232

2017 [01/12] / **GBR** - Li, Q. - Xu, L. - Luo, K.W. - Li, X.F. - Huang, W.Q. - Wang, L.L. - Yu, Y.B. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2017, Roč. 5, č. 18, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 4426 - 4434

2017 [01/12] / **DEU** - Du, Y.Y. - He, F. - Hua, Z.L. - Wu, Z.J. - Li, M.L. - Li, J.S. - Huang, K.K. - Shi, J.L. **In: European Journal of Inorganic Chemistry**. Weinheim: John Wiley & Sons. Wiley-VCH, 2017, č. 19, [tlačená forma] [online]. ISSN 1434-1948. ISSN (online) 1099-0682. - SCIE ; WOS CC, s. 2573 - 2579

2017 [01/12] / **GBR** - Albani, D. - Li, Q. - Vile, G. - Mitchell, S. - Almora-Barrios, N. - Witte, P.T. - Lopez, N. - Perez-Ramirez, J. **In: Green Chemistry**: an international journal and green chemistry resource: cutting-edge research for a greener sustainable future. Cambridge: The Royal Society of Chemistry, 2017, Roč. 19, č. 10, [tlačená forma] [online]. ISSN 1463-9262. ISSN (online) 1463-9270. - SCIE ; WOS CC, s. 2361 - 2370

2017 [01/12] / **USA** - Takagi, M. - Taketsugu, T. - Kino, H. - Tateyama, Y. - Terakura, K. - Maeda, S. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 18, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 184110

2017 [01/12] / **USA** - Almora-Barrios, N. - Cano, I. - van Leeuwen, P.W.N.M. - Lopez, N. **In: ACS Catalysis**. Washington: American Chemical Society, 2017, Roč. 7, č. 6, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 3949 - 3954

2017 [01/12] / **DEU** - Musso, T. - Kumar, P.V. - Grossman, J.C. - Foster, A.S. **In: Advanced electronic materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2017, Roč. 3, č. 6, [online]. ISSN (online) 2199-160X. - SCIE ; WOS CC, s. Art. No. 1600318

2017 [01/12] / **USA** - Cervinka, C. - Fulem, M. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2017, Roč. 13, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2840 - 2850

2017 [01/12] / Levita, G. - Righi, M.C. **In: ChemPhysChem**, 2017, Roč. 18, č. 11. - SCIE ; WOS CC, s. 1475 - 1480

2017 [01/12] / Fumanal, M. - Novoa, J.J. - Ribas-Arino, J. **In: Chemistry-A European Journal**, 2017, Roč. 23, č. 32. - SCIE ; WOS CC, s. 7772 - 7784

2017 [01/12] / **USA** - Li, S.S. - Ji, W.X. - Li, P. - Hu, S.J. - Cai, L. - Zhang, C.W. - Yan, S.S. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2017, Roč. 9, č. 25, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 21515 - 21523

2017 [01/12] / **NLD** - Bacaksiz, C. - Senger, R.T. - Sahin, H. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2017, Roč. 409, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 426 - 430

2017 [01/12] / **DEU** - Hart, L.S. - Webb, J.L. - Dale, S. - Bending, S.J. - Mucha-Kruczynski, M. - Wolverson, D. - Chen, C.Y. - Avila, J. - Asensio, M.C. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2017, Roč. 7, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 5145

2017 [01/12] / **GBR** - Singh, B. - Gupta, M.K. - Mishra, S.K. - Mittal, R. - Sastry, P.U. - Rols, S. - Chaplot, S.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 27, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 17967 - 17984

2017 [01/12] / **NLD** - Nasresfahani, S. - Safaiee, R. - Sheikhi, M.H. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2017, Roč. 662, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 93 - 101

2017 [01/12] / **GBR** - Ren, M.J. - Li, M.M. **In: Japanese Journal of Applied Physics**. Tokyo: Japan Society of Applied Physics, 2017, Roč. 56, č. 9, [tlačená forma] [online]. ISSN 0021-4922. ISSN (online) 1347-4065. - SCIE ; WOS CC, s. Art. No. 095201

2017 [01/12] / **NLD** - Lei, J. - Xu, M.C. - Hu, S.J. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2017, Roč. 416, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 681 - 685

2017 [01/12] / **NLD** - Rubio-Pereda, P. - Galicia-Hernandez, J.M. - Cocoletzi, G.H. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2017, Roč. 416, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 266 - 272

2017 [01/12] / **GBR** - Liu, J.H. - Kan, X. - Amin, B. - Gan, L.Y. - Zhao, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 32253 - 32261

2017 [01/12] / **NLD** - Fang, B.C. - Li, J.J. - Zhao, N.Q. - Shi, C.S. - Ma, L.Y. - He, C.N. - He, F. - Liu, E.Z. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2017, Roč. 425, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 811 - 822

2017 [01/12] / Beltran, A. - Gracia, L. - Andres, J. - Longo, E. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 49. - SCIE ; WOS CC, s. 27624 - 27642

2017 [01/12] / **USA** - Wang, K.C. - Stanev, T.K. - Valencia, D. - Charles, J. - Henning, A. - Sangwan, V.K. - Lahiri, A. - Mejia, D. - Sarangapani, P. - Povolotskyi, M. - Afzalian, A. - Maassen, J. - Klimeck, G. - Hersam, M.C. - Lauhon, L.J. -

Stern, N.P. - Kubis, T. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2017, Roč. 122, č. 22, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 224302

2017 [01/12] / **GBR** - Unsal, E. - Senger, R.T. - Sahin, H. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2017, Roč. 5, č. 46, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 12249 - 12255

2017 [01/12] / Onen, A. - Kecik, D. - Durgun, E. - Ciraci, S. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 48. - SCIE ; WOS CC, s. 27098 - 27110

2017 [01/12] / **DEU** - Wang, D.C. - Chen, L. - Liu, H.M. - Shi, C.M. - Wang, X.L. - Cui, G.L. - Zhang, P.H. - Chen, Y.Q. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2017, Roč. 7, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 17089

2017 [01/12] / **USA** - Li, S.S. - Ji, W.X. - Hu, S.J. - Zhang, C.W. - Yan, S.S. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2017, Roč. 9, č. 47, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 41443 - 41453

2017 [01/12] / **GBR** - Li, S.L. - Yin, H. - Kan, X. - Gan, L.Y. - Schwingenschlogl, U. - Zhao, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 44, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 30069 - 30077

2017 [01/12] / **GBR** - Kim, S.J. - Park, B. - Noh, S.H. - Yoon, H.S. - Oh, J. - Yoo, S. - Kang, K. - Han, B. - Jun, S.C. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2017, Roč. 9, č. 41, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 15934 - 15944

2017 [01/12] / **GBR** - Luo, X.K. - Wang, G.Z. - Huang, Y.H. - Wang, B. - Yuan, H.K. - Chen, H. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 41, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 28216 - 28224

2017 [01/12] / **DEU** - Yoon, G. - Kim, D.H. - Park, I. - Chang, D. - Kim, B. - Lee, B. - Oh, K. - Kang, K. **In: Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2017, Roč. 27, č. 40, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCIE ; WOS CC, s. Art. No. 1702887

2017 [01/12] / **GBR** - Wang, L. - Wang, Q. - Huang, J.M. - Li, W.Q. - Chen, G.H. - Yang, Y.H. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 39, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 26765 - 26775

2017 [01/12] / **GBR** - Ma, X.C. - Wu, X. - Zhao, X.W. - Sun, H. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 25456 - 25462

2017 [01/12] / **NLD** - Liu, X. - Cheng, X.L. - Lu, Y.P. **In: Physics Letters A**: General Physics, Nonlinear Science, Statistical Physics, Atomic, Molecular and Cluster Physics, Plasma and Fluid Physics, Condensed Matter, Cross-disciplinary Physics, Biological Physics, Nanosciences, Quantum Physics, Optical physics. Amsterdam: Elsevier, 2017, Roč. 381, č. 37, [tlačená forma] [online]. ISSN 0375-9601. ISSN (online) 1873-2429. - SCIE ; WOS CC, s. 3211 - 3216

2017 [01/12] / **GBR** - Mou, Z.Y. - Tian, Y.H. - Kertesz, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 36, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 24761 - 24768

2017 [01/12] / **NLD** - Mortazavi, B. - Rahaman, O. - Ahzi, S. - Rabczuk, T. **In: Applied Materials Today**. Amsterdam: Elsevier, 2017, Roč. 8, [tlačená forma] [online]. ISSN 2352-9407. ISSN (online) 2352-9415. - SCIE ; WOS CC, s. 60 - 67

2017 [01/12] / **NLD** - Li, L.L. - Zhang, H. - Cheng, X.L. **In: Computational Materials Science**. Amsterdam: Elsevier, 2017, Roč. 137, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 119 - 124

2017 [01/12] / **GBR** - Guan, Z.Y. - Ni, S. - Hu, S.L. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2017, Roč. 7, č. 72, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 45393 - 45399

2017 [01/12] / **GBR** - Liang, D. - Quhe, R.G. - Chen, Y.J. - Wu, L.Y. - Wang, Q. - Guan, P.F. - Wang, S.M. - Lu, P.F. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2017, Roč. 7, č. 67, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 42455 - 42461

2017 [01/12] / **USA** - Yanagisawa, S. - Hamada, I. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2017, Roč. 121, č. 4, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 045501

2017 [01/12] / **GBR** - Tian, X.X. - Wang, T. - Jiao, H.J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 3, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 2186 - 2192

2017 [01/12] / **USA** - Esters, M. - Hennig, R.G. - Johnson, D.C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 96, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s.

2017 [01/12] / Netrattana, P. - Reunchan, P. **In: Siam Physics Congress**, 2017, Roč. 901. - SCIE ; WOS CC, s. Art. No. 012102

2016 [01/12] / **DEU** - Navarrete-Lopez, A.M. - San-Roman, M.L. - Zicovich-Wilson, C.M. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2016, Roč. 135, č. 5, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 136

2016 [01/12] / **NLD** - Sarker, P. - Huda, M.N. **In: Computational Materials Science**. Amsterdam: Elsevier, 2016, Roč. 111, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 359 - 365

2016 [01/12] / Liu, F. - Wang, T.C. **In: Carbon**, 2016, Roč. 96. - SCIE ; WOS CC, s. 1175 - 1180

2016 [01/12] / **GBR** - Erba, A. - Maul, J. - Civalleri, B. **In: Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 52, č. 9, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCIE ; WOS CC, s. 1820 - 1823

2016 [01/12] / **GBR** - Cheung, P.M. - Berger, R.F. - Zakharov, L.N. - Gilbertson, J.D. **In: Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 52, č. 22, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCIE ; WOS CC, s. 4156 - 4159

2016 [01/12] / **GBR** - Feng, L.P. - Jiang, W.Z. - Su, J. - Zhou, L.Q. - Liu, Z.T. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 8, č. 12, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 6507 - 6513

2016 [01/12] / Porsev, V.V. - Bandura, A.V. - Evarestov, R.A. **In: Lithuanian Journal of Physics**, 2016, Roč. 56, č. 2.

ISSN 1392-1932. - SCIE ; WOS CC, s. 79 - 85

2016 [01/12] / **GBR** - Yang, J.W. - Yuan, Y.H. - Hua, Z. **In: Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2016, Roč. 114, č. 14, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCIE ; WOS CC, s. 2157 - 2163

2016 [01/12] / **GBR** - Bian, X. - Wang, Q. - Wang, X.Y. - Wang, L. - Li, W.Q. - Chen, G.H. - Zhu, H.J. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 6, č. 78, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 74973 - 74981

2016 [01/12] / **GBR** - Pandey, K.K. **In: New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2016, Roč. 40, č. 9, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCIE ; WOS CC, s. 7831 - 7839

2016 [01/12] / **GBR** - de Oliveira, R.C. - Gracia, L. - Assis, M. - Li, M.S. - Andres, J. - Longo, E. - Cavalcante, L.S. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 34, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 6483 - 6491

2016 [01/12] / **GBR** - Bacaksiz, C. - Sahin, H. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 6, č. 92, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 89708 - 89714

2016 [01/12] / **DEU** - Zhao, X.Y. - Li, Q. - Yu, T.T. - Yang, M. - Fink, K. - Shen, X.D. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2016, Roč. 6, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 19448

2016 [01/12] / Gan, L.Y. - Zhang, Q.Y. - Guo, C.S. - Schwingenschloegl, U. - Zhao, Y. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 4. - SCIE ; WOS CC, s. 2119 - 2125

2016 [01/12] / **USA** - Cervinka, C. - Fulem, M. - Ruzicka, K. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 144, č. 6, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 064505

2016 [01/12] / **USA** - Onen, A. - Kecik, D. - Durgun, E. - Ciraci, S. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 085431

2016 [01/12] / **GBR** - Tonner, R. - Rosenow, P. - Jakob, P. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 8, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 6316 - 6328

2016 [01/12] / **USA** - Bacaksiz, C. - Cahangirov, S. - Rubio, A. - Senger, R.T. - Peeters, F.M. - Sahin, H. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 12, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 125403

2016 [01/12] / Gueddida, S. - Gruber, M. - Miyamachi, T. - Beaurepaire, E. - Wulfhekel, W. - Alouani, M. **In: Journal of Physical Chemistry Letters**, 2016, Roč. 7, č. 5. - SCIE ; WOS CC, s. 900 - 904

2016 [01/12] / Lechner, C. - Pannier, B. - Baranek, P. - Forero-Martinez, N.C. - Vach, H. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 9. - SCIE ; WOS CC, s. 5083 - 5100

2016 [01/12] / **DEU** - Tonkikh, A.A. - Voloshina, E.N. - Werner, P. - Blumtritt, H. - Senkovskiy, B. - Guntherodt, G. - Parkin, S.S.P. - Dedkov, Y.S. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2016, Roč. 6, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 23547

2016 [01/12] / Zhang, Q. - Yin, L. - Mi, W.B. - Wang, X.C. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 11. - SCIE ; WOS CC, s. 6156 - 6164

2016 [01/12] / Rego, C.R.C. - Oliveira, L.N. - Tereshchuk, P. - Da Silva, J.L.F. **In: Journal of Physics-Condensed Matter**, 2016, Roč. 28, č. 12. - SCIE ; WOS CC, s. Art. No. 129501

2016 [01/12] / Cervinka, C. - Fulem, M. - Stoffel, R.P. - Dronskowski, R. **In: Journal of Physical Chemistry A**, 2016, Roč. 120, č. 12. - SCIE ; WOS CC, s. 2022 - 2034

2016 [01/12] / **NLD** - Nicolini, P. - Polcar, T. **In: Computational Materials Science**. Amsterdam: Elsevier, 2016, Roč. 115, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 158 - 169

2016 [01/12] / **USA** - Menendez, C. - Lobato, A. - Abbasi-Perez, D. - Fernandez-Nunez, J. - Baonza, V.G. - Recio, J.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 14, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 144112

2016 [01/12] / **DEU** - Wang, Y.P. - Ji, W.X. - Zhang, C.W. - Li, S.S. - Li, F. - Li, P. - Ren, M.J. - Chen, X.L. - Yuan, M. - Wang, P.J. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2016, Roč. 173, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 379 - 384

2016 [01/12] / **USA** - Besse, R. - Sabino, F.P. - Da Silva, J.L.F. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 16, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 165205

2016 [01/12] / **USA** - Paier, J. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2016, Roč. 146, č. 5, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 861 - 885

2016 [01/12] / Schon, J.C. - Oligschleger, C. - Cortes, J. **In: Zeitschrift fur Naturforschung Section b-A Journal of Chemical Sciences**, 2016, Roč. 71, č. 5. - SCIE ; WOS CC, s. 351 - 374

2016 [01/12] / **USA** - He, Y.M. - Yang, Y. - Zhang, Z.H. - Gong, Y.J. - Zhou, W. - Hu, Z.L. - Ye, G.L. - Zhaug, X. - Bianco, E. - Lei, S.D. - Jin, Z.H. - Zou, X.L. - Yang, Y.C. - Zhang, Y. - Xie, E.Q. - Lou, J. - Yakobson, B. - Vajtai, R. - Li, B. - Ajayan, P. **In: Nano letters**. Washington: American Chemical Society, 2016, Roč. 16, č. 5, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 3314 - 3320

2016 [01/12] / **NLD** - Salehi, H. - Moaddeli, M. - Amiri, P. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2016, Roč. 647, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 96 - 102

2016 [01/12] / **USA** - Borycz, J. - Paier, J. - Verma, P. - Darago, L.E. - Xiao, D.J. - Truhlar, D.G. - Long, J.R. - Gagliardi, L. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2016, Roč. 55, č. 10, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 4924 - 4934

2016 [01/12] / **USA** - Gueddida, S. - Alouani, M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 18, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 184433

2016 [01/12] / **GBR** - Wei, H.L. - Shi, Y.R. - Liu, Y.F. **In: Semiconductor Science and Technology**. Bristol: Institute of Physics. IOP Publishing, 2016, Roč. 31, č. 6, [tlačená forma] [online]. ISSN 0268-1242. ISSN (online) 1361-6641. - SCIE ; WOS CC, s. Art. No. 065016

2016 [01/12] / **GBR** - Guo, Y.H. - Wang, Z.F. - Zhang, L.Z. - Shen, X.D. - Liu, F. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 21, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 14449 - 14453

2016 [01/12] / **GBR** - Bai, Y.J. - Deng, K.M. - Kan, E.J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 23, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 15765 - 15773

2016 [01/12] / **USA** - Lee, J.H. - Park, J.H. - Soon, A. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 2, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 024108

2016 [01/12] / **FRA** - Oliveira, B.G. **In: Comptes Rendus Chimie**. [s.l.]: Elsevier, 2016, Roč. 19, č. 8, [tlačená forma] [online]. ISSN 1631-0748. ISSN (online) 1878-1543. - SCIE ; WOS CC, s. 995 - 1002

2016 [01/12] / **GBR** - Fumanal, M. - Deumal, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 30, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 20738 - 20749

2016 [01/12] / **USA** - Zhu, Z. - Peelaers, H. - Van de Walle, C.G. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 085426

2016 [01/12] / **NLD** - Qiu, W.H. - Ye, H. - Yu, Z.Y. - Liu, Y.M. **In: Superlattices and Microstructures**: a journal devoted to the science and technology of synthetic microstructures, microdevices, surfaces and interfaces. Amsterdam: Elsevier, 2016, Roč. 97, [tlačená forma] [online]. ISSN 0749-6036. ISSN (online) 1096-3677. - SCIE ; WOS CC, s. 250 - 257

2016 [01/12] / **USA** - Liu, Z.X. - De Jesus, L.R. - Banerjee, S. - Mukherjee, P.P. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2016, Roč. 8, č. 35, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 23028 - 23036

2016 [01/12] / **NLD** - Mortazavi, B. - Dianat, A. - Cuniberti, G. - Rabczuk, T. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2016, Roč. 213, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 865 - 870

2016 [01/12] / Schwerdtfeger, P. - Tonner, R. - Moyano, G.E. - Pahl, E. **In: Angewandte Chemie-International Edition**, 2016, Roč. 55, č. 40. - SCIE ; WOS CC, s. 12200 - 12205

2016 [01/12] / Levita, G. - Restuccia, P. - Righi, M.C. **In: Carbon**, 2016, Roč. 107. - SCIE ; WOS CC, s. 878 - 884

2016 [01/12] / **NLD** - Mortazavi, B. - Dianat, A. - Rahaman, O. - Cuniberti, G. - Rabczuk, T. **In: Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2016, Roč. 329, [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCIE ; WOS CC, s. 456 -

461

2016 [01/12] / **NLD** - Souissi, M. - Chen, Y. - Sluiter, M.H.F. - Numakura, H. **In: Computational Materials Science**. Amsterdam: Elsevier, 2016, Roč. 124, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 249 - 258

2016 [01/12] / **USA** - Kecik, D. - Durgun, E. - Ciraci, S. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 20, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 205409

2016 [01/12] / **GBR** - Li, Q. - Xu, L. - Luo, K.W. - Huang, W.Q. - Wang, L.L. - Li, X.F. - Huang, G.F. - Yu, Y.B. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 33094 - 33102

2016 [01/12] / **NLD** - Hernandez-Tamargo, C.E. - Roldan, A. - de Leeuw, N.H. **In: Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2016, Roč. 237, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCIE ; WOS CC, s. 192 - 203

2016 [01/12] / **DEU** - Srour, J. - Badawi, M. - Hassan, F.E.H. - Postnikov, A.V. **In: Physica Status Solidi B-Basic Solid State Physics**. Weinheim: John Wiley & Sons. Wiley-VCH, 2016, Roč. 253, č. 8, [tlačená forma] [online]. ISSN 0370-1972. ISSN (online) 1521-3951. - SCIE ; WOS CC, s. 1472 - 1475

2016 [01/12] / **DEU** - Hu, X.H. - Kou, L.Z. - Sun, L.T. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2016, Roč. 6, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 31122

2016 [01/12] / **USA** - Zhou, Y.N. - Chen, W. - Cui, P. - Zeng, J. - Lin, Z.N. - Kaxiras, E. - Zhang, Z.Y. **In: Nano letters**. Washington: American Chemical Society, 2016, Roč. 16, č. 10, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 6058 - 6063

2016 [01/12] / **DEU** - Guijarro, A. - Verges, J.A. - San-Fabian, E. - Chiappe, G. - Louis, E. **In: ChemPhysChem**, 2016, Roč. 17, č. 21. - SCIE ; WOS CC, s. 3548 - 3557

2016 [01/12] / **GBR** - Hernandez-Tamargo, C.E. - Barzaga, R. - Mikosch, H. - Martinez, J.A. - Herrera, J.A. - Farias, M.H. - Hernandez, M.P. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 43, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 29987 - 29998

2016 [01/12] / **NLD** - Saghatforoush, L. - Khoshtarkib, Z. - Keypour, H. - Hakimi, M. **In: Polyhedron**: The International Journal for Research in Inorganic Chemistry. Amsterdam: Elsevier, 2016, Roč. 119, [tlačená forma] [online]. ISSN 0277-5387. ISSN (online) 1873-3719. - SCIE ; WOS CC, s. 160 - 174

2016 [01/12] / **DEU** - Liang, S.H. - Yang, H.X. - Yang, H.W. - Tao, B.S. - Djeffal, A. - Chshiev, M. - Huang, W.C. - Li, X.G. - Ferri, A. - Desfeux, R. - Mangin, S. - Lacour, D. - Hehn, M. - Copie, O. - Dumesnil, K. - Lu, Y. **In: Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2016, Roč. 28, č. 46, [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCIE ; WOS CC, s. 10204 - 10210

2016 [01/12] / **DEU** - Lari, G.M. - Groninger, O.G. - Li, Q. - Mondelli, C. - Lopez, N. - Perez-Ramirez, J. **In: ChemSusChem**. Weinheim: John Wiley & Sons. Wiley-VCH, 2016, Roč. 9, č. 24, [tlačená forma] [online]. ISSN 1864-5631. ISSN (online) 1864-564X. - SCIE ; WOS CC, s. 3407 - 3418

2016 [01/12] / **GBR** - Zhang, Y.Y. - Hao, F. - Xiao, H. - Liu, C. - Shi, X.Y. - Chen, X. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2016, Roč. 41, č. 48, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 23067 - 23074

2016 [01/12] / Vela, S. - Souto, M. - Ratera, I. - Rovira, C. - Veciana, J. **In: Journal of Physical Chemistry A**, 2016, Roč. 120, č. 51. - SCIE ; WOS CC, s. 10297 - 10303

2016 [01/12] / **USA** - Novko, D. - Tremblay, J.C. - Blanco-Rey, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 24, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 244701

2015 [01/12] / **GBR** - Wang, T. - Tian, X.X. - Yang, Y. - Li, Y.W. - Wang, J.G. - Beller, M. - Jiao, H.J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 3, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 1907 - 1917

2015 [01/12] / **NLD** - Matczak, P. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2015, Roč. 1051, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 110 - 122

2015 [01/12] / **GBR** - Liu, H.S. - Han, N.N. - Zhao, J.J. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 5, č. 23, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 17572 - 17581

2015 [01/12] / **GBR** - Feng, L.P. - Su, J. - Liu, Z.T. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 5, č. 26, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 20538 - 20544

2015 [01/12] / **GBR** - Vela, S. - Deumal, M. - Shiga, M. - Novoa, J.J. - Ribas-Arino, J. **In: Chemical Science**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 6, č. 4, [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCIE ; WOS CC, s. 2371 - 2381

2015 [01/12] / **GBR** - Liu, S.L. - Tian, X.X. - Wang, T. - Wen, X.D. - Li, Y.W. - Wang, J.G. - Jiao, H.J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 8811 - 8821

2015 [01/12] / **GBR** - Zhang, R.W. - Zhang, C.W. - Luan, H.X. - Ji, W.X. - Wang, P.J. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 5, č. 45, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 35377 - 35383

2015 [01/12] / **GBR** - Zhang, H. - Wang, J. - Tian, Z.X. - Liu, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 21, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 13821 - 13828

2015 [01/12] / **GBR** - Reilly, A.M. - Tkatchenko, A. **In: Chemical Science**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 6, č. 6, [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCIE ; WOS CC, s. 3289 - 3301

2015 [01/12] / Singh, T. - Kumar, J. - Sastri, O.S.K.S. **In: Proceedings of the International Conference on Condensed Matter Physics**, 2015, Roč. 1661. - SCIE ; WOS CC, s. Art. No. 110024

2015 [01/12] / **GBR** - Vela, S. - Fumanal, M. - Ribas-Arino, J. - Robert, V. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 16306 - 16314

2015 [01/12] / **GBR** - Shan, X.Y. - Wang, Q. - Bian, X. - Li, W.Q. - Chen, G.H. - Zhu, H.J. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 5, č. 96, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 78625 -

78633

2015 [01/12] / **GBR** - George, J. - Wang, A. - Deringer, V.L. - Wang, R.M. - Dronskowski, R. - Englert, U. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 38, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 7414 - 7422

2015 [01/12] / **USA** - Chen, W. - Cui, P. - Zhu, W.G. - Kaxiras, E. - Gao, Y.F. - Zhang, Z.Y. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045408

2015 [01/12] / **USA** - Wang, V. - Kawazoe, Y. - Geng, W.T. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045433

2015 [01/12] / **USA** - Garcia-Muelas, R. - Li, Q. - Lopez, N. **In: ACS Catalysis**. Washington: American Chemical Society, 2015, Roč. 5, č. 2, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1027 - 1036

2015 [01/12] / Bachhuber, F. - von Appen, J. - Dronskowski, R. - Schmidt, P. - Nilges, T. - Pfitzner, A. - Weihrich, R. **In: Zeitschrift fur Kristallographie-Crystalline Materials**, 2015, Roč. 230, č. 2. - SCIE ; WOS CC, s. 107 - 115

2015 [01/12] / Liu, X.H. - George, J. - Maintz, S. - Dronskowski, R. **In: Angewandte Chemie-International Edition**, 2015, Roč. 54, č. 6. - SCIE ; WOS CC, s. 1954 - 1959

2015 [01/12] / Mondal, K. - Kamal, C. - Banerjee, A. - Chakrabarti, A. - Ghanty, T.K. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 6. - SCIE ; WOS CC, s. 3192 - 3198

2015 [01/12] / **JPN** - Obata, M. - Nakamura, M. - Hamada, I. - Oda, T. **In: Journal of the Physical Society of Japan**. Tokio: The Physical Society of Japan, 2015, Roč. 84, č. 2, [tlačená forma] [online]. ISSN 0031-9015. ISSN (online) 1347-4073. - SCIE ; WOS CC, s. Art. No. 024715

2015 [01/12] / Lee, S.H. - Jhi, S.H. **In: Journal of Physics-Condensed Matter**, 2015, Roč. 27, č. 7. - SCIE ; WOS CC, s. Art. No. 075301

2015 [01/12] / **USA** - Bacaksiz, C. - Sahin, H. - Ozaydin, H.D. - Horzum, S. - Senger, R.T. - Peeters, F.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 085430

2015 [01/12] / **USA** - Almora-Barrios, N. - Pogodin, S. - Bellarosa, L. - Garcia-Melchor, M. - Revilla-Lopez, G. - Garcia-Rates, M. - Vazquez-Garcia, A.B. - Hernandez-Ariznavarreta, P. - Lopez, N. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2015, Roč. 7, č. 6, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 928 - 935

2015 [01/12] / Stoffel, R.P. - Deringer, V.L. - Simon, R.E. - Hermann, R.P. - Dronskowski, R. **In: Journal of Physics-Condensed Matter**, 2015, Roč. 27, č. 8. - SCIE ; WOS CC, s. Art. No. 085402

2015 [01/12] / **USA** - Ahouari, H. - Rousse, G. - Rodriguez-Carvajal, J. - Sougrati, M.T. - Saubanere, M. - Courty, M. - Recham, N. - Tarascon, J.M. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2015, Roč. 27, č. 5, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 1631 - 1639

2015 [01/12] / Revilla-Lopez, G. - Blonski, P. - Lopez, N. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 10. -

SCIE ; WOS CC, s. 5478 - 5483

2015 [01/12] / **GBR** - Feng, L.P. - Su, J. - Li, D.P. - Liu, Z.T. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 10, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 6700 - 6704

2015 [01/12] / Bocquet, M.L. - Coasne, B. - Pellenq, R. - Ulm, F.J. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 12. - SCIE ; WOS CC, s. 6511 - 6517

2015 [01/12] / **USA** - Lee, Y. - Hwang, Y. - Chung, Y.C. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2015, Roč. 7, č. 13, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 7163 - 7169

2015 [01/12] / **DEU** - Zhang, R.W. - Zhang, C.W. - Ji, W.X. - Ren, M.J. - Li, F. - Yuan, M. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2015, Roč. 156, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 89 - 94

2015 [01/12] / Wu, R.T. - Yan, L.H. - Zhang, Y.F. - Ren, J.H. - Bao, D.L. - Zhang, H.G. - Wang, Y.L. - Du, S.X. - Huan, Q. - Gao, H.J. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 15. - SCIE ; WOS CC, s. 8208 - 8212

2015 [01/12] / Li, Q.F. - Duan, C.G. - Wan, X.G. - Kuo, J.L. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 16. - SCIE ; WOS CC, s. 8662 - 8670

2015 [01/12] / **USA** - Symalla, F. - Shallcross, S. - Beljakov, I. - Fink, K. - Wenzel, W. - Meded, V. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 20, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 205412

2015 [01/12] / **USA** - Liang, L.B. - Zhu, P. - Meunier, V. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 142, č. 18, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 184708

2015 [01/12] / Zhang, R.G. - Liu, F. - Zhao, X.J. - Wang, B.J. - Ling, L.X. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 19. - SCIE ; WOS CC, s. 10355 - 10364

2015 [01/12] / **USA** - Vile, G. - Almora-Barrios, N. - Lopez, N. - Perez-Ramirez, J. **In: ACS Catalysis**. Washington: American Chemical Society, 2015, Roč. 5, č. 6, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 3767 - 3778

2015 [01/12] / Zhao, K. - Wang, Y. - Sui, Y. - Xin, C. - Wang, X.J. - Wang, Y. - Liu, Z.G. - Li, B.S. **In: Physica Status Solidi-Rapid Research Letters**, 2015, Roč. 9, č. 6. - SCIE ; WOS CC, s. 379 - 383

2015 [01/12] / **USA** - Guler-Kilic, S. - Kilic, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 245204

2015 [01/12] / Ohfuchi, M. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 23. - SCIE ; WOS CC, s. 13200 - 13206

2015 [01/12] / **CHN** - Yan, L.H. - Wu, R.T. - Bao, D.L. - Ren, J.H. - Zhang, Y.F. - Zhang, H.G. - Huang, L. - Wang, Y.L. - Du, S.X. - Huan, Q. - Gao, H.J. **In: Chinese Physics B**. Peking: Chinese Physical Society, 2015, Roč. 24, č. 7, [tlačená forma] [online]. ISSN 1674-1056. ISSN (online) 2058-3834. - SCIE ; WOS CC, s. Art. No. 076802

2015 [01/12] / **USA** - Altenburg, S.J. - Lattelais, M. - Wang, B. - Bocquet, M.L. - Berndt, R. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2015, Roč. 137, č. 29, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 9452 - 9458

2015 [01/12] / **NLD** - Park, J. - Yu, B.D. - Hong, S. **In: Current Applied Physics**. Amsterdam: Elsevier. Elsevier Science, 2015, Roč. 15, č. 8, [tlačená forma] [online]. ISSN 1567-1739. ISSN (online) 1878-1675. - SCIE ; WOS CC, s. 885 - 891

2015 [01/12] / **USA** - Delgado, M. - Sommer, S.K. - Swanson, S.P. - Berger, R.F. - Seda, T. - Zalcharov, L.N. - Gilbertson, J.D. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2015, Roč. 54, č. 15, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 7239 - 7248

2015 [01/12] / **DEU** - Li, S.S. - Zhang, C.W. - Ji, W.X. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2015, Roč. 164, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 150 - 156

2015 [01/12] / Wang, J. - Li, D. - Zhang, H.J. - Wang, Y.L. - Meng, J.J. - Niu, Y. - Zhao, H.M. - Liang, C.J. **In: Journal of Physics D-Applied Physics**, 2015, Roč. 48, č. 32. - SCIE ; WOS CC, s. Art. No. 325002

2015 [01/12] / **USA** - Caffrey, N.M. - Armiento, R. - Yakimova, R. - Abrikosov, I.A. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 92, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 081409

2015 [01/12] / **USA** - Levita, G. - Molinari, E. - Polcar, T. - Righi, M.C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 92, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 085434

2015 [01/12] / **USA** - Gong, K. - Zhang, L. - Liu, L. - Zhu, Y. - Yu, G.H. - Grutter, P. - Guo, H. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2015, Roč. 118, č. 9, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 093902

2015 [01/12] / **DEU** - Shen, Y.Q. - Oganov, A.R. - Qian, G.R. - Zhang, J. - Dong, H.F. - Zhu, Q. - Zhou, Z.X. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2015, Roč. 5, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 14204

2015 [01/12] / Cannella, C.B. - Goldman, N. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 37. - SCIE ; WOS CC, s. 21605 - 21611

2015 [01/12] / Porsev, V.V. - Bandura, A.V. - Evarestov, R.A. **In: ChemPhysChem**, 2015, Roč. 16, č. 14. - SCIE ; WOS CC, s. 3007 - 3014

2015 [01/12] / **USA** - Kecik, D. - Bacaksiz, C. - Senger, R.T. - Durgun, E. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 92, č. 16, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 165408

2015 [01/12] / Rego, C.R.C. - Oliveira, L.N. - Tereshchuk, P. - Da Silva, J.L.F. **In: Journal of Physics-Condensed Matter**, 2015, Roč. 27, č. 41. - SCIE ; WOS CC, s. Art. No. 415502

2015 [01/12] / **NLD** - Dri, F.L. - Wu, X.W. - Moon, R.J. - Martini, A. - Zavattieri, P.D. **In: Computational Materials**

Science. Amsterdam: Elsevier, 2015, Roč. 109, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 330 - 340

2015 [01/12] / **CHE** - Xu, R.L. - Liu, J. - Chen, F. - Liu, N.H. - Cai, Y.X. - Liu, X.Q. - Song, X. - Dong, M.D. - Wang, L. **In: Nano research**. Peking: Tshinghua Press, 2015, Roč. 8, č. 11, [tlačená forma] [online]. ISSN 1998-0124. ISSN (online) 1998-0000. - SCIE ; WOS CC, s. 3505 - 3511

2015 [01/12] / **NLD** - Pandey, K.K. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2015, Roč. 1073, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCO, s. 20 - 26

2015 [01/12] / **GBR** - Pandey, K.K. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 5, č. 128, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 105668 - 105677

2015 [01/12] / **USA** - Wagner, M. - Berkebile, S. - Netzer, F.P. - Ramsey, M.G. **In: ACS Nano**. Washington: American Chemical Society, 2015, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 12070 - 12078

2015 [01/12] / Ding, Y. - Wang, Y.L. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 49. - SCIE ; WOS CC, s. 27848 - 27854

2015 [01/12] / Wang, V. - Liu, Y.C. - Kawazoe, Y. - Geng, W.T. **In: Journal of Physical Chemistry Letters**, 2015, Roč. 6, č. 24. - SCIE ; WOS CC, s. 4876 - 4883

2015 [01/12] / **NLD** - Ambrusi, R.E. - Garcia, S.G. - Pronsato, M.E. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2015, Roč. 324, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 710 - 717

2014 [01/12] / Fumanal, M. - Vela, S. - Ribas-Arino, J. - Novoa, J.J. **In: Chemistry-An Asian Journal**, 2014, Roč. 9, č. 12. - SCIE ; WOS CC, s. 3612 - 3622

2014 [01/12] / **GBR** - Dri, F.L. - Shang, S.L. - Hector, L.G. - Saxe, P. - Liu, Z.K. - Moon, R.J. - Zavattieri, P.D. **In: Modelling and simulation in materials science and engineering**. Bristol: Institute of Physics. IOP Publishing, 2014, Roč. 22, č. 8, [online] [tlačená forma]. ISSN 0965-0393. ISSN (online) 1361-651X. - SCIE ; WOS CC, s. Art. No. 085012

2014 [01/12] / Brandenburg, J.G. - Grimme, S. **Prediction and Calculation of Crystal Structures: Methods and Applications.Book Series: Topics in Current Chemistry** [textový dokument (print)] . Berlin: Springer, 2014. 1 vyd. - BKCI-S ; WOS CC, s. 1 - 23

2014 [01/12] / George, J. - Deringer, V.L. - Dronskowski, R. **In: Journal of Physical Chemistry A**, 2014, Roč. 118, č. 17. - SCIE ; WOS CC, s. 3193 - 3200

2014 [01/12] / **DEU** - Zhang, L.Z. - Du, S.X. - Sun, J.T. - Huang, L. - Meng, L. - Xu, W.Y. - Pan, L.D. - Pan, Y. - Wang, Y.L. - Hofer, W.A. - Gao, H.J. **In: Advanced Materials Interfaces**. Weinheim: John Wiley & Sons. Wiley-VCH, 2014, Roč. 1, č. 3, [online]. ISSN 2196-7350. - SCIE ; WOS CC, s. Art. No. 1300104

2014 [01/12] / Liu, S.L. - Tian, X.X. - Wang, T. - Wen, X.D. - Li, Y.W. - Wang, J.G. - Jiao, H.J. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 45. - SCIE ; WOS CC, s. 26139 - 26154

2014 [01/12] / **NLD** - Zhang, Y.G. - Sa, B.S. - Zhou, J. - Sun, Z.M. **In: Computational Materials Science**. Amsterdam: Elsevier, 2014, Roč. 81, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 163 - 169

2014 [01/12] / **GBR** - Wang, V. - Liu, R.J. - He, H.P. - Yang, C.M. - Ma, L. **In: Solid State Communications**: an International Journal. Oxford: Elsevier, 2014, Roč. 177, [tlačená forma] [online]. ISSN 0038-1098. ISSN (online) 1879-2766. - SCIE ; WOS CC, s. 74 - 79

2014 [01/12] / **GBR** - Deringer, V.L. - Pan, F. - George, J. - Muller, P. - Dronskowski, R. - Englert, U. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 2, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 135 - 138

2014 [01/12] / **GBR** - Kulish, V.V. - Malyi, O.I. - Ng, M.F. - Chen, Z. - Manzhos, S. - Wu, P. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 9, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 4260 - 4267

2014 [01/12] / **GBR** - Fernandez, N. - Ferro, Y. - Carissan, Y. - Marchois, J. - Allouche, A. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 5, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 1957 - 1966

2014 [01/12] / **GBR** - Hu, W. - Xi, N. - Wu, X.J. - Li, Z.Y. - Yang, J.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 15, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 6957 - 6962

2014 [01/12] / **GBR** - Fischer, M. - Bell, R.G. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 10, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 1934 - 1949

2014 [01/12] / **GBR** - Li, S.S. - Zhang, C.W. - Ji, W.X. - Li, F. - Wang, P.J. - Hu, S.J. - Yan, S.S. - Liu, Y.S. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 30, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 15968 - 15978

2014 [01/12] / **GBR** - Hussain, T. - Panigrahi, P. - Ahuja, R. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 17, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 8100 - 8105

2014 [01/12] / **GBR** - Li, S.S. - Zhang, C.W. - Ji, W.X. - Li, F. - Wang, P.J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 41, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 22861 - 22866

2014 [01/12] / **GBR** - Revilla-Lopez, G. - Lopez, N. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 35, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 18933 - 18940

2014 [01/12] / **GBR** - Liu, Y.X. - Duan, D.F. - Tian, F.B. - Huang, X.L. - Li, D. - Zhao, Z.L. - Sha, X.J. - Chu, B.H. - Zhang, H.D. - Liu, B.B. - Cui, T. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 4, č. 71, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 37569 - 37574

2014 [01/12] / **GBR** - Li, X.X. - Yang, J.L. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2014, Roč. 2, č. 34, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 7071 - 7076

2014 [01/12] / **GBR** - Deringer, V.L. - Stoffel, R.P. - Togo, A. - Eck, B. - Meven, M. - Dronskowski, R. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of

Chemistry, 2014, Roč. 16, č. 47, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 10907 - 10915

2014 [01/12] / **GBR** - Vela, S. - Novoa, J.J. - Ribas-Arino, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 27012 - 27024

2014 [01/12] / **GBR** - Feng, G. - Yang, D.Q. - Kong, D.J. - Liu, J.W. - Lu, Z.H. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 4, č. 89, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 47906 - 47920

2014 [01/12] / **USA** - Azuri, I. - Adler-Abramovich, L. - Gazit, E. - Hod, O. - Kronik, L. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2014, Roč. 136, č. 3, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 963 - 969

2014 [01/12] / **GBR** - Wang, X. - Cheng, X.Y. - Zhang, Y.T. - Li, R.H. - Xing, W.W. - Zhang, P.C. - Chen, X.Q. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 26974 - 26982

2014 [01/12] / **USA** - Luder, J. - Sanyal, B. - Eriksson, O. - Puglia, C. - Brena, B. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045416

2014 [01/12] / **USA** - Dong, L. - Dongare, A.M. - Namburu, R.R. - O'Regan, T.P. - Dubey, M. **In: Applied Physics Letters**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 104, č. 5, [tlačená forma] [online]. ISSN 0003-6951. ISSN (online) 1077-3118. - SCIE ; WOS CC, s. Art. No. 053107

2014 [01/12] / **NLD** - Sa, B.S. - Zhou, J. - Ahuja, R. - Sun, Z.M. **In: Computational Materials Science**. Amsterdam: Elsevier, 2014, Roč. 82, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 66 - 69

2014 [01/12] / **DEU** - Kim, H. **In: Journal of the Korean Physical Society**. Berlín: Springer Nature, 2014, Roč. 64, č. 4, [tlačená forma] [online]. ISSN 0374-4884. ISSN (online) 1976-8524. - SCIE ; WOS CC, s. 547 - 553

2014 [01/12] / Deringer, V.L. - Stoffel, R.P. - Dronskowski, R. **In: Crystal Growth and Design**, 2014, Roč. 14, č. 2. - SCIE ; WOS CC, s. 871 - 878

2014 [01/12] / **USA** - Almora-Barrios, N. - Novell-Leruth, G. - Whiting, P. - Liz-Marzan, L.M. - Lopez, N. **In: Nano letters**. Washington: American Chemical Society, 2014, Roč. 14, č. 2, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 871 - 875

2014 [01/12] / Jiang, S.Q. - Huang, X.L. - Duan, D.F. - Zheng, S.K. - Li, F.F. - Yang, X. - Zhou, Q. - Liu, B.B. - Cui, T. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 6. - SCIE ; WOS CC, s. 3236 - 3243

2014 [01/12] / **USA** - He, J.G. - Hummer, K. - Franchini, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075409

2014 [01/12] / **USA** - Yang, K. - Liu, L.W. - Zhang, L.Z. - Xiao, W.D. - Fei, X.M. - Chen, H. - Du, S.X. - Ernst, K.H. - Goo, H.J. **In: ACS Nano**. Washington: American Chemical Society, 2014, Roč. 8, č. 3, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 2246 - 2251

2014 [01/12] / Gan, L.Y. - Zhang, Q.Y. - Cheng, Y.C. - Schwingenschlogl, U. **In: Journal of Physical Chemistry Letters**, 2014, Roč. 5, č. 8. - SCIE ; WOS CC, s. 1445 - 1449

2014 [01/12] / Ramos-Sanchez, G. - Balbuena, P.B. **In: Journal of Electroanalytical Chemistry**, 2014, Roč. 716. ISSN 0022-0728. - SCIE ; WOS CC, s. 23 - 30

2014 [01/12] / Moellmann, J. - Grimme, S. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 14. - SCIE ; WOS CC, s. 7615 - 7621

2014 [01/12] / **USA** - Deringer, V.L. - Stoffel, R.P. - Dronskowski, R. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 9, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 094303

2014 [01/12] / **USA** - Hirsch, A. - Azuri, I. - Addadi, L. - Weiner, S. - Yang, K.S. - Curtarolo, S. - Kronik, L. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2014, Roč. 26, č. 9, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 2934 - 2942

2014 [01/12] / **USA** - Shi, W. - Chen, J.M. - Xi, J.Y. - Wang, D. - Shuai, Z.G. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2014, Roč. 26, č. 8, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 2669 - 2677

2014 [01/12] / Vile, G. - Almora-Barrios, N. - Mitchell, S. - Lopez, N. - Perez-Ramirez, J. **In: Chemistry-A European Journal**, 2014, Roč. 20, č. 20. - SCIE ; WOS CC, s. 5926 - 5937

2014 [01/12] / **GBR** - Chittari, B.L. **In: Philosophical Magazine Letters**. Oxfordshire: Taylor & Francis Group, 2014, Roč. 94, č. 5, [tlačená forma] [online]. ISSN 0950-0839. ISSN (online) 1362-3036. - SCIE ; WOS CC, s. 278 - 287

2014 [01/12] / **GBR** - Vela, S. - Mota, F. - Deumal, M. - Suizu, R. - Shuku, Y. - Mizuno, A. - Awaga, K. - Shiga, M. - Novoa, J.J. - Ribas-Arino, J. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2014, Roč. 5, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 4411

2014 [01/12] / **DEU** - Malberg, F. - Brandenburg, J.G. - Reckien, W. - Holloczki, O. - Grimme, S. - Kirchner, B. **In: Beilstein Journal of Organic Chemistry**. Frankfurt nad Mohanom: Beilstein-Institut zur Förderung der Chemischen Wissenschaften, 2014, Roč. 10, [tlačená forma]. ISSN 2195-951X. ISSN (online) 1860-5397. - SCIE ; WOS CC, s. 1299 - 1307

2014 [01/12] / Levita, G. - Cavaleiro, A. - Molinari, E. - Polcar, T. - Righi, M.C. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 25. - SCIE ; WOS CC, s. 13809 - 13816

2014 [01/12] / **USA** - Eames, C. - Clark, J.M. - Rousse, G. - Tarascon, J.M. - Islam, M.S. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2014, Roč. 26, č. 12, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 3672 - 3678

2014 [01/12] / **GBR** - Chen, P. - Nishiyama, Y. - Mazeau, K. **In: Cellulose**. London: Blackie Academic & Professional, 2014, Roč. 21, č. 4, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 2207 - 2217

2014 [01/12] / **USA** - Jo, S. - Lee, S. - Yun, K.H. - Hwang, Y. - Chung, Y.C. **In: IEEE Transactions on Magnetics**: a Publication of the IEEE Magnetics Society. New York: Institute of Electrical and Electronics Engineers. IEEE Magnetics Society, 2014, Roč. 50, č. 8, [tlačená forma] [online]. ISSN 0018-9464. ISSN (online) 1941-0069. - SCIE ; WOS CC, s. Art. No. 1600104

2014 [01/12] / **GBR** - Kim, J.S. - Yang, J.H. - Jeong, Y.C. - Kim, D.H. - Baek, S.B. - Kim, Y.C. **In: Japanese Journal of Applied Physics**. Tokyo: Japan Society of Applied Physics, 2014, Roč. 53, č. 8, [tlačená forma] [online]. ISSN 0021-4922.

ISSN (online) 1347-4065. - SCIE ; WOS CC, s. Art. No. 0804

2014 [01/12] / Egger, D.A. - Kronik, L. **In: Journal of Physical Chemistry Letters**, 2014, Roč. 5, č. 15. - SCIE ; WOS CC, s. 2728 - 2733

2014 [01/12] / Garcia-Muelas, R. - Lopez, N. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 31. - SCIE ; WOS CC, s. 17531 - 17537

2014 [01/12] / Liao, J.M. - Sa, B.S. - Zhou, J. - Ahuja, R. - Sun, Z.M. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 31. - SCIE ; WOS CC, s. 17594 - 17599

2014 [01/12] / **USA** - Li, X.X. - Wu, X.J. - Yang, J.L. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2014, Roč. 136, č. 31, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 11065 - 11069

2014 [01/12] / **GBR** - Kim, D. - Lee, S. - Hwang, Y. - Yun, K.H. - Chung, Y.C. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2014, Roč. 39, č. 25, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 13189 - 13194

2014 [01/12] / **NLD** - Porsev, V.V. - Bandura, A.V. - Evarestov, R.A. **In: Acta Materialia**. Amsterdam: Acta Materialia, 2014, Roč. 75, [tlačená forma] [online]. ISSN 1359-6454. ISSN (online) 1873-2453. - SCIE ; WOS CC, s. 246 - 258

2014 [01/12] / Wang, J.J. - Li, J.M. - Fang, L.L. - Sun, Q. - Jia, Y. **In: Tribology Letters**, 2014, Roč. 55, č. 3. - SCIE ; WOS CC, s. 405 - 412

2014 [01/12] / **USA** - Schweinfurth, D. - Demeshko, S. - Hohloch, S. - Steinmetz, M. - Brandenburg, J.G. - Dechert, S. - Meyer, F. - Grimme, S. - Sarkar, B. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2014, Roč. 53, č. 16, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 8203 - 8212

2014 [01/12] / Cho, S.B. - Chung, Y.C. **In: Carbon**, 2014, Roč. 77. - SCIE ; WOS CC, s. 208 - 214

2014 [01/12] / Li, F.Y. - Tu, K.X. - Chen, Z.F. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 36. - SCIE ; WOS CC, s. 21264 - 21274

2014 [01/12] / **USA** - Yang, J.H. - Baek, S.B. - Kim, Y.C. **In: Journal of Nanoscience and Nanotechnology**. Valencia: American Scientific Publishers, 2014, Roč. 14, č. 10, [tlačená forma] [online]. ISSN 1533-4880. ISSN (online) 1533-4899. - SCIE ; WOS CC, s. 7954 - 7960

2014 [01/12] / **NLD** - Liu, X.Y. - Zhang, J.M. - Xu, K.W. - Ji, V. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2014, Roč. 313, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 405 - 410

2014 [01/12] / **USA** - Hansen, A. - Bannwarth, C. - Grimme, S. - Petrovic, P. - Werle, C. - Djukic, J.P. **In: ChemistryOpen**. Hoboken: John Wiley & Sons. Wiley Blackwell, 2014, Roč. 3, č. 5, [online]. ISSN (online) 2191-1363. - SCIE ; WOS CC, s. 177 - 189

2014 [01/12] / Li, S.S. - Zhang, C.W. - Yan, S.S. - Hu, S.J. - Ji, W.X. - Wang, P.J. - Li, P. **In: Journal of Physics-Condensed Matter**, 2014, Roč. 26, č. 39. - SCIE ; WOS CC, s. Art. No. 395003

2014 [01/12] / **USA** - Brandenburg, J.G. - Bender, G. - Ren, J.J. - Hansen, A. - Grimme, S. - Eckert, H. - Daniliuc, C.G. - Kehr, G. - Erker, G. **In: Organometallics**. Washington, D. C.: American Chemical Society. ACS Publications, 2014, Roč.

33, č. 19, [tlačená forma] [online]. ISSN 0276-7333. ISSN (online) 1520-6041. - SCIE ; WOS CC, s. 5358 - 5364

2014 [01/12] / **USA** - Shwetha, G. - Kanchana, V. - Valsakumar, M.C. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2014, Roč. 116, č. 13, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 133510

2014 [01/12] / **USA** - Sorescu, D.C. - Byrd, E.F.C. - Rice, B.M. - Jordan, K.D. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4982 - 4994

2014 [01/12] / Kropp, T. - Paier, J. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 41. - SCIE ; WOS CC, s. 23690 - 23700

2014 [01/12] / Zhang, R.W. - Zhang, C.W. - Ji, W.X. - Hu, S.J. - Yan, S.S. - Li, S.S. - Li, P. - Wang, P.J. - Liu, Y.S. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 43. - SCIE ; WOS CC, s. 25278 - 25283

2014 [01/12] / **USA** - Zhu, Q. - Sharma, V. - Oganov, A.R. - Ramprasad, R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 141, č. 15, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 154102

2014 [01/12] / **USA** - Al-Hamdani, Y.S. - Alfe, D. - von Lilienfeld, O.A. - Michaelides, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 141, č. 18, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 18530

2014 [01/12] / Shojaei, F. - Kang, H.S. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 44. - SCIE ; WOS CC, s. 25626 - 25632

2014 [01/12] / **USA** - Deringer, V.L. - Dronskowski, R. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2014, Roč. 116, č. 17, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 173703

2014 [01/12] / **USA** - Musso, T. - Kumar, P.V. - Foster, A.S. - Grossman, J.C. **In: ACS Nano**. Washington: American Chemical Society, 2014, Roč. 8, č. 11, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 11432 - 11439

2014 [01/12] / Liu, L. - Siegel, D.A. - Chen, W. - Liu, P.Z. - Guo, J.J. - Duscher, G. - Zhaog, C. - Wang, H. - Wang, W.L. - Bai, X.D. - McCarty, K.F. - Zhang, Z.Y. - Gu, G. **In: Proceedings of the National Academy of Sciences of the United States of**, 2014, Roč. 111, č. 47. - SCIE ; WOS CC, s. 16670 - 16675

2014 [01/12] / Li, Q.F. - Wan, X.G. - Duan, C.G. - Kuo, J.L. **In: Journal of Physics D-Applied Physics**, 2014, Roč. 47, č. 46. - SCIE ; WOS CC, s. Art. No. 465302

2014 [01/12] / Liu, H.S. - Han, N.N. - Zhao, J.J. **In: Journal of Physics-Condensed Matter**, 2014, Roč. 26, č. 47. - SCIE ; WOS CC, s. Art. No. 475303

2014 [01/12] / Boukhvalov, D.W. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 47. - SCIE ; WOS CC, s. 27594 - 27598

2013 [01/12] / **GBR** - Hu, W. - Wu, X.J. - Li, Z.Y. - Yang, J.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 16, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 5753 - 5757

2013 [01/12] / **GBR** - Yuan, L. - Li, Z.Y. - Yang, J.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 2, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 497 - 503

2013 [01/12] / **GBR** - Cho, S.B. - Chung, Y.C. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2013, Roč. 1, č. 8, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 1595 - 1600

2013 [01/12] / **GBR** - Lee, S. - Lee, M. - Chung, Y.C. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 9, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 3243 - 3248

2013 [01/12] / **GBR** - Wang, Q. - Wei, L. - Sullivan, M. - Yang, S.W. - Chen, Y. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 3, č. 9, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 3046 - 3053

2013 [01/12] / **GBR** - Grimme, S. - Steinmetz, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 38, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 16031 - 16042

2013 [01/12] / **GBR** - Ramos-Sanchez, G. - Balbuena, P.B. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 28, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 11950 - 11959

2013 [01/12] / **GBR** - Kim, D. - Lee, S. - Jo, S. - Chung, Y.C. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 30, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 12757 - 12761

2013 [01/12] / **GBR** - Li, F.Y. - Chen, Z.F. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 5, č. 12, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 5321 - 5333

2013 [01/12] / **GBR** - Le, N.B. - Woods, L.M. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 3, č. 25, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 10014 - 10018

2013 [01/12] / **GBR** - Maganas, D. - Roemelt, M. - Havecker, M. - Trunschke, A. - Knop-Gericke, A. - Schlogl, R. - Neese, F. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 19, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 7260 - 7276

2013 [01/12] / **USA** - Li, L.H. - Zheng, X.L. - Wang, J.J. - Sun, Q. - Xu, Q. **In: ACS Sustainable Chemistry & Engineering**. Washington: American Chemical Society, 2013, Roč. 1, č. 1, [online]. ISSN (online) 2168-0485. - SCIE ; WOS CC, s. 144 - 151

2013 [01/12] / **USA** - Chen, W. - Santos, E.J.G. - Zhu, W.G. - Kaxiras, E. - Zhang, Z.Y. **In: Nano letters**. Washington: American Chemical Society, 2013, Roč. 13, č. 2, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 509 - 514

2013 [01/12] / **USA** - Shishkina, A.V. - Zhurov, V.V. - Stash, A.I. - Vener, M.V. - Pinkerton, A.A. - Tsirelson, V.G. **In: Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2013, Roč. 13, č. 2, [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCIE ; WOS CC, s. 816 - 828

2013 [01/12] / **CHE** - Zhou, H.T. - Zhang, L.Z. - Mao, J.H. - Li, G. - Zhang, Y. - Wang, Y.L. - Du, S.X. - Hofer, W.A. -

Gao, H.J. **In: Nano research**. Peking: Tshinghua Press, 2013, Roč. 6, č. 2, [tlačená forma] [online]. ISSN 1998-0124. ISSN (online) 1998-0000. - SCIE ; WOS CC, s. 131 - 137

2013 [01/12] / Li, C. - Yang, S.X. - Li, S.S. - Xia, J.B. - Li, J.B. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 1. - SCIE ; WOS CC, s. 483 - 488

2013 [01/12] / **GBR** - Sawinski, P.K. - Deringer, V.L. - Dronskowski, R. **In: Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2013, Roč. 42, č. 42, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCIE ; WOS CC, s. 15080 - 15087

2013 [01/12] / **GBR** - Hu, W. - Wu, X.J. - Li, Z.Y. - Yang, J.L. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 5, č. 19, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 9062 - 9066

2013 [01/12] / **USA** - Gueddida, S. - Alouani, M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 87, č. 14, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 144413

2013 [01/12] / **NLD** - Wang, Y.S. - Li, X.F. - Wang, F. - Xu, B. - Zhang, J. - Sun, Q. - Jia, Y. **In: Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2013, Roč. 415, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCIE ; WOS CC, s. 26 - 30

2013 [01/12] / **USA** - Hu, W. - Li, Z.Y. - Yang, J.L. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 138, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124706

2013 [01/12] / Penschke, C. - Paier, J. - Sauer, J. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 10. - SCIE ; WOS CC, s. 5274 - 5285

2013 [01/12] / **DEU** - Djeghloul, F. - Ibrahim, F. - Cantoni, M. - Bowen, M. - Joly, L. - Boukari, S. - Ohresser, P. - Bertran, F. - Le Fevre, P. - Thakur, P. - Scheurer, F. - Miyamachi, T. - Mattana, R. - Seneor, P. - Jaafar, A. - Rinaldi, C. - Javaid, S. - Arabski, J. - Kappler, J.P. - Wulfhekel, W. - Brookes, N.B. - Bertacco, R. - Taleb-Ibrahimi, A. - Alouani, M. - Beaurepaire, E. - Weber, W. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2013, Roč. 3, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 1272

2013 [01/12] / **USA** - Wang, Y.S. - Wang, F.S. - Xu, B. - Zhang, J. - Sun, Q. - Jia, Y. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2013, Roč. 113, č. 6, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 064309

2013 [01/12] / Liu, H.S. - Gao, J.F. - Zhao, J.J. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 20. - SCIE ; WOS CC, s. 10353 - 10359

2013 [01/12] / **USA** - Weber, A.P. - Caruso, A.N. - Vescovo, E. - Ali, M.E. - Tarafder, K. - Janjua, S.Z. - Sadowski, J.T. - Oppeneer, P.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 87, č. 18, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 184411

2013 [01/12] / **USA** - Zahid, F. - Liu, L. - Zhu, Y. - Wang, J. - Guo, H. **In: AIP Advances**. Melville: American Institute of Physics, 2013, Roč. 3, č. 5, [online]. ISSN (online) 2158-3226. - SCIE ; WOS CC, s. Art. No. 052111

2013 [01/12] / Goldman, N. - Srinivasan, S.G. - Hamel, S. - Fried, L.E. - Gaus, M. - Elstner, M. **In: Journal of Physical**

Chemistry C, 2013, Roč. 117, č. 15. - SCIE ; WOS CC, s. 7885 - 7894

2013 [01/12] / Kou, L.Z. - Tang, C. - Frauenheim, T. - Chen, C.F. **In: Journal of Physical Chemistry Letters**, 2013, Roč. 4, č. 8. - SCIE ; WOS CC, s. 1328 - 1333

2013 [01/12] / **USA** - Ehrlich, S. - Moellmann, J. - Grimme, S. **In: Accounts of Chemical Research**. Washington: American Chemical Society, 2013, Roč. 46, č. 4, [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCIE ; WOS CC, s. 916 - 926

2013 [01/12] / **GBR** - Lee, S. - Lee, M. - Choi, H. - Yoo, D.S. - Chung, Y.C. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2013, Roč. 38, č. 11, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 4611 - 4617

2013 [01/12] / **USA** - Piotrowski, M.J. - Nomiyama, R.K. - Da Silva, J.L.F. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 88, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075421

2013 [01/12] / Deringer, V.L. - Dronskowski, R. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 29. - SCIE ; WOS CC, s. 15075 - 15089

2013 [01/12] / **USA** - Moellmann, J. - Grimme, S. **In: Organometallics**. Washington, D. C.: American Chemical Society. ACS Publications, 2013, Roč. 32, č. 14, [tlačená forma] [online]. ISSN 0276-7333. ISSN (online) 1520-6041. - SCIE ; WOS CC, s. 3784 - 3787

2013 [01/12] / **USA** - Yamauchi, K. - Hamada, I. - Oguchi, T. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 88, č. 3, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 035110

2013 [01/12] / **USA** - Espejo, C. - Rangel, T. - Romero, A.H. - Gonze, X. - Rignanese, G.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 87, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 245114

2013 [01/12] / **USA** - Marques, M.P.M. - Valero, R. - Parker, S.F. - Toinkinson, J. - de Carvalho, L.A.E.B. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2013, Roč. 117, č. 21, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 6421 - 6429

2013 [01/12] / **USA** - Tran, F. - Hutter, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 138, č. 20, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 204103

2013 [01/12] / **USA** - Sa, B.S. - Sun, Z.M. - Kaewmaraya, T. - Zhou, J. - Ahuja, R. **In: Science of advanced materials**. Stevenson Ranch: American Scientific Publishers, 2013, Roč. 5, č. 10, [tlačená forma] [online]. ISSN 1947-2935. ISSN (online) 1947-2943. - SCIE ; WOS CC, s. 1493 - 1497

2013 [01/12] / **USA** - Dzade, N.Y. - Roldan, A. - de Leeuw, N.H. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 139, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124708

2013 [01/12] / **USA** - Jiang, X.P. - Kharche, N. - Kohl, P. - Boykin, T.B. - Klimeck, G. - Luisier, M. - Ajayan, P.M. - Nayak, S.K. **In: Applied Physics Letters**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 103, č. 13, [tlačená

forma] [online]. ISSN 0003-6951. ISSN (online) 1077-3118. - SCIE ; WOS CC, s. Art. No. 133107

2013 [01/12] / **NLD** - Lee, S. - Chung, Y.C. **In: Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2013, Roč. 205, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCIE ; WOS CC, s. 160 - 164

2013 [01/12] / **NLD** - Jeong, Y.C. - Baek, S.B. - Kim, D.H. - Kim, J.S. - Kim, Y.C. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2013, Roč. 280, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 207 - 211

2013 [01/12] / **NLD** - Song, N.H. - Lv, J. - Wang, Y.S. **In: Computational Materials Science**. Amsterdam: Elsevier, 2013, Roč. 77, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 31 - 34

2013 [01/12] / Tereshchuk, P. - Da Silva, J.L.F. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 33. - SCIE ; WOS CC, s. 16942 - 16952

2013 [01/12] / **USA** - Gan, L.Y. - Zhang, Q.Y. - Cheng, Y.C. - Schwingenschlogl, U. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 88, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235310

2013 [01/12] / **USA** - Vile, G. - Baudouin, D. - Remediakis, I.N. - Coperet, C. - Lopez, N. - Perez-Ramirez, J. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2013, Roč. 5, č. 12, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 3750 - 3759

2013 [01/12] / **GBR** - Dri, F.L. - Hector, L.G. - Moon, R.J. - Zavattieri, P.D. **In: Cellulose**. London: Blackie Academic & Professional, 2013, Roč. 20, č. 6, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 2703 - 2718

2013 [01/12] / **DEU** - Liu, H.S. - Gao, J.F. - Zhao, J.J. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2013, Roč. 3, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 3238

2013 [01/12] / **USA** - Kang, J. - Li, J.B. - Li, S.S. - Xia, J.B. - Wang, L.W. **In: Nano letters**. Washington: American Chemical Society, 2013, Roč. 13, č. 11, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 5485 - 5490

2013 [01/12] / **NLD** - Biswal, M. - Body, M. - Legein, C. - Sadoc, A. - Boucher, F. **In: Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2013, Roč. 207, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCIE ; WOS CC, s. 208 - 217

2013 [01/12] / **NLD** - Babu, K.R. - Vaitheeswaran, G. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2013, Roč. 586, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 44 - 50

2013 [01/12] / **USA** - Hu, W. - Li, Z.Y. - Yang, J.L. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 139, č. 15, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 154704

2013 [01/12] / **USA** - Caffrey, N.M. - Ferriani, P. - Marocchi, S. - Heinze, S. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 88, č. 15, [tlačená forma] [online]. ISSN 2469-9950.

ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 155403

2013 [01/12] / Jones, P.M. - Tang, H. - Hsia, Y.T. - Yan, X.P. - Kiely, J.D. - Huang, J.W. - Platt, C. - Ma, X.D. - Stirniman, M. - Dinh, L. **In: Advances in Tribology**, 2013, Roč. 2013. - SCIE ; WOS CC, s. Art. No. 850473

2013 [01/12] / Kharche, N. - Nayak, S.K. **Graphene, Carbon Nanotubes, and Nanostructures: Techniques and Applications** [textový dokument (print)] . Boca Raton: Taylor & Francis Group. CRC Press, 2013. 1 vyd. - BKCI-S ; WOS CC, s. 25 - 39

2013 [01/12] / **GBR** - Niwa, M. - Suzuki, K. - Morishita, N. - Sastre, G. - Okumura, K. - Katada, N. **In: Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 3, č. 8, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCIE ; WOS CC, s. 1919 - 1927

2013 [01/12] / **NLD** - Wang, J.J. - Wang, F. - Li, J.M. - Sun, Q. - Yuan, P.F. - Jia, Y. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2013, Roč. 608, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 74 - 79

2013 [01/12] / Brandenburg, J.G. - Alessio, M. - Civalleri, B. - Peintinger, M.F. - Bredow, T. - Grimme, S. **In: Journal of Physical Chemistry A**, 2013, Roč. 117, č. 38. - SCIE ; WOS CC, s. 9282 - 9292

2013 [01/12] / Tang, Q. - Zhou, Z. - Shen, P.W. - Chen, Z.F. **In: ChemPhysChem**, 2013, Roč. 14, č. 9. - SCIE ; WOS CC, s. 1787 - 1792

2013 [01/12] / **USA** - Ma, J.W. - Habrioux, A. - Morais, C. - Lewera, A. - Vogel, W. - Verde-Gomez, Y. - Ramos-Sanchez, G. - Balbuena, P.B. - Alonso-Vante, N. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 9, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1940 - 1950

2013 [01/12] / **NLD** - Babu, K.R. - Vaitheeswaran, G. **In: Solid State Sciences**. Amsterdam: Elsevier. Elsevier Masson, 2013, Roč. 23, [tlačená forma]. ISSN 1293-2558. ISSN (online) 1873-3085. - SCIE ; WOS CC, s. 17 - 25

2012 [01/12] / **USA** - Jayaramulu, K. - Reddy, S.K. - Hazra, A. - Balasubramanian, S. - Maji, T.K. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2012, Roč. 51, č. 13, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 7103 - 7111

2012 [01/12] / **USA** - Reckien, W. - Janetzko, F. - Peintinger, M.F. - Bredow, T. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2012, Roč. 33, č. 25, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 2023 - 2031

2012 [01/12] / **USA** - Volkova, E.I. - Jones, I.A. - Brooks, R. - Zhu, Y. - Bichoutskaia, E. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 86, č. 10, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s.

2012 [01/12] / **USA** - Shwetha, G. - Kanchana, V. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 86, č. 11, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s.

2012 [01/12] / Liu, C.S. - Pilania, G. - Wang, C.C. - Ramprasad, R. **In: Journal of Physical Chemistry A**, 2012, Roč. 116, č. 37. - SCIE ; WOS CC, s. 9347 - 9352

2012 [01/12] / Park, H. - Lee, J.Y. - Shin, S. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 37. - SCIE ; WOS CC, s. 20054 - 20061

2012 [01/12] / **NLD** - Kang, H.S. **In: Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2012, Roč. 405, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCIE ; WOS CC, s. 148 - 154

2012 [01/12] / Minniti, M. - Diaz, C. - Cunado, J.L.F. - Politano, A. - Maccariello, D. - Martin, F. - Farias, D. - Miranda, R. **In: Journal of Physics-Condensed Matter**, 2012, Roč. 24, č. 35. - SCIE ; WOS CC, s.

2012 [01/12] / Delbe, K. - Mansot, J.L. - Thomas, P. - Baranek, P. - Boucher, F. - Vangelisti, R. - Billaud, D. **In: Tribology Letters**, 2012, Roč. 47, č. 3. - SCIE ; WOS CC, s. 367 - 379

2012 [01/12] / **NLD** - Wang, Y.S. - Wang, F. - Li, M. - Xu, B. - Sun, Q. - Jia, Y. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2012, Roč. 258, č. 22, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 8874 - 8879

2012 [01/12] / Rana, M.K. - Koh, H.S. - Hwang, J. - Siegel, D.J. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 32. - SCIE ; WOS CC, s. 16957 - 16968

2012 [01/12] / Meng, L. - Wu, R.T. - Zhang, L.Z. - Li, L.F. - Du, S.X. - Wang, Y.L. - Gao, H.J. **In: Journal of Physics-Condensed Matter**, 2012, Roč. 24, č. 31. - SCIE ; WOS CC, s.

2012 [01/12] / **CHN** - Zheng, Z.Y. - Zhao, J.J. **In: Acta Physico-Chimica Sinica**. Peking: Peking University Press, 2012, Roč. 28, č. 8. ISSN 1000-6818. ISSN (online) 1872-1508. - SCIE ; WOS CC, s. 1809 - 1814

2012 [01/12] / **USA** - Otero-de-la-Roza, A. - Johnson, E.R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2012, Roč. 137, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s.

2012 [01/12] / Blonski, P. - Lopez, N. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 29. - SCIE ; WOS CC, s. 15484 - 15492

2012 [01/12] / Breuer, T. - Celik, M.A. - Jakob, P. - Tonner, R. - Witte, G. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 27. - SCIE ; WOS CC, s. 14491 - 14503

2012 [01/12] / **USA** - Li, Y.F. - Li, F.Y. - Chen, Z.F. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2012, Roč. 134, č. 27, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 11269 - 11275

2012 [01/12] / Park, J. - Hong, S. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 26. - SCIE ; WOS CC, s. 13890 - 13895

2012 [01/12] / **NLD** - Wang, Y.S. - Yuan, P.F. - Li, M. - Jiang, W.F. - Sun, Q. - Jia, Y. **In: Computational Materials Science**. Amsterdam: Elsevier, 2012, Roč. 60, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 181 - 185

2012 [01/12] / **USA** - Hamada, I. - Yamauchi, K. - Oguchi, T. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 85, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s.

2012 [01/12] / **NLD** - Baek, S.B. - Kim, D.H. - Kim, Y.C. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2012, Roč. 258, č. 17, [tlačená forma] [online]. ISSN

0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 6341 - 6344

2012 [01/12] / **USA** - Slawinska, J. - Wlasny, I. - Dabrowski, P. - Klusek, Z. - Zasada, I. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 85, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s.

2012 [01/12] / **USA** - Bjorkman, T. - Gulans, A. - Krasheninnikov, A.V. - Nieminen, R.M. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 108, č. 23, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s.

2012 [01/12] / **USA** - Pereira, A.L.J. - Lisboa, P.N. - Acuna, J. - Brandt, I.S. - Pasa, A.A. - Zanatta, A.R. - Vilcarromero, J. - Beltran, A. - da Silva, J.H.D. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2012, Roč. 111, č. 11, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s.

2012 [01/12] / **USA** - Pereira, A.L.J. - Gracia, L. - Santamaria-Perez, D. - Vilaplana, R. - Manjon, F.J. - Errandonea, D. - Nalin, M. - Beltran, A. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 85, č. 17, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s.

2012 [01/12] / Fang, H.J. - Kamakoti, P. - Zang, J. - Cundy, S. - Paur, C. - Ravikovitch, P.I. - Sholl, D.S. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 19. - SCIE ; WOS CC, s. 10692 - 10701

2012 [01/12] / Ataca, C. - Sahin, H. - Ciraci, S. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 16. - SCIE ; WOS CC, s. 8983 - 8999

2012 [01/12] / **USA** - Mugarza, A. - Robles, R. - Krull, C. - Korytar, R. - Lorente, N. - Gambardella, P. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 85, č. 15, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s.

2012 [01/12] / Kang, H.S. - Kim, Y.S. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 14. - SCIE ; WOS CC, s. 8167 - 8173

2012 [01/12] / **USA** - Lingam, C.B. - Babu, K.R. - Tewari, S.P. - Vaitheeswaran, G. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2012, Roč. 33, č. 9, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 987 - 997

2012 [01/12] / **USA** - Al-Saidi, W.A. - Voora, V.K. - Jordan, K.D. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2012, Roč. 8, č. 4, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 1503 - 1513

2012 [01/12] / Brgoch, J. - Miller, G.J. **In: Journal of Physical Chemistry A**, 2012, Roč. 116, č. 9. - SCIE ; WOS CC, s. 2234 - 2243

2012 [01/12] / **NLD** - Li, M. - Zhang, J.Y. - Zhang, Y. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2012, Roč. 527, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 63 - 66

2012 [01/12] / Tang, Q. - Zhou, Z. - Chen, Z.F. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 6. - SCIE ; WOS CC, s. 4119 - 4125

2012 [01/12] / Kim, H. - Choi, J.M. - Goddard, W.A. **In: Journal of Physical Chemistry Letters**, 2012, Roč. 3, č. 3. -

SCIE ; WOS CC, s. 360 - 363

2012 [01/12] / **DEU** - Noh, J.Y. - Kim, H. **In: Journal of the Korean Physical Society**. Berlín: Springer Nature, 2012, Roč. 60, č. 3, [tlačená forma] [online]. ISSN 0374-4884. ISSN (online) 1976-8524. - SCIE ; WOS CC, s. 410 - 414

2012 [01/12] / Goldman, N. - Fried, L.E. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 3. - SCIE ; WOS CC, s. 2198 - 2204

2012 [01/12] / **GBR** - Di Sante, D. - Stroppa, A. - Picozzi, S. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2012, Roč. 14, č. 42, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 14673 - 14681

2012 [01/12] / **GBR** - Frayret, C. - Izgorodina, E.I. - MacFarlane, D.R. - Villesuzanne, A. - Barres, A.L. - Politano, O. - Rebeix, D. - Poizot, P. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2012, Roč. 14, č. 32, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 11398 - 11412

2012 [01/12] / **GBR** - Yuan, L. - Li, Z.Y. - Yang, J.L. - Hou, J.G. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2012, Roč. 14, č. 22, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 8179 - 8184

2012 [01/12] / **USA** - Huang, B. - Lee, H. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 86, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 245406

2012 [01/12] / **USA** - Gunka, P.A. - Dranka, M. - Piechota, J. - Zukowska, G.Z. - Zalewska, A. - Zachara, J. **In: Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2012, Roč. 12, č. 11, [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCIE ; WOS CC, s. 5663 - 5670

2012 [01/12] / Moellmann, J. - Ehrlich, S. - Tonner, R. - Grimme, S. **In: Journal of Physics-Condensed Matter**, 2012, Roč. 24, č. 42. - SCIE ; WOS CC, s. Art. No. 424206

2012 [01/12] / **USA** - Klimes, J. - Michaelides, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2012, Roč. 137, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No.120901

2012 [01/12] / Lopez, N. - Almora-Barrios, N. - Carchini, G. - Blonski, P. - Bellarosa, L. - Garcia-Muelas, R. - Novell-Leruth, G. - Garcia-Mota, M. **In: Catalysis Science & Technology**, 2012, Roč. 2, č. 12. - SCIE ; WOS CC, s. 2405 - 2417

2012 [01/12] / **NLD** - Li, M. - Zhang, J.Y. - Zhang, Y. **In: Catalysis Communications**. Amsterdam: Elsevier, 2012, Roč. 29, [tlačená forma]. ISSN 1566-7367. ISSN (online) 1873-3905. - SCIE ; WOS CC, s. 175 - 179

2011 [01/12] / **USA** - Slawinska, J. - Zasada, I. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2011, Roč. 84, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235445

2011 [01/12] / Parthasarathi, R. - Bellesia, G. - Chundawat, S.P.S. - Dale, B.E. - Langan, P. - Gnanakaran, S. **In: Journal of Physical Chemistry A**, 2011, Roč. 115, č. 49. - SCIE ; WOS CC, s. 14191 - 14202

2011 [01/12] / Ehrlich, S. - Moellmann, J. - Reckien, W. - Bredow, T. - Grimme, S. **In: ChemPhysChem**, 2011, Roč. 12, č. 17. - SCIE ; WOS CC, s. 3414 - 3420

2011 [01/12] / **USA** - Marom, N. - Tkatchenko, A. - Rossi, M. - Gobre, V.V. - Hod, O. - Scheffler, M. - Kronik, L. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2011, Roč. 7, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 3944 - 3951

2011 [01/12] / **USA** - Kharche, N. - Nayak, S.K. **In: Nano letters**. Washington: American Chemical Society, 2011, Roč. 11, č. 12, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 5274 - 5278

2011 [01/12] / Li, C. - Li, J.B. - Wu, F.M. - Li, S.S. - Xia, J.B. - Wang, L.W. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 46. - SCIE ; WOS CC, s. 23221 - 23225

2011 [01/12] / **USA** - Lee, T.B. - Mckee, M.L. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2011, Roč. 50, č. 22, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 11412 - 11422

2011 [01/12] / **USA** - Ramasubramaniam, A. - Naveh, D. - Towe, E. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2011, Roč. 84, č. 20, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 205325

2011 [01/12] / **USA** - Duong, T. - Gibbons, S. - Kinra, R. - Arroyave, R. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2011, Roč. 110, č. 9, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 093504

2011 [01/12] / **USA** - Yamauchi, K. - Hamada, I. - Huang, H.B. - Oguchi, T. **In: Applied Physics Letters**. Melville: American Institute of Physics. AIP Publishing, 2011, Roč. 99, č. 18, [tlačená forma] [online]. ISSN 0003-6951. ISSN (online) 1077-3118. - SCIE ; WOS CC, s. Art. No. 181904

2011 [01/12] / Maschio, L. - Civalleri, B. - Ugliengo, P. - Gavezzotti, A. **In: Journal of Physical Chemistry A**, 2011, Roč. 115, č. 41. - SCIE ; WOS CC, s. 11179 - 11186

2011 [01/12] / Allen, J.P. - Scanlon, D.O. - Parker, S.C. - Watson, G.W. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 40. - SCIE ; WOS CC, s. 19916 - 19924

2011 [01/12] / **USA** - Kang, H.S. - Pramanik, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2011, Roč. 135, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124708

2011 [01/12] / **USA** - Allen, J.P. - Scanlon, D.O. - Watson, G.W. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2011, Roč. 84, č. 11, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 115141

2011 [01/12] / Voora, V.K. - Al-Saidi, W.A. - Jordan, K.D. **In: Journal of Physical Chemistry A**, 2011, Roč. 115, č. 34. - SCIE ; WOS CC, s. 9695 - 9703

2011 [01/12] / **USA** - Nisar, J. - Arhammar, C. - Jamstorp, E. - Ahuja, R. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2011, Roč. 84, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075120

2011 [01/12] / **USA** - Kharche, N. - Zhou, Y. - O'Brien, K.P. - Kar, S. - Nayak, S.K. **In: ACS Nano**. Washington: American Chemical Society, 2011, Roč. 5, č. 8, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 6096 - 6101

2011 [01/12] / **USA** - Stroppa, A. - Di Sante, D. - Horiuchi, S. - Tokura, Y. - Vanderbilt, D. - Picozzi, S. **In: Physical**

Review B. College Park: American Institute of Physics. American Physical Society, 2011, Roč. 84, č. 1, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 014101

2011 [01/12] / **DEU** - Park, J. - Yu, B.D. - Hong, S. **In: Journal of the Korean Physical Society**. Berlín: Springer Nature, 2011, Roč. 59, č. 1, [tlačená forma] [online]. ISSN 0374-4884. ISSN (online) 1976-8524. - SCIE ; WOS CC, s. 196 - 199

2011 [01/12] / **USA** - Slawinska, J. - Dabrowski, P. - Zasada, I. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2011, Roč. 83, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 245429

2011 [01/12] / Tang, Q. - Li, F.Y. - Zhou, Z. - Chen, Z.F. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 24. - SCIE ; WOS CC, s. 11983 - 11990

2011 [01/12] / **USA** - Wen, X.D. - Hoffmann, R. - Ashcroft, N.W. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2011, Roč. 133, č. 23, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 9023 - 9035

2011 [01/12] / Pramanik, A. - Kang, H.S. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 22. - SCIE ; WOS CC, s. 10971 - 10978

2011 [01/12] / **USA** - Tafipolsky, M. - Engels, B. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2011, Roč. 7, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 1791 - 1803

2011 [01/12] / **USA** - Stradi, D. - Barja, S. - Diaz, C. - Garnica, M. - Borca, B. - Hinarejos, J.J. - Sanchez-Portal, D. - Alcami, M. - Arnau, A. - de Parga, A.L.V. - Miranda, R. - Martin, F. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2011, Roč. 106, č. 18, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s. Art. No. 186102

2011 [01/12] / **USA** - Pei, Y. - Zeng, X.C. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2011, Roč. 109, č. 9, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 093514

2011 [01/12] / **USA** - Grimme, S. - Ehrlich, S. - Goerigk, L. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2011, Roč. 32, č. 7, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 1456 - 1465

2011 [01/12] / Stroppa, A. - Jain, P. - Barone, P. - Marsman, M. - Perez-Mato, J.M. - Cheetham, A.K. - Kroto, H.W. - Picozzi, S. **In: Angewandte Chemie-International Edition**, 2011, Roč. 50, č. 26. - SCIE ; WOS CC, s. 5847 - 5850

ADC_028: / Sklenák, Štěpán (Autor) (10%) - Andrikopoulos, Prokopis C. (Autor) (10%) - Boekfa, Bundet (Autor) (10%) - Jansang, Bavornpon (Autor) (10%) - Nováková, Jana (Autor) (10%) - Benco, Ľubomír (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (10%) - Hafner, Jürgen (Autor) (10%) - Dědeček, Jiří (Autor) (10%) - Sobalík, Zdeněk (Autor) (10%): **N2O decomposition over Fe-zeolites: Structure of the active sites and the origin of the distinct reactivity of Fe-ferrierite, Fe-ZSM-5, and Fe-beta. A combined periodic DFT and multispectral study**. – text, ilustr., graf., tab. – [recenzované]. – DOI 10.1016/j.jcat.2010.04.008. – CCC ; SCO ; WOS CC.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – Roč. 272, č. 2 (2010), s. 262-274 [tlačená forma] [online]
Počet všetkých autorov: 10

[článok]
Lit.: 75
[OV 120 Chémia, chemická technológia a biotechnológie]

Ohlasy (100):

2025 [01/20] / **GBR** - Centi, Gabrile - Perathoner, Siglinda. **Zeolites in Environmental Catalysis**. DOI 10.1039/9781837676859-00453 In: **Zeolites from Fundamentals to Emerging Applications**. London: The Royal Society of Chemistry, 2025, s. 453-481 [tlačená forma] [online]. ISBN [9781837675456, 9781837676859]. - SCO, s. 453 - 481

2025 [01/20] / **NLD** - Makova, Anna S. - Chesnokova, Alena V. - Kustov, Alexander L. - Leonov, Alexander V. - Pribytkov, Petr V. - Plenkin, Danil S. - Ter-Akopyan, Marina N. - Kustov, Leonid M. **Decomposition of N2O on different iron-containing catalysts** [elektronický dokument]. DOI 10.71267/mencom.7530 In: **Mendeleev communications**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 35, č. 2, s. 234-236 [tlačená forma] [online]. ISSN 0959-9436. ISSN (online) 1364-551X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 234 - 236

2025 [01/20] / **NLD** - Makova, Anna S. - Mashkin, Mikhail Yu - Mishin, Igor V. - Kapustin, Gennady I. - Tkachenko, Olga P. - Kalmykov, Konstantin B. - Kustov, Alexander L. - Kustov, Leonid M. **Synthesis of zeolites with a ferrierite structure by hydrothermal and solvothermal methods and their activity in N2O decomposition** [elektronický dokument]. DOI 10.1016/j.colsurfa.2025.138472 In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2025, Roč. 727, art. no. 138472 [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 138472

2025 [01/20] / **GBR** - Liu, Ning - Zhang, Tingting - Dai, Chengna - Xu, Ruinian - Yu, Gangqiang - Wang, Ning - Chen, Biaohua. **2D spatial structure-favored, tandem catalysis-boosted direct transformation of methane to methanol over Cu-FER** [elektronický dokument]. DOI 10.1039/d5sc02092a In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 28, s. 13082-13095 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 13082 - 13095

2025 [01/20] / **USA** - Wang, Shuo - Li, Chenchen - Liu, Chong - Zhuang, Wei. **On the Heterogeneity of Iron-Oxo Species in Zeolites for the Oxidation of Methane to Methanol by Nitrous Oxide: A Theoretical Perspective** [elektronický dokument]. DOI 10.1002/cctc.202401416 In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2025, Roč. 17, č. 1, art. no. e202401416 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **DEU** - Moore, Rio G. - Crawford, James M. **Isolated and Paired Metal Sites in Zeolites Using Solid-State Ion Exchange** [elektronický dokument]. DOI 10.1002/anie.202505186 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 64, č. 23, art. no. e202505186 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2024 [01/20] / **DEU** - Kornas, Agnieszka - Mlekodaj, Kinga - Tabor, Edyta. **Nature and Redox Properties of Iron Sites in Zeolites Revealed by Mössbauer Spectroscopy** [elektronický dokument]. DOI 10.1002/cplu.202300543 In: **ChemPlusChem**: a Genuinely Multidisciplinary Journal Centering on Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 89, č. 5, art. no. e202300543 [online]. ISSN (online) 2192-6506. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **CHE** - Yuan, Ning - Gao, Congru - Sun, Xiuliang - Li, Jianwei. **Density Functional Theory Study of Mechanism of Reduction of N2O by CO over Fe-ZSM-5 Zeolites**. DOI 10.3390/catal14010049 In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 14, č. 1, art. no. 49 [online]. ISSN 2073-4344. - SCO ; CCC ; WOS CC, s. art. no. 49

2024 [01/20] / **USA** - Liu, Chunli - Liu, Yonghua - Xu, Gaomou - Wang, Tao. **Associative-Distal Mechanism of the Haber-Bosch Process on a Ferrierite Catalyst with Spatially Isolated Dual Molybdenum Sites** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c01107 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 16, s. 6711-6718 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 6711 - 6718

2024 [01/20] / **NLD** - Campa, Maria Cristina - Pietrogiacomi, Daniela - Catracchia, Carlotta - Morpurgo, Simone - Olszowka, Joanna - Mlekodaj, Kinga - Lemishka, Mariia - Dedecek, Jiri - Kornas, Agnieszka - Tabor, Edyta. **Fe-MOR and Fe-FER as catalysts for abatement of N2O with CH4: in situ UV–vis DRS and operando FTIR study**. DOI 10.1016/j.apcatb.2023.123360 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2024, Roč. 342, art. no. 123360 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s. art. no. 123360

2024 [01/20] / **GBR** - Zhang, Yan - Du, Jinpeng - Shan, Yulong - Wang, Fei - Liu, Jingjing - Wang, Meng - Liu, Zhi - Yan, Yong - Xu, Guangyan - He, Guangzhi - Shi, Xiaoyan - Lian, Zhihua - Yu, Yunbo - Shan, Wenpo - He, Hong. **Toward synergetic reduction of pollutant and greenhouse gas emissions from vehicles: a catalysis perspective** [elektronický dokument]. DOI 10.1039/d4cs00140k In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 54, č. 3, s. 1151-1215 [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO ; CCC ; WOS CC, s. 1151 - 1215

2024 [01/20] / **GBR** - Antúnez-García, Joel - Ponce-Ruiz, Jesus L.A. - Núñez-González, Roberto - Petranovskii, Vitalii - Murrieta-Rico, Fabian N. - Serrato, Armando Reyes - Shelyapina, Marina G. - Xiao, Mufei - Zamora, Jonathan. **Theoretical investigation of Fe and Cu cations hosted within the MOR zeolite framework** [elektronický dokument]. DOI 10.1016/j.mtcomm.2024.110418 In: **Materials today. Communications.**. Oxford: Elsevier, 2024, Roč. 41, art. no. 110418 [online]. ISSN (online) 2352-4928. - SCO ; CCC ; WOS CC, s. art. no. 110418

2024 [01/20] / **USA** - Xiao, Peipei - Wang, Lizhuo - Toyoda, Hiroto - Wang, Yong - Nakamura, Kengo - Huang, Jun - Osuga, Ryota - Nishibori, Maiko - Gies, Hermann - Yokoi, Toshiyuki. **Revealing Active Sites and Reaction Pathways in Direct Oxidation of Methane over Fe-Containing CHA Zeolites Affected by the Al Arrangement** [elektronický dokument]. DOI 10.1021/jacs.4c11773 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2024, Roč. 146, č. 46, s. 31969-31981 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC, s. 31969 - 31981

2024 [01/20] / **NLD** - Makova, Anna S. - Timofeeva, Maria N. - Tkachenko, Olga P. - Panchenko, Valentina N. - Leonov, Alexander V. - Kapustin, Gennady I. - Davshan, Nikolay A. - Kalmykov, Konstantin B. - Kustov, Alexander L. - Ter-Akopyan, Marina N. - Kustov, Leonid M. **Effect of microwave irradiation on the synthesis of zeolite with ferrierite structure: Study of acid and catalytic properties** [elektronický dokument]. DOI 10.1016/j.colsurfa.2024.135321 In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2024, Roč. 703, art. no. 135321 [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO ; CCC ; WOS CC, s. art. no. 135321

2024 [01/20] / **IND** - Dutta, Buddhadeb. **Metal Incorporated Zeolites as Heterogeneous Catalysts in the Selective Partial Oxidation of Methane to Methanol: A Review** [elektronický dokument]. DOI 10.14233/ajchem.2024.32083 In: **Asian Journal of Chemistry**: an International Peer reviewed Research Journal of Chemistry. Ghaziabad: Asian Publication Corporation, 2024, Roč. 36, č. 9, s. 1977-1987 [tlačená forma] [online]. ISSN 0970-7077. ISSN (online) 0975-427X. - SCO, s. 1977 - 1987

2024 [01/20] / **USA** - Zhu, Zhan Jun - He, Zhen Hong - Tian, Yue - Wang, Sen Wang - Sun, Yong Chang - Wang, Kuan - Wang, Weitao - Zhang, Zhi Fang - Liu, Jiajie - Liu, Zhao Tie. **Mass-Transfer Enhancement in the CO2 Oxidative Dehydrogenation of Propane over GaN Supported on Zeolite Nanosheets with a Short b-Axis and Hierarchical Pores** [elektronický dokument]. DOI 10.1021/acscatal.4c02599 In: **ACS Catalysis**. Washington: American Chemical Society,

2024, Roč. 14, č. 13, s. 10376-10391 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 10376 - 10391

2023 [01/20] / **USA** - Liu, Chunli - Xu, Gaomou - Wang, Tao. **Theoretical Approach toward a Mild Condition Haber-Bosch Process on the Zeolite Catalyst with Confined Dual Active Sites** [elektronický dokument]. DOI 10.1021/jacsau.3c00546 In: **JACS Au**. Washington: American Chemical Society, 2023, Roč. 3, č. 12, s. 3374-3380 [online]. ISSN (online) 2691-3704. - SCO ; WOS CC, s. 3374 - 3380

2023 [01/20] / **USA** - Cheng, Jie - Zheng, Dahai - Yu, Gangqiang - Xu, Ruinian - Dai, Chengna - Liu, Ning - Wang, Ning - Chen, Biaohua. **N2O Catalytic Decomposition and NH3-SCR Coupling Reactions over Fe-SSZ-13 Catalyst: Mechanisms and Interactions Unraveling via Experiments and DFT Calculations** [elektronický dokument]. DOI 10.1021/acscatal.2c04747 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 2, s. 934-947 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 934 - 947

2023 [01/20] / **USA** - Gokce, Iklim - Ozbek, M. Olus - Ipek, Bahar. **Conditions for higher methanol selectivity for partial CH4 oxidation over Fe-MOR using N2O as the oxidant and comparison to Fe-SSZ-13, Fe-SSZ-39, Fe-FER, and Fe-ZSM-5** [elektronický dokument]. DOI 10.1016/j.jcat.2023.115113 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2023, Roč. 427, art. no. 115113 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. art. no. 115113

2023 [01/20] / **USA** - Dummer, Nicholas F. - Willock, David J. - He, Qian - Howard, Mark J. - Lewis, Richard J. - Qi, Guodong - Taylor, Stuart H. - Xu, Jun - Bethell, Don - Kiely, Christopher J. - Hutchings, Graham J. **Methane Oxidation to Methanol** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00439 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6359-6411 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; WOS CC, s. 6359 - 6411

2023 [01/20] / **CHE** - Kotolevich, Yulia - Khramov, Evgenii - Sánchez-López, Perla - Pestryakov, Alexey - Zubavichus, Yan - Antúnez-Garcia, Joel - Petranovskii, Vitalii. **Formation of Ag-Fe Bimetallic Nano-Species on Mordenite Depending on the Initial Ratio of Components** [elektronický dokument]. DOI 10.3390/ma16083026 In: **Materials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 16, č. 8, art. no. 3026 [online]. ISSN (online) 1996-1944. - SCO ; CCC ; WOS CC, s. art. no. 3026

2023 [01/20] / **USA** - Mlekodaj, Kinga - Lemishka, Mariia - Kornas, Agnieszka - Wierzbicki, Dominik K. - Olszowka, Joanna E. - Jirglová, Hana - Dedecek, Jiri - Tabor, Edyta. **Evolution of Active Oxygen Species Originating from O<inf>2</inf> Cleavage over Fe-FER for Application in Methane Oxidation** [elektronický dokument]. DOI 10.1021/acscatal.2c06099 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 5, s. 3345-3355 [online]. ISSN (online) 2155-5435. - SCO, s. 3345 - 3355

2023 [01/20] / **CHE** - Kotolevich, Yulia - Zepeda-Partida, Trino - Yocupicio-Gaxiola, Rosario - Antúnez-Garcia, Joel - Pelaez, Luis - Avalos-Borja, Miguel - Vázquez-Salas, Pedro Jovanni - Fuentes-Moyado, Sergio - Petranovskii, Vitalii. **Influence of the Valence of Iron on the NO Reduction by CO over Cu-Fe-Mordenite**. DOI 10.3390/catal13030484 In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 3, art. no. 484 [online]. ISSN 2073-4344. - SCO ; CCC ; WOS CC, s. art. no. 484

2022 [01/20] / **CHE** - Szymaszek-Wawryca, A. - Summa, P. - Duraczynska, D. - Diaz, U. - Motak, M. **Hydrotalcite-Modified Clinoptilolite as the Catalyst for Selective Catalytic Reduction of NO with Ammonia (NH3-SCR)** In: **materials**, 2022, Roč. 15, č. 22. - SCO, s. Art. No. 7884

2022 [01/20] / **GBR** - Buttignol, F. - Rentsch, D. - Alxneit, I. - Garbujo, A. - Biasi, P. - Krocher, O. - Ferri, D. **Aging of industrial Fe-zeolite based catalysts for nitrous oxide abatement in nitric acid production plants** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 12, č. 24, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 7308 - 7321

2022 [01/20] / **USA** - Nicholas, K.M. - Lander, C. - Shao, Y. **Computational Evaluation of Potential Molecular Catalysts for Nitrous Oxide Decomposition** [elektronický dokument] In: **Inorganic Chemistry**. Washington: American Chemical Society, 2022, Roč. 61, č. 37, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO, s. 14591 - 14605

2022 [01/20] / **USA** - Bickel, E.E. - Hoffman, A.J. - Lee, S. - Snider, H.E. - Nimlos, C.T. - Zamiechowski, N.K. - Hibbitts, D.D. - Gounder, R. **Altering the Arrangement of Framework Al Atoms in MEL Zeolites Using Mixtures of Tetrabutylammonium and Sodium Structure-Directing Agents** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 15, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 6835 - 6852

2022 [01/20] / **USA** - Rhoda, H.M. - Heyer, A.J. - Snyder, B.E.R. - Plessers, D. - Bols, M.L. - Schoonheydt, R.A. - Sels, B.F. - Solomon, E.I. **Second-Sphere Lattice Effects in Copper and Iron Zeolite Catalysis** [elektronický dokument] In: **Chemical Reviews**. Washington: American Chemical Society, 2022, Roč. 122, č. 14, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO, s. 12207 - 12243

2022 [01/20] / **USA** - Li, L.-Y. - Wang, Z.-Y. - Yang, S.-Y. - Chen, J.-G. - He, Z.-H. - Wang, K. - Luo, Q.-X. - Liu, Z.-W. - Liu, Z.-T. **Understanding the Role of Fe Doping in Tuning the Size and Dispersion of GaN Nanocrystallites for CO2-Assisted Oxidative Dehydrogenation of Propane** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 14, [online]. ISSN (online) 2155-5435. - SCO, s. 8527 - 8543

2022 [01/20] / **USA** - Bickel, Elizabeth E. - Hoffman, Alexander J. - Lee, Songhyun - Snider, Hannah E. - Nimlos, Claire T. - Zamiechowski, Natalie K. - Hibbitts, David D. - Gounder, Rajamani. **Altering the Arrangement of Framework Al Atoms in MEL Zeolites Using Mixtures of Tetrabutylammonium and Sodium Structure-Directing Agents** [elektronický dokument]. DOI 10.1021/acs.chemmater.2c01083 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 15, s. 6835-6852 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 6835 - 6852

2022 [01/20] / **USA** - Rhoda, Hannah M. - Heyer, Alexander J. - Snyder, Benjamin E.R. - Plessers, Dieter - Bols, Max L. - Schoonheydt, Robert A. - Sels, Bert F. - Solomon, Edward I. **Second-Sphere Lattice Effects in Copper and Iron Zeolite Catalysis** [elektronický dokument]. DOI 10.1021/acs.chemrev.1c00915 In: **Chemical Reviews**. Washington: American Chemical Society, 2022, Roč. 122, č. 14, s. 12207-12243 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO, s. 12207 - 12243

2022 [01/20] / **USA** - Li, Long Yao - Wang, Zhong Yu - Yang, Shao Yan - Chen, Jian Gang - He, Zhen Hong - Wang, Kuan - Luo, Qun Xing - Liu, Zhong Wen - Liu, Zhao Tie. **Understanding the Role of Fe Doping in Tuning the Size and Dispersion of GaN Nanocrystallites for CO2-Assisted Oxidative Dehydrogenation of Propane** [elektronický dokument]. DOI 10.1021/acscatal.2c01989 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 14, s. 8527-8543 [online]. ISSN (online) 2155-5435. - SCO, s. 8527 - 8543

2022 [01/20] / **CHE** - Szymaszek-Wawryca, Agnieszka - Summa, Paulina - Duraczyńska, Dorota - Díaz, Urbano - Motak, Monika. **Hydrotalcite-Modified Clinoptilolite as the Catalyst for Selective Catalytic Reduction of NO with Ammonia (NH<inf>3</inf>-SCR)** [elektronický dokument]. DOI 10.3390/ma15227884 In: **Materials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 15, č. 22, art. no. 7884 [online]. ISSN (online) 1996-1944. - SCO, s. art. no. 7884

2022 [01/20] / **GBR** - Buttignol, Filippo - Rentsch, Daniel - Alxneit, Ivo - Garbujo, Alberto - Biasi, Pierdomenico - Kröcher, Oliver - Ferri, Davide. **Aging of industrial Fe-zeolite based catalysts for nitrous oxide abatement in nitric acid production plants** [elektronický dokument]. DOI 10.1039/d2cy01486f In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 12, č. 24, s. 7308-7321 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 7308 - 7321

2022 [01/20] / **USA** - Nicholas, Kenneth M. - Lander, Chance - Shao, Yihan. **Computational Evaluation of Potential Molecular Catalysts for Nitrous Oxide Decomposition** [elektronický dokument]. DOI 10.1021/acs.inorgchem.2c01598 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2022, Roč. 61, č. 37, s. 14591-14605 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO, s. 14591 - 14605

2022 [01/20] / **NLD** - Kang, Bin - Li, Ming - Di, Zhaoying - Guo, Xiaonan - Wei, Ying - Jia, Jingbo - Zhang, Runduo. **Role of Al pairs on effective N2O decomposition over the ZSM-5 zeolite catalyst** [elektronický dokument]. DOI 10.1016/j.cattod.2022.01.018 In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2022, Roč. 402, s. 17-26 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO, s. 17 - 26

2021 [01/20] / **DEU** - Denisova, K.O. - Il'in, A.A. - Il'in, A.P. - Sakharova, Y .N. **Effect of Catalyst Composition and Process Conditions on the Catalytic Efficiency of Cobalt Ferrite in the Decomposition of Nitrogen(I) Oxide** [elektronický dokument] In: **Russian Journal of Physical Chemistry A**. Cham: Springer Nature, 2021, Roč. 95, č. 10, [tlačená forma] [online]. ISSN 0036-0244. ISSN (online) 1531-863X. - SCO, s. 2014 - 2019

2021 [01/20] / **USA** - Bickel, E.E. - Nimlos, C.T. - Gounder, R. **Developing quantitative synthesis-structure-function relations for framework aluminum arrangement effects in zeolite acid catalysis** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 399, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 75 - 85

2021 [01/20] / **PRK** - Kwak, S.J. - Kim, H.S. - Park, N. - Park, M.-J. - Lee, W.B. **Recent progress on Al distribution over zeolite frameworks: Linking theories and experiments** In: **Korean Journal of Chemical Engineering**, 2021, Roč. 38, č. 6. - SCO, s. 1117 - 1128

2021 [01/20] / **GBR** - Aranifard, S. - Bell, A.T. - Keil, F.J. - Heyden, A. **Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 in the presence of nitric oxide based on parameters obtained from first-principles calculations** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 10, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 3539 - 3555

2021 [01/20] / **USA** - Olszowka, J.E. - Lemishka, M. - Mlekodaj, K. - Kubat, P. - Rutkowska-Zbik, D. - Dedecek, J. - Tabor, E. **Determination of Zn Speciation, Siting, and Distribution in Ferrierite Using Luminescence and FTIR Spectroscopy** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 17. - SCO, s. 9060 - 9073

2021 [01/20] / **CHE** - Zeng, J. - Wang, Y. - Diao, F. - Qiu, L. - Chang, H. **Selective Catalytic Reduction of N2O by CO over Fe-Beta Zeolites Catalysts: Influence of Iron Species Distribution** In: **Catalysis Surveys from Asia**, 2021, Roč. 25, č. 1. - SCO, s. 58 - 67

2021 [01/20] / **NLD** - Denardin, F.G. - Muniz, A.R. - Perez-Lopez, O.W. **Experimental and DFT analysis of the acid and reduction properties of Fe-Cu/ZSM-5** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2021, Roč. 314, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 110860

2021 [01/20] / **NLD** - Nguyen, T.P.T. - Yang, K.H. - Kim, M.H. - Hong, Y.S. **Selective catalytic reduction of NO by NH3 over Fe2O3-promoted V2O5/TiO2-based catalysts with high Fe2O3-to-V2O5 ratios** [elektronický dokument] In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2021, Roč. 360, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO, s. 305 - 316

2020 [01/12] / **USA** - Zhang, T. - Qiu, Y. - Liu, G. - Chen, J. - Peng, Y. - Liu, B. - Li, J. **Nature of active Fe species and reaction mechanism over high-efficiency Fe/CHA catalysts in catalytic decomposition of N2O** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2020, Roč. 392, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 322 - 335

2020 [01/12] / **USA** - Sanahuja-Parejo, O. - Veses, A. - Lopez, J.M. - Callen, M.S. - Solsona, B. - Richards, N. - Taylor, S.H. - Garcia, T. **Insights into the production of upgraded biofuels using Mg-loaded mesoporous ZSM-5 zeolites** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2020, Roč. 12, č. 20, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 5236 - 5249

2020 [01/12] / **DEU** - Zhao, G. - Drewery, M. - Mackie, J. - Oliver, T. - Kennedy, E.M. - Stockenhuber, M. **The Catalyzed Conversion of Methane to Value-Added Products** [elektronický dokument] In: **Energy Technology**: generation, conversion, storage, distribution. Weinheim: John Wiley & Sons. Wiley-VCH, 2020, Roč. 8, č. 8, [tlačená forma] [online]. ISSN 2194-4288. ISSN (online) 2194-4296. - SCO, s. Art. No. 1900665

2020 [01/12] / **GBR** - Zhuang, W. - Liu, X. - Chen, L. - Liu, P. - Wen, H. - Zhou, Y. - Wang, J. **One-pot hydrothermal synthesis of ultrafine Pd clusters within Beta zeolite for selective oxidation of alcohols** [elektronický dokument] In: **Green Chemistry**: an international journal and green chemistry resource: cutting-edge research for a greener sustainable future. Cambridge: The Royal Society of Chemistry, 2020, Roč. 22, č. 13, [tlačená forma] [online]. ISSN 1463-9262. ISSN (online) 1463-9270. - SCO, s. 4199 - 4209

2020 [01/12] / Ma, J. - Yang, D. - Yu, F. - Lai, H. - Feng, F. - Chang, S. **The effect of different silicon-aluminum ratios on selective catalytic reduction performance of Fe-Beta molecular sieves** In: **Gongneng Cailiao/Journal of Functional Materials**, 2020, Roč. 51, č. 5. - SCO, s. 5202 - 5207

2020 [01/12] / **USA** - Zhao, G. - Adesina, A. - Kennedy, E. - Stockenhuber, M. **Formation of Surface Oxygen Species and the Conversion of Methane to Value-Added Products with N2O as Oxidant over Fe-Ferrierite Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 2, [online]. ISSN (online) 2155-5435. - SCO, s. 1406 - 1416

2019 [01/12] / Biturini, N.F. - Santos, A.P.N.M. - Batista, M.S. **In: Reaction Kinetics Mechanisms and Catalysis**, 2019, Roč. 126, č. 1. - SCIE ; WOS CC, s. 341 - 352

2019 [01/12] / Zhu, N. - Lian, Z.H. - Zhang, Y. - Shan, W.P. - He, H. **In: Chinese Chemical Letters**, 2019, Roč. 30, č. 4. ISSN 1001-7417. - SCIE ; WOS CC, s. 867 - 870

2019 [01/12] / Mahyuddin, M.H. - Shiota, Y. - Yoshizawa, K. **In: Catalysis Science & Technology**, 2019, Roč. 9, č. 8. - SCIE ; WOS CC, s. 1744 - 1768

2019 [01/12] / Xie, W.M. - Chen, H.Y. - He, D.S. - Zhang, Y. - Fu, L.J. - Ouyang, J. - Yang, H.M. **In: Surface & Coatings Technology**, 2019, Roč. 367. - SCIE ; WOS CC, s. 118 - 126

2018 [01/12] / **USA** - Liu, J. - Wei, Y.J. - Li, P.Z. - Zhang, P.P. - Su, W. - Sun, Y. - Zou, R.Q. - Zhao, Y.L. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 5, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 3865 - 3874

2018 [01/12] / **USA** - Snyder, B.E.R. - Bols, M.L. - Schoonheydt, R.A. - Sels, B.F. - Solomon, E.I. **In: Chemical Reviews**. Washington: American Chemical Society, 2018, Roč. 118, č. 5, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 2718 - 2768

2018 [01/12] / **NLD** - Avdeev, V.I. - Bedilo, A.F. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2018, Roč. 695, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 222 - 227

2018 [01/12] / **USA** - Wang, A.Y. - Wang, Y.L. - Walter, E.D. - Kukkadapu, R.K. - Guo, Y.L. - Lu, G.Z. - Weber, R.S. - Wang, Y. - Peden, C.H.F. - Gao, F. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2018, Roč. 358, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 199 - 210

2018 [01/12] / **USA** - Richards, N. - Nowicka, E. - Carter, J.H. - Morgan, D.J. - Dummer, N.F. - Golunski, S. - Hutchings, G.J. **In: Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2018, Roč. 61, č. 18-19, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCIE ; WOS CC, s. 1983 - 1992

2018 [01/12] / Berlier, G. - Crocella, V. - Signorile, M. - Borfecchia, E. - Bonino, F. - Bordiga, S. **In: Structure and Reactivity of Metals in Zeolite Materials**, 2018, Roč. 178. - SCIE ; WOS CC, s. 91 - 154

2017 [01/12] / Melian-Cabrera, I. - van Eck, E.R.H. - Espinosa, S. - Siles-Quesada, S. - Falco, L. - Kentgens, A.P.M. - Kapteijn, F. - Moulijn, J.A. **In: Applied Catalysis B-environmental**, 2017, Roč. 203. - SCIE ; WOS CC, s. 218 - 226

2017 [01/12] / **USA** - Mahyuddin, M.H. - Shiota, Y. - Staykov, A. - Yoshizawa, K. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2017, Roč. 56, č. 17, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 10370 - 10380

2017 [01/12] / de Moura, A.P.N. - Batista, M.D. **In: Materia-Rio de Janeiro**, 2017, Roč. 22, č. 3. - SCIE ; WOS CC, s. Art. No. 0

2016 [01/12] / Grzybek, G. - Stelmachowski, P. - Gudyka, S. - Indyka, P. - Sojka, Z. - Guillen-Hurtado, N. - Rico-Perez, V. - Bueno-Lopez, A. - Kotarba, A. **In: Applied Catalysis B-environmental**, 2016, Roč. 180. - SCIE ; WOS CC, s. 622 - 629

2016 [01/12] / **USA** - Kaczmarczyk, J. - Zasada, F. - Janas, J. - Indyka, P. - Piskorz, W. - Kotarba, A. - Sojka, Z. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 2, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1235 - 1246

2016 [01/12] / **USA** - Zhang, R.D. - Liu, N. - Lei, Z.G. - Chen, B.H. **In: Chemical Reviews**. Washington: American Chemical Society, 2016, Roč. 116, č. 6, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 3658 - 3721

2016 [01/12] / **GBR** - Szanyi, J. - Gao, F. - Kwak, J.H. - Kollar, M. - Wang, Y.L. - Peden, C.H.F. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 15, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 10473 - 10485

2016 [01/12] / **NLD** - Wu, M.F. - Wang, H. - Zhong, L.S. - Zhang, X.Y. - Hao, Z.P. - Shen, Q. - Wei, W. - Qian, G.R. - Sun, Y.H. **In: Chinese Journal of Catalysis**: the Journal of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and the Chinese Chemical Society. Amsterdam: Elsevier, 2016, Roč. 37, č. 6, [tlačená forma]. ISSN 1872-2067. ISSN (online) 0253-9837. - SCIE ; WOS CC, s. 898 - 907

2016 [01/12] / **USA** - Zhang, W. - Xie, J.Y. - Hou, W. - Liu, Y.Q. - Zhou, Y. - Wang, J. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2016, Roč. 8, č. 35, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 23122 - 23132

2015 [01/12] / **USA** - Xue, Z.W. - Shen, Y.S. - Shen, S.B. - Li, C.L. - Zhu, S.M. **In: Journal of industrial and engineering chemistry**. New York: Elsevier. Elsevier Science, 2015, Roč. 30, [tlačená forma] [online]. ISSN 1226-086X. ISSN (online) 1876-794X. - SCIE ; WOS CC, s. 98 - 105

2015 [01/12] / **USA** - Xie, P.F. - Luo, Y.J. - Ma, Z. - Huang, C.Y. - Miao, C.X. - Yue, Y.H. - Hua, W.M. - Gao, Z. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2015, Roč. 330, [tlačená forma] [online]. ISSN 0021-9517.

ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 311 - 322

2015 [01/12] / Mao, Y. - Wang, H.F. - Hu, P. **In: : International journal of quantum chemistry,** 2015, Roč. 115, č. 10. - SCIE ; WOS CC, s. 618 - 630

2015 [01/12] / Liu, X. - Yang, Z.Y. - Li, Y.P. - Zhang, F.Z. **In: Journal of Molecular Catalysis A-Chemical**, 2015, Roč. 396. - SCIE ; WOS CC, s. 181 - 187

2014 [01/12] / **GBR** - Ates, A. **In: Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 4, č. 7, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCIE ; WOS CC, s. 2031 - 2041

2014 [01/12] / **NLD** - Rutkowska, M. - Chmielarz, L. - Jablonska, M. - Van Oers, C.J. - Cool, P. **In: Journal of Porous Materials**. Dordrecht: Springer Nature. Springer, 2014, Roč. 21, č. 1, [tlačená forma] [online]. ISSN 1380-2224. ISSN (online) 1573-4854. - SCIE ; WOS CC, s. 91 - 98

2014 [01/12] / **USA** - Krivoruchenko, D.S. - Kucherov, A.V. - Telegina, N.S. - Bokarev, D.A. - Selvam, P. - Stakheev, A.Y. **In: Russian Chemical Bulletin**. [s.l.]: Springer Nature, 2014, Roč. 63, č. 2, [tlačená forma] [online]. ISSN 1066-5285. ISSN (online) 1573-9171. - SCIE ; WOS CC, s. 389 - 395

2014 [01/12] / Inger, M. - Wilk, M. - Saramok, M. - Grzybek, G. - Grodzka, A. - Stelmachowski, P. - Makowski, W. - Kotarba, A. - Sojka, Z. **In: Industrial and Engineering Chemistry Research**, 2014, Roč. 53, č. 25. - SCIE ; WOS CC, s. 10335 - 10342

2014 [01/12] / Horvath, B. - Sustek, M. - Skriniarova, J. - Omastova, M. - Dobrocka, E. - Hronec, M. **In: Applied Catalysis A-General**, 2014, Roč. 481. - SCIE ; WOS CC, s. 71 - 78

2014 [01/12] / **USA** - Moretti, G. - Fierro, G. - Ferraris, G. - Andreozzi, G.B. - Naticchioni, V. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2014, Roč. 318, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 1 - 13

2014 [01/12] / **NLD** - Ma, N. - Liu, X.F. - Zhang, B.Q. **In: Materials letters**. Amsterdam: Elsevier. North-Holland, 2014, Roč. 131, [tlačená forma] [online]. ISSN 0167-577X. ISSN (online) 1873-4979. - SCIE ; WOS CC, s. 67 - 70

2013 [01/12] / **USA** - Sirijaraensre, J. - Limtrakul, J. **In: Structural Chemistry**: an international journal concerned with energy, structure, and their relationships to chemical, physical, and biological properties: Computational and Experimental Studies of Chemical and Biological Systems. New York: Springer Nature, 2013, Roč. 24, č. 4, [tlačená forma]. ISSN 1040-0400. ISSN (online) 1572-9001. - SCIE ; WOS CC, s. 1307 - 1318

2013 [01/12] / Boron, P. - Chmielarz, L. - Gurgul, J. - Latka, K. - Shishido, T. - Krafft, J.M. - Dzwigaj, S. **In: Applied Catalysis B-environmental**, 2013, Roč. 138. - SCIE ; WOS CC, s. 434 - 445

2013 [01/12] / **USA** - Goldsmith, B.R. - Sanderson, E.D. - Bean, D. - Peters, B. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 138, č. 20, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 204105

2013 [01/12] / **USA** - Wang, J.Y. - Xia, H.A. - Ju, X.H. - Feng, Z.C. - Fan, F.T. - Li, C. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2013, Roč. 300, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 876 - 888

2013 [01/12] / **USA** - Wang, J.Y. - Li, G.N. - Ju, X.H. - Xia, H.A. - Fan, F.T. - Wang, J.H. - Feng, Z.C. - Li, C. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2013, Roč. 301, [tlačená forma] [online]. ISSN 0021-9517. ISSN

(online) 1090-2694. - SCIE ; WOS CC, s. 77 - 82

2013 [01/12] / **USA** - Yang, Z.W. - Yang, G. - Liu, X.C. - Han, X.W. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2013, Roč. 143, č. 3, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 260 - 266

2013 [01/12] / **NLD** - Dai, C.N. - Lei, Z.G. - Wang, Y.L. - Zhang, R.D. - Chen, B.H. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2013, Roč. 167, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 254 - 266

2013 [01/12] / Li, G.N. - Pidko, E.A. - van Santen, R.A. - Li, C. - Hensen, E.J.M. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 1. - SCIE ; WOS CC, s. 413 - 426

2013 [01/12] / **USA** - Li, G.N. - Pidko, E.A. - Filot, I.A.W. - van Santen, R.A. - Li, C. - Hensen, E.J.M. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2013, Roč. 308, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 386 - 397

2012 [01/12] / **USA** - Liu, N. - Zhang, R.D. - Chen, B.H. - Li, Y.P. - Li, Y.X. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2012, Roč. 294, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 99 - 112

2012 [01/12] / **NLD** - Obalova, L. - Jiratova, K. - Karaskova, K. - Chromcakova, Z. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2012, Roč. 191, č. 1, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 116 - 120

2012 [01/12] / **NLD** - Hussain, M. - Fino, D. - Russo, N. **In: Journal of Hazardous Materials**: Environmental Control, Risk Assessment, Impact and Management. Amsterdam: Elsevier, 2012, Roč. 211, [tlačená forma] [online]. ISSN 0304-3894. ISSN (online) 1873-3336. - SCIE ; WOS CC, s. 255 - 265

2012 [01/12] / Maier, S.M. - Jentys, A. - Janousch, M. - van Bokhoven, J.A. - Lercher, J.A. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 9. - SCIE ; WOS CC, s. 5846 - 5856

2011 [01/12] / **USA** - Li, G.N. - Pidko, E.A. - van Santen, R.A. - Feng, Z.C. - Li, C. - Hensen, E.J.M. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2011, Roč. 284, č. 2, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 194 - 206

2011 [01/12] / **NLD** - Maniak, G. - Stelmachowski, P. - Stanek, J.J. - Kotarba, A. - Sojka, Z. **In: Catalysis Communications**. Amsterdam: Elsevier, 2011, Roč. 15, č. 1, [tlačená forma]. ISSN 1566-7367. ISSN (online) 1873-3905. - SCIE ; WOS CC, s. 127 - 131

2011 [01/12] / **NLD** - Inger, M. - Kowalik, P. - Saramok, M. - Wilk, M. - Stelmachowski, P. - Maniak, G. - Granger, P. - Kotarba, A. - Sojka, Z. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2011, Roč. 176, č. 1, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 365 - 368

2011 [01/12] / Chu, Z.K. - Fu, G. - Guo, W.P. - Xu, X. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 30. - SCIE ; WOS CC, s. 14754 - 14761

2011 [01/12] / Liu, N. - Chen, B.H. - Li, Y.P. - Zhang, R.D. - Liang, X. - Li, Y.D. - Lei, Z.G. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 26. - SCIE ; WOS CC, s. 12883 - 12890

2011 [01/12] / van Eck, E.R.H. - Pieterse, J.A.Z. - Kentgens, A.P.M. **In: Solid State Nuclear Magnetic Resonance**:

Including research on Dynamic Nuclear Polarization, 2011, Roč. 39, č. 3-4, [tlačená forma]. ISSN 0926-2040. ISSN (online) 1527-3326. - SCIE ; WOS CC, s. 99 - 105

2011 [01/12] / **GBR** - Lv, Y.A. - Zhuang, G.L. - Wang, J.G. - Jia, Y.B. - Xie, Q. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2011, Roč. 13, č. 27, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 12472 - 12477

ADC_029: / Track, Anna M. (Autor) (9.091%) - Rissner, Ferdinand (Autor) (9.091%) - Heimel, Georg (Autor) (9.091%) - Romaner, Lorenz (Autor) (9.091%) - Kaefer, Daniel (Autor) (9.091%) - Bashir, Asif (Autor) (9.091%) - Rangger, Gerold M. (Autor) (9.091%) - Hofmann, Oliver T. (Autor) (9.091%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (9.091%) - Witte, Gregor (Autor) (9.091%) - Zojer, Egbert (Autor) (9.09%): **Simultaneously Understanding the Geometric and Electronic Structure of Anthraceneselenolate on Au(111): A Combined Theoretical and Experimental Study**. – CCC ; SCO ; WOS CC.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 114, č. 6 (2010), s. 2677-2684 [tlačená forma] [online]
Počet všetkých autorov: 11
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]

Kvartil Q:
2009, AIS - Nanoscience & nanotechnology - Q1; **2009, JIF** - Chemistry, physical - Q1; **2009, JIF** - Materials science, multidisciplinary - Q1; **2009, JIF** - Nanoscience & nanotechnology - Q1

Ohlasy (22):
2024 [01/20] / **FRA** - Balasundaram, N. - Sivalingam, K. - Kasu, Yamini - Polepaka, Sanjeeva - Hamza, Laeth H.J. **Investigation of prefabricated concrete slabs for interior and exterior walls** [elektronický dokument]. DOI 10.1051/e3sconf/202456411004 In: **E3S Web of Conferences**: International Conference on SDGs and Bibliometric Studies (ICoSBi 2024) . Les Ulis: Édition Diffusion Presse Sciences, 2024, art. no. 11004 [online]. ISSN 2555-0403. ISSN (online) 2267-1242. - SCO, s. art. no. 11004

2023 [01/20] / **USA** - Liu, Yangbiao - Notz, Sebastian - Lang, Heinrich - Zharnikov, Michael. **Pyrene-Terminated Self-Assembled Monolayers on Au Substrate: Molecular Organization and Charge Transport Properties** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c05201 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 38, s. 19290-19300 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 19290 - 19300

2021 [01/20] / **NLD** - Kang, H. - Seong, S. - Ito, E. - Isoshima, T. - Hara, M. - Yoon, H.J. - Noh, J. **Comparative study of structural order, thermal desorption behavior, and work function change of self-assembled monolayers of pentafluorobenzenethiols and tetrafluorobenzenethiols on Au(1 1 1)** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 555, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 149671

2021 [01/20] / **GBR** - Guo, Y. **Research on Design Method and Construction Key Points of Prefabricated Building Structure Combined with Machinery** In: **Journal of Physics: Conference Series**, 2021, Roč. 1744, č. 2. - SCO, s. Art. No. 022091

2020 [01/12] / Werner, P. - Wachter, T. - Asyuda, A. - Wiesner, A. - Kind, M. - Bolte, M. - Weinhardt, L. - Terfort, A. -

Zharnikov, M. **Electron Transfer Dynamics and Structural Effects in Benzonitrile Monolayers with Tuned Dipole Moments by Differently Positioned Fluorine Atoms** In: **ACS Applied Materials and Interfaces**, 2020, Roč. 12, č. 35. - SCO, s. 39859 - 39869

2019 [01/12] / **DEU** - Kang, X. - Zhu, M.Z. **In: Small**. Weinheim: John Wiley & Sons, 2019, Roč. 15, č. 43, [tlačená forma] [online]. ISSN 1613-6810. ISSN (online) 1613-6829. - SCIE ; WOS CC, s. Art. No. 1902703

2018 [01/12] / Saranya, G. - Senthilkumar, K. **In: Computational Chemistry Methodology in Structural Biology and Materials Sciences**, 2018. - SCIE ; WOS CC, s. 209 - 241

2018 [01/12] / Wachter, T. - Troster, A. - Hock, S. - Terfort, A. - Zharnikov, M. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 7. - SCIE ; WOS CC, s. 4105 - 4115

2017 [01/12] / **USA** - Liu, Z.F. - Egger, D.A. - Refaely-Abramson, S. - Kronik, L. - Neaton, J.B. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 092326

2015 [01/12] / **USA** - Ossowski, J. - Wachter, T. - Silies, L. - Kind, M. - Noworolska, A. - Blobner, F. - Gnatek, D. - Rysz, J. - Bolte, M. - Feulner, P. - Terfort, A. - Cyganik, P. - Zharnikov, M. **In: ACS Nano**. Washington: American Chemical Society, 2015, Roč. 9, č. 4, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 4508 - 4526

2015 [01/12] / **USA** - Egger, D.A. - Liu, Z.F. - Neaton, J.B. - Kronik, L. **In: Nano letters**. Washington: American Chemical Society, 2015, Roč. 15, č. 4, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 2448 - 2455

2014 [01/12] / **USA** - Hohman, J.N. - Thomas, J.C. - Zhao, Y.X. - Auluck, H. - Kim, M. - Vijselaar, W. - Kommeren, S. - Terfort, A. - Weiss, P.S. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2014, Roč. 136, č. 22, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 8110 - 8121

2014 [01/12] / **DEU** - Li, H. - Ratcliff, E.L. - Sigdel, A.K. - Giordano, A.J. - Marder, S.R. - Berry, J.J. - Bredas, J.L. **In: Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2014, Roč. 24, č. 23, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCIE ; WOS CC, s. 3593 - 3603

2013 [01/12] / Romashov, L.V. - Ananikov, V.P. **In: Chemistry-A European Journal**, 2013, Roč. 19, č. 52. - SCIE ; WOS CC, s. 17640 - 17660

2013 [01/12] / Kronik, L. - Morikawa, Y. **Understanding the Metal-Molecule Interface from First Principles** In: **Molecule-Metal Interface**. Oxford: Blackwell, 2013. - BKCI-S ; WOS CC, s. 51 - 88

2013 [01/12] / Cornil, D. - Cornil, J. **In: Journal of Electron Spectroscopy and Related Phenomena**, 2013, Roč. 189. ISSN 03682048. - SCIE ; WOS CC, s. 32 - 38

2012 [01/12] / **NLD** - Turchanin, A. - Golzhauser, A. **In: Progress in Surface Science**. Amsterdam: Elsevier, 2012, Roč. 87, č. 5-8. ISSN 0079-6816. ISSN (online) 1878-4240. - SCIE ; WOS CC, s. 108 - 162

2012 [01/12] / **DEU** - Hamoudi, H. - Kao, P. - Nefedov, A. - Allara, D.L. - Zharnikov, M. **In: Beilstein Journal of Nanotechnology**. Frankfurt nad Mohanom: Beilstein-Institut zur Förderung der Chemischen Wissenschaften, 2012, Roč. 3, [online]. ISSN (online) 2190-4286. - SCIE ; WOS CC, s. 12 - 24

2011 [01/12] / Aqua, T. - Cohen, H. - Sinai, O. - Frydman, V. - Bendikov, T. - Krepel, D. - Hod, O. - Kronik, L. - Naaman, R. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 50. - SCIE ; WOS CC, s. 24888 - 24892

2011 [01/12] / Aqua, T. - Cohen, H. - Sinai, O. - Frydman, V. - Bendikoy, T. - Krepel, D. - Hod, O. - Kronik, L. - Naaman, R. **In: Journal of Physical Chemistry C**, 2011, Roč. 115, č. 50. - SCIE ; WOS CC, s. 24888 - 24892

2011 [01/12] / **USA** - Biller, A. - Tamblyn, I. - Neaton, J.B. - Kronik, L. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2011, Roč. 135, č. 16, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 164706

2011 [01/12] / **USA** - Fatemi, V. - Kamenetska, M. - Neaton, J.B. - Venkataraman, L. **In: Nano letters**. Washington: American Chemical Society, 2011, Roč. 11, č. 5, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 1988 - 1992

2011 - spolu : 3

ADC_030: / Bučko, Tomáš (Autor) [UKOPRCFZ] (25%) - Tunega, Daniel (Autor) (25%) - Ángyán, János G. (Autor) (25%) - Hafner, Jürgen (Autor) (25%): **Ab Initio Study of Structure and Interconversion of Native Cellulose Phases**. – CCC ; SCO ; WOS CC.
In: *The Journal of Physical Chemistry A* [textový dokument (print)] [elektronický dokument] : Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. – Washington (USA) : American Chemical Society. – ISSN 1089-5639. – ISSN (online) 1520-5215. – Roč. 115, č. 135 (2011), s. 10097-10105 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,131 - 2011
SJR: 1,422 - 2011
CiteScore: 4,9 - 2011

Ohlasy (41):
2024 [01/20] / **USA** - Lee, Juhyung - Lee, Byeoksong - Park, Nae Man - Park, Ji Sang - Kang, Joongoo. **Molecular Surface Doping of Cellulose Nanocrystals: A High-Throughput Computational Study** [elektronický dokument]. DOI 10.1021/acs.chemmater.4c02045 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2024, Roč. 36, č. 23, art. no. 11421 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC, s. art. no. 11421

2024 [01/20] / **DEU** - Xia, Qian - Wang, Jun - Jiang, Jian - Hu, Anfu - Wu, Jian - Lu, Xinbo - Xiao, Weiqiang - Zhou, Guojun - Zhuang, Guilin. **Adsorption and diffusion properties of tobacco composition and additive: a multiscale theoretical study** [elektronický dokument]. DOI 10.1007/s00214-023-03084-8 In: **Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2024, Roč. 143, č. 1, art. no. 10 [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCO ; CCC ; WOS CC, s. art. no. 10

2022 [01/20] / **NLD** - Krichen, F. - Walha, S. - Abdelmouleh, M. **Hirshfeld surface analysis of the intermolecular interaction networks in cellulose Ialpha and Ibeta** [elektronický dokument] In: **Carbohydrate Research**: An International Journal of Molecular Glycoscience. Amsterdam: Elsevier, 2022, Roč. 518, [tlačená forma] [online]. ISSN 0008-6215. ISSN (online) 1873-426X. - SCO, s. Art. No. 108600

2022 [01/20] / **USA** - Chen, P. - Zhao, C. - Wang, H. - Li, Y. - Tan, G. - Shao, Z. - Nishiyama, Y. - Hu, T. - Wohlert, J. **Quantifying the Contribution of the Dispersion Interaction and Hydrogen Bonding to the Anisotropic Elastic Properties of Chitin and Chitosan** [elektronický dokument] In: **Biomacromolecules**. Washington: American Chemical Society, 2022, Roč. 23, č. 4, [tlačená forma] [online]. ISSN 1525-7797. ISSN (online) 1526-4602. - SCO, s. 1633 - 1642

2021 [01/20] / **GBR** - Chen, P. - Nishiyama, Y. - Wohlert, J. **Quantifying the influence of dispersion interactions on the elastic properties of crystalline cellulose** [elektronický dokument] In: **Cellulose**. London: Blackie Academic & Professional, 2021, Roč. 28, č. 17, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCO, s. 10777 - 10786

2021 [01/20] / **NLD** - Chi, Y. - Huang, B. - Saafi, M. - Fullwood, N. - Lambert, C. - Whale, E. - Hepworth, D. - Ye, J. **2D bio-based nanomaterial as a green route to amplify the formation of hydrate phases of cement composites: Atomistic simulations and analytical characterization** [elektronický dokument] In: **Construction and Building Materials**: An international journal dedicated to the investigation and innovative use of materials in construction and repair. Amsterdam: Elsevier, 2021, Roč. 299, [tlačená forma] [online]. ISSN 0950-0618. ISSN (online) 1879-0526. - SCO, s. Art. No. 123867

2020 [01/12] / **GBR** - Dumitrica, T. **In: Carbohydrate polymers**. Oxford: Elsevier, 2020, Roč. 230, [tlačená forma] [online]. ISSN 0144-8617. ISSN (online) 1879-1344. - SCIE ; WOS CC, s. Art. No. 115624

2020 [01/12] / **USA** - Qiao, Q. - Li, X.B. - Huang, L.L. **In: Journal of Chemical and Engineering Data**: the ACS journal for data. Washington DC: American Chemical Society, 2020, Roč. 65, č. 2, [tlačená forma] [online]. ISSN 0021-9568. ISSN (online) 1520-5134. - SCIE ; WOS CC, s. 360 - 372

2020 [01/12] / **USA** - Zhang, H. - Guo, Y. - Bourell, D.L. - Meng, D. **Effects of ingredient proportions on the performance of a-Cellulose/PLA mixtures used for laser sintering** [elektronický dokument] In: **BioResources**. Raleigh: NC State University, 2020, Roč. 15, č. 3, [online]. ISSN (online) 1930-2126. - SCO, s. 5886 - 5898

2020 [01/12] / **GBR** - Lousada, C.M. **Wood cellulose as a hydrogen storage material** [elektronický dokument] In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2020, Roč. 45, č. 29, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO, s. 14907 - 14914

2020 [01/12] / Angyan, J. - Dobson, J. - Jansen, G. - Gould, T. **London Dispersion Forces in Molecules, Solids and Nano-structures: An Introduction to Physical Models and Computational Methods** In: **RSC Theoretical and Computational Chemistry Series**. London: Royal Society of Chemistry, 2020. - SCO, s. 1 - 434

2019 [01/12] / **GBR** - Makarem, M. - Lee, C.M. - Kafle, K. - Huang, S.X. - Chae, I. - Yang, H. - Kubicki, J.D. - Kim, S.H. **In: Cellulose**. London: Blackie Academic & Professional, 2019, Roč. 26, č. 1, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 35 - 79

2018 [01/12] / **GBR** - Dai, Y.H. - Zhong, Z.S. - Gong, S.S. **In: Materials Research Express**. Bristol: Institute of Physics. IOP Publishing, 2018, Roč. 5, č. 6, [online]. ISSN (online) 2053-1591. - SCIE ; WOS CC, s. Art. No. 065904

2018 [01/12] / Lousada, C.M. - Sophonrat, N. - Yang, W.H. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 23. - SCIE ; WOS CC, s. 12168 - 12176

2018 [01/12] / **GBR** - Oehme, D.P. - Yang, H. - Kubicki, J.D. **In: Cellulose**. London: Blackie Academic & Professional, 2018, Roč. 25, č. 7, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 3755 - 3777

2018 [01/12] / **GBR** - Chen, P. - Ogawa, Y. - Nishiyama, Y. - Ismail, A.E. - Mazeau, K. **In: Cellulose**. London: Blackie

Academic & Professional, 2018, Roč. 25, č. 8, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 4345 - 4355

2018 [01/12] / **DEU** - Kubicki, J.D. - Yang, H. - Sawada, D. - O'Neill, H. - Oehme, D. - Cosgrove, D. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2018, Roč. 8, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 13983

2017 [01/12] / Feng, Q.G. - Noumbissi, R. - Biswas, K. - Koizumi, H. **In: : International journal of quantum chemistry,** 2017, Roč. 117, č. 10. - SCIE ; WOS CC, s. Art. No. 25357

2017 [01/12] / **NLD** - Hayakawa, D. - Nishiyama, Y. - Mazeau, K. - Ueda, K. **In: Carbohydrate Research**: An International Journal of Molecular Glycoscience. Amsterdam: Elsevier, 2017, Roč. 449, [tlačená forma] [online]. ISSN 0008-6215. ISSN (online) 1873-426X. - SCIE ; WOS CC, s. 103 - 113

2016 [01/12] / **DEU** - Navarrete-Lopez, A.M. - San-Roman, M.L. - Zicovich-Wilson, C.M. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2016, Roč. 135, č. 5, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 136

2016 [01/12] / **USA** - Deringer, V.L. - Englert, U. - Dronskowski, R. **In: Biomacromolecules**. Washington: American Chemical Society, 2016, Roč. 17, č. 3, [tlačená forma] [online]. ISSN 1525-7797. ISSN (online) 1526-4602. - SCIE ; WOS CC, s. 996 - 1003

2016 [01/12] / Zhu, Q. - Oganov, A.R. - Zeng, Q.F. - Zhou, X.F. **Structure prediction and its applications in computational materials design** In: **Chemical Modelling**. Cambridge: Royal Soc. Chemistry, 2016. - BKCI-S ; WOS CC, s. 219 - 248

2015 [01/12] / **USA** - Lopez, C.A. - Bellesia, G. - Redondo, A. - Langan, P. - Chundawat, S.P.S. - Dale, B.E. - Marrink, S.J. - Gnanakaran, S. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2015, Roč. 119, č. 2, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 465 - 473

2015 [01/12] / Thiyam, P. - Persson, C. - Parsons, D.F. - Huang, D. - Buhmann, S.Y. - Bostrom, M. **In: Colloids and Surfaces A-Physicochemical and Engineering Aspects**, 2015, Roč. 470. - SCIE ; WOS CC, s. 316 - 321

2015 [01/12] / **NLD** - Dri, F.L. - Wu, X.W. - Moon, R.J. - Martini, A. - Zavattieri, P.D. **In: Computational Materials Science**. Amsterdam: Elsevier, 2015, Roč. 109, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 330 - 340

2015 [01/12] / **USA** - Zhu, C.T. - Dobryden, I. - Ryden, J. - Oberg, S. - Holmgren, A. - Mathew, A.P. **In: Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2015, Roč. 31, č. 45, [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCIE ; WOS CC, s. 12390 - 12400

2015 [01/12] / **NLD** - Ishikawa, T. - Hayakawa, D. - Miyamoto, H. - Ozawa, M. - Ozawa, T. - Ueda, K. **In: Carbohydrate Research**: An International Journal of Molecular Glycoscience. Amsterdam: Elsevier, 2015, Roč. 417, [tlačená forma] [online]. ISSN 0008-6215. ISSN (online) 1873-426X. - SCIE ; WOS CC, s. 72 - 77

2015 [01/12] / **USA** - Lee, C.M. - Kubicki, J.D. - Fan, B.X. - Zhong, L.H. - Jarvis, M.C. - Kim, S.H. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2015, Roč. 119, č. 49, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 15138 - 15149

2014 [01/12] / **GBR** - Dri, F.L. - Shang, S.L. - Hector, L.G. - Saxe, P. - Liu, Z.K. - Moon, R.J. - Zavattieri, P.D. **In: Modelling and simulation in materials science and engineering**. Bristol: Institute of Physics. IOP Publishing, 2014, Roč. 22, č. 8, [online] [tlačená forma]. ISSN 0965-0393. ISSN (online) 1361-651X. - SCIE ; WOS CC, s. Art. No. 085012

2014 [01/12] / **USA** - Zhu, Q. - Sharma, V. - Oganov, A.R. - Ramprasad, R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 141, č. 15, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 154102

2014 [01/12] / **GBR** - Chen, P. - Nishiyama, Y. - Mazeau, K. **In: Cellulose**. London: Blackie Academic & Professional, 2014, Roč. 21, č. 4, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 2207 - 2217

2014 [01/12] / **NLD** - Kobayashi, T. - Hayakawa, D. - Khishigjargal, T. - Ueda, K. **In: Carbohydrate Research**: An International Journal of Molecular Glycoscience. Amsterdam: Elsevier, 2014, Roč. 388, [tlačená forma] [online]. ISSN 0008-6215. ISSN (online) 1873-426X. - SCIE ; WOS CC, s. 61 - 66

2014 [01/12] / **GBR** - Kubicki, J.D. - Watts, H.D. - Zhao, Z. - Zhong, L.H. **In: Cellulose**. London: Blackie Academic & Professional, 2014, Roč. 21, č. 2, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 909 - 926

2013 [01/12] / **GBR** - Dri, F.L. - Hector, L.G. - Moon, R.J. - Zavattieri, P.D. **In: Cellulose**. London: Blackie Academic & Professional, 2013, Roč. 20, č. 6, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 2703 - 2718

2013 [01/12] / **USA** - Lee, C.M. - Mohamed, N.M.A. - Watts, H.D. - Kubicki, J.D. - Kim, S.H. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2013, Roč. 117, č. 22, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 6681 - 6692

2013 [01/12] / **GBR** - Kubicki, J.D. - Mohamed, M.N.A. - Watts, H.D. **In: Cellulose**. London: Blackie Academic & Professional, 2013, Roč. 20, č. 1, [tlačená forma] [online]. ISSN 0969-0239. ISSN (online) 1572-882X. - SCIE ; WOS CC, s. 9 - 23

2013 [01/12] / Bostrom, M. - Huang, D. - Yang, W.H. - Persson, C. - Sernelius, B.E. **In: EPL**, 2013, Roč. 104, č. 6. - SCIE ; WOS CC, s. Art. No. 63003

2013 [01/12] / Brumm, P.J. **In: Biofuels-Uk**, 2013, Roč. 4, č. 6. - SCIE ; WOS CC, s. 669 - 681

2012 [01/12] / **USA** - Bellesia, G. - Chundawat, S.P.S. - Langan, P. - Redondo, A. - Dale, B.E. - Gnanakaran, S. **In: Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2012, Roč. 116, č. 28, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCIE ; WOS CC, s. 8031 - 8037

2012 [01/12] / Breuer, T. - Celik, M.A. - Jakob, P. - Tonner, R. - Witte, G. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 27. - SCIE ; WOS CC, s. 14491 - 14503

2011 [01/12] / Parthasarathi, R. - Bellesia, G. - Chundawat, S.P.S. - Dale, B.E. - Langan, P. - Gnanakaran, S. **In: Journal of Physical Chemistry A**, 2011, Roč. 115, č. 49. - SCIE ; WOS CC, s. 14191 - 14202

ADC_031: / Benco, Ľubomír (Autor) (34%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (33%) - Hafner, Jürgen (Autor) (33%): **Dehydrogenation of propane over Zn-MOR. Static and dynamic reaction energy diagram**. – CCC ; SCO ; WOS CC.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – Roč. 277, č. 1 (2011), s. 104-116 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 2,224 - 2011
SJR: 3,092 - 2011
CiteScore: 10 - 2011

Ohlasy (40):

2023 [01/20] / **USA** - Ji, Xiangyang - Ma, Yue - Sun, Xiao - Song, Shaojia - Yang, Kun - Huang, Weixin - Xu, Chunming - Feng, Bohan - Liu, Jian - Song, Weiyu. **Photothermal Propane Dehydrogenation Catalyzed by VOx-Doped TiO2 Nanoparticles** [elektronický dokument]. DOI 10.1021/acsanm.3c00794 In: **ACS applied nano materials**. Washington: American Chemical Society, 2023, Roč. 6, č. 7, s. 6354-6364 [online]. ISSN (online) 2574-0970. - SCO ; CCC ; WOS CC, s. 6354 - 6364

2023 [01/20] / **USA** - Berger, Fabian - Rybicki, Marcin - Sauer, Joachim. **Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites** [elektronický dokument]. DOI 10.1021/acscatal.2c05493 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 3, s. 2011-2024 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 2011 - 2024

2022 [01/20] / **USA** - Rybicki, Marcin - Sillar, Kaido - Sauer, Joachim. **Dual-Site Model for Ab Initio Calculations of Gibbs Free Energies and Enthalpies of Adsorption: Methane in Zeolite Mobile Five (H-MFI)** [elektronický dokument]. DOI 10.1021/acs.jpclett.2c03302 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2022, Roč. 13, č. 50, s. 11595-11600 [online]. ISSN (online) 1948-7185. - SCO, s. 11595 - 11600

2022 [01/20] / **USA** - Ma, R. - Gao, J. - Kou, J. - Dean, D.P. - Breckner, C.J. - Liang, K. - Zhou, B. - Miller, J.T. - Zou, G. **Insights into the Nature of Selective Nickel Sites on Ni/Al2O3Catalysts for Propane Dehydrogenation** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 20, [online]. ISSN (online) 2155-5435. - SCO, s. 12607 - 12616

2022 [01/20] / **USA** - De Wispelaere, K. - Plessow, P.N. - Studt, F. **Toward Computing Accurate Free Energies in Heterogeneous Catalysis: a Case Study for Adsorbed Isobutene in H-ZSM-5** [elektronický dokument] In: **ACS Physical Chemistry Au**. Washington: American Chemical Society, 2022, Roč. 2, č. 5, [online]. ISSN (online) 2694-2445. - SCO, s. 399 - 406

2022 [01/20] / **USA** - Song, S. - Yang, K. - Zhang, P. - Wu, Z. - Li, J. - Su, H. - Dai, S. - Xu, C. - Li, Z. - Liu, J. - Song, W. **Silicalite-1 Stabilizes Zn-Hydride Species for Efficient Propane Dehydrogenation** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5997 - 6006

2021 [01/20] / **USA** - Van der Mynsbrugge, J. - Bell, A.T. **Challenges for the theoretical description of the mechanism and kinetics of reactions catalyzed by zeolites** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 404, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 832 - 849

2021 [01/20] / **NLD** - Liu, Y. - Zhang, G. - Wang, J. - Zhu, J. - Zhang, X. - Miller, J.T. - Song, C. - Guo, X. **Promoting propane dehydrogenation with CO2 over Ga2O3/SiO2 by eliminating Ga-hydrides** [elektronický dokument] In: **Chinese Journal of Catalysis**: the Journal of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and

the Chinese Chemical Society. Amsterdam: Elsevier, 2021, Roč. 42, č. 12, [tlačená forma]. ISSN 1872-2067. ISSN (online) 0253-9837. - SCO, s. 2225 - 2233

2021 [01/20] / **USA** - Liu, J. - Liu, Y. - Liu, H. - Fu, Y. - Chen, Z. - Zhu, W. **Silicalite-1 Supported ZnO as an Efficient Catalyst for Direct Propane Dehydrogenation** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2021, Roč. 13, č. 22, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 4780 - 4786

2021 [01/20] / **CHN** - Tian, H.-F. - He, H.-H. - Liao, J.-K. - Zha, F. - Guo, X.-J. - Tang, X.-H. **Catalytic performance of different zeolites for propane and CO2coupling to propylene** In: **Ranliao Huaxue Xuebao/Journal of Fuel Chemistry and Technology**, 2021, Roč. 49, č. 4. ISSN 02532409. - SCO, s. 495 - 503

2021 [01/20] / **GBR** - Du, Y.-J. - Hu, W.-D. - Wang, C.-M. - Zhou, J. - Yang, G. - Wang, Y.-D. - Yang, W.-M. **First-principles microkinetic analysis of Lewis acid sites in Zn-ZSM-5 for alkane dehydrogenation and its implication to methanol-to-aromatics conversion** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 6, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 2031 - 2046

2020 [01/12] / **NLD** - Wang, Y.-L. - Wang, X.-X. - Zhu, Y.-A. - Zhu, K.-K. - Chen, D. - Zhou, X.-G. **Shape selectivity in acidic zeolite catalyzed 2-pentene skeletal isomerization from first principles** [elektronický dokument] In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 347, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO, s. 115 - 123

2020 [01/12] / Cabana, N.C. - Serra, R.R. - Boix, A.V. - Bolcatto, P.G. **Geometries and Interaction Energies of Toluene on CsxNa1-xMordenite** In: **Physica Status Solidi (B) Basic Research**, 2020, Roč. 257, č. 9. - SCO, s. Art. No. 2000131

2019 [01/12] / **USA** - Chen, C. - Hu, Z.P. - Ren, J.T. - Zhang, S.M. - Wang, Z. - Yuan, Z.Y. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 2, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 868 - 877

2019 [01/12] / Chen, C. - Sun, M.L. - Hu, Z.P. - Ren, J.T. - Zhang, S.M. - Yuan, Z.Y. **In: Catalysis Science & Technology**, 2019, Roč. 9, č. 8. - SCIE ; WOS CC, s. 1979 - 1988

2019 [01/12] / **USA** - Bailleul, S. - Rogge, S.M.J. - Vanduyfhuys, L. - Van Speybroeck, V. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 16, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 3993 - 4010

2018 [01/12] / Van der Mynsbrugge, J. - Janda, A. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ChemPhysChem**, 2018, Roč. 19, č. 4. - SCIE ; WOS CC, s. 341 - 358

2018 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Vanduyfhuys, L. - Demuynck, R. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 10, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 189 - 228

2017 [01/12] / Chibani, S. - Medlej, I. - Lebegue, S. - Angyan, J.G. - Cantrel, L. - Badawi, M. **In: ChemPhysChem**, 2017, Roč. 18, č. 12. - SCIE ; WOS CC, s. 1642 - 1652

2016 [01/12] / De Wispelaere, K. - Bailleul, S. - Van Speybroeck, V. **In: Catalysis Science & Technology**, 2016, Roč. 6, č. 8. - SCIE ; WOS CC, s. 2686 - 2705

2016 [01/12] / **USA** - De Wispelaere, K. - Wondergem, C.S. - Ensing, B. - Hemelsoet, K. - Meijer, E.J. - Weckhuysen, B.M. - Van Speybroeck, V. - Ruiz-Martinez, J. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 3, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1991 - 2002

2016 [01/12] / **USA** - Ghashghaee, M. - Ghambarian, M. - Azizi, Z. **In: Structural Chemistry**: an international journal concerned with energy, structure, and their relationships to chemical, physical, and biological properties: Computational and Experimental Studies of Chemical and Biological Systems. New York: Springer Nature, 2016, Roč. 27, č. 2, [tlačená forma]. ISSN 1040-0400. ISSN (online) 1572-9001. - SCIE ; WOS CC, s. 467 - 475

2016 [01/12] / **USA** - Coperet, C. - Estes, D.P. - Larmier, K. - Searles, K. **In: Chemical Reviews**. Washington: American Chemical Society, 2016, Roč. 116, č. 15, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 8463 - 8505

2016 [01/12] / Conte, M. - Hippler, M. **In: Journal of Physical Chemistry A**, 2016, Roč. 120, č. 34. - SCIE ; WOS CC, s. 6677 - 6687

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2015 [01/12] / **CHE** - Larsson, R. **In: Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2015, Roč. 20, č. 2, [online]. ISSN (online) 1420-3049. - SCIE ; WOS CC, s. 2529 - 2535

2015 [01/12] / **NLD** - Sun, Y.N. - Gao, Y.N. - Wu, Y.M. - Shan, H.H. - Wang, G.W. - Li, C.Y. **In: Catalysis Communications**. Amsterdam: Elsevier, 2015, Roč. 60, [tlačená forma]. ISSN 1566-7367. ISSN (online) 1873-3905. - SCIE ; WOS CC, s. 42 - 45

2015 [01/12] / De Wispelaere, K. - Ensing, B. - Ghysels, A. - Meijer, E.J. - Van Speybroeck, V. **In: Chemistry-A European Journal**, 2015, Roč. 21, č. 26. - SCIE ; WOS CC, s. 9385 - 9396

2015 [01/12] / **USA** - Erichsen, M.W. - De Wispelaere, K. - Hemelsoet, K. - Moors, S.L.C. - Deconinck, T. - Waroquier, M. - Svelle, S. - Van Speybroeck, V. - Olsbye, U. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2015, Roč. 328, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 186 - 196

2015 [01/12] / Itadani, A. - Sogawa, Y. - Oda, A. - Ohkubo, T. - Yumura, T. - Kobayashi, H. - Sato, M. - Kuroda, Y. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 37. - SCIE ; WOS CC, s. 21483 - 21496

2014 [01/12] / **GBR** - Xing, B. - Wang, G.C. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 6, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 2621 - 2629

2014 [01/12] / **GBR** - Mao, Y.M. - Zhou, Y. - Wen, H.M. - Xie, J.Y. - Zhang, W. - Wang, J. **In: New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2014, Roč. 38, č. 7, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCIE ; WOS CC, s. 3295 - 3301

2014 [01/12] / **GBR** - Van Speybroeck, V. - De Wispelaere, K. - Van der Mynsbrugge, J. - Vandichel, M. - Hemelsoet, K. - Waroquier, M. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 43, č. 21, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7326 - 7357

2013 [01/12] / Oda, A. - Torigoe, H. - Itadani, A. - Ohkubo, T. - Yumura, T. - Kobayashi, H. - Kuroda, Y. **In: Journal of**

Physical Chemistry C, 2013, Roč. 117, č. 38. - SCIE ; WOS CC, s. 19525 - 19534

2013 [01/12] / **USA** - Moors, S.L.C. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 11, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2556 - 2567

2013 [01/12] / Patrylak, K.I. - Patrylak, L.K. - Repetskyi, I.A. **In: Theoretical and Experimental Chemistry**, 2013, Roč. 49, č. 3. - SCIE ; WOS CC, s. 143 - 157

2013 [01/12] / Hemelsoet, K. - Van der Mynsbrugge, J. - De Wispelaere, K. - Waroquier, M. - Van Speybroeck, V. **In: ChemPhysChem**, 2013, Roč. 14, č. 8. - SCIE ; WOS CC, s. 1526 - 1545

2013 [01/12] / **CHN** - Wang, C. - Wei, Z.Z. - Lu, Y.K. - Xing, B. - Wang, G.C. **In: Acta Physico-Chimica Sinica**. Peking: Peking University Press, 2013, Roč. 29, č. 4. ISSN 1000-6818. ISSN (online) 1872-1508. - SCIE ; WOS CC, s. 723 - 730

2013 [01/12] / **GBR** - Kling, D.P. - Machado, E.S.A. - Chagas, H.C. - dos Santos, A.P.A. - Rosenbach, N. - Carneiro, J.W. - Mota, C.J.A. **In: Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 49, č. 40, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCIE ; WOS CC, s. 4480 - 4482

2012 [01/12] / **CHE** - Li, F.M. - Yang, H.Q. - Ju, T.Y. - Li, X.Y. - Hu, C.W. **In: International journal of molecular sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2012, Roč. 13, č. 7, [online] [tlačená forma]. ISSN 1661-6596. ISSN (online) 1422-0067. - SCIE ; WOS CC, s. 9278 - 9297

ADC_032: / Bučko, Tomáš (Autor) [UKOPRCFZ] (25%) - Benco, Ľubomír (Autor) (25%) - Hafner, Jürgen (Autor) (25%) - Ángyán, János G. (Autor) (25%): **Monomolecular cracking of propane over acidic chabazite: An ab initio molecular dynamics and transition path sampling study**. – CCC ; SCO ; WOS CC.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – Roč. 279, č. 1 (2011), s. 220-228 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 2,224 - 2011
SJR: 3,092 - 2011
CiteScore: 10 - 2011

Ohlasy (83):
2025 [01/20] / **NLD** - Yu, Lingjing - Nie, Hong - Yang, Ping - Wang, Linmeng - Feng, Shihao - Gao, Hongyi - Wang, Ge. **Recent advances in hydrotreating and hydrocracking catalysts for the preparation of light aromatics: Influencing factors, catalytic mechanisms and performance relationship descriptors** [elektronický dokument]. DOI 10.1016/j.ccr.2025.216444 In: **Coordination Chemistry Reviews**. Amsterdam: Elsevier, 2025, Roč. 529, art. no. 216444 [tlačená forma] [online]. ISSN 0010-8545. ISSN (online) 1873-3840. - SCO ; CCC ; WOS CC, s. art. no. 216444

2025 [01/20] / **GBR** - Fedik, Nikita - Li, Wei - Lubbers, Nicholas - Nebgen, Benjamin - Tretiak, Sergei - Li, Ying Wai. **Challenges and opportunities for machine learning potentials in transition path sampling: alanine dipeptide and azobenzene studies** [elektronický dokument]. DOI 10.1039/d4dd00265b In: **Digital Discovery**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 4, č. 5, s. 1158-1175. ISSN (online) 2635098X. - SCO ; WOS CC, s. 1158 - 1175

2025 [01/20] / **NLD** - Zhang, Nan - Ma, Jinghong - Li, Ruifeng - Han, Peide - Jiao, Haijun. **Al-distribution and acidity of HZSM-5: Theory and practice** [elektronický dokument]. DOI 10.1016/j.mcat.2025.114865 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2025, Roč. 574, art. no. 114865 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO ; CCC ; WOS CC, s. art. no. 114865

2025 [01/20] / **DEU** - Verma, Rahul - Sahoo, Sudhir K. **Recent Advances and Challenges in Modeling Catalytic Reactions in Zeolites** [elektronický dokument]. DOI 10.1002/slct.202501858 In: **Chemistry Select**. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 10, č. 41, art. no. e01858 [online]. ISSN (online) 2365-6549. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. e01858

2024 [01/20] / **USA** - Sauer, Joachim. **The future of computational catalysis** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115482 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 433, art. no. 115482 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. art. no. 115482

2024 [01/20] / **NLD** - Peng, Yajing - Liu, Weina - Ma, Bowen - Zhang, Jinshun - Liu, Yuhui - Su, Yan - Yang, Yanqiang. **Double-proton transfer triggering mechanism of nitromethane caused by intermolecular hydrogen bonding at low temperature** [elektronický dokument]. DOI 10.1016/j.arabjc.2023.105579 In: **Arabian Journal of Chemistry**. Amsterdam: Elsevier, 2024, Roč. 17, č. 2, art. no. 105579 [tlačená forma] [online]. ISSN 1878-5352. ISSN (online) 1878-5379. - SCO ; WOS CC, s. art. no. 105579

2023 [01/20] / **RUS** - Nazarova, Galina Y. - Ivashkina, Elena N. - Maltsev, Vladislav V. **Calculation of thermodynamic and kinetic parameters of catalytic cracking reactions on lewis and bronsted acid sites** [elektronický dokument]. DOI 10.18799/24131830/2023/7/4220 In: **Bulletin of the Tomsk Polytechnic University**: Geo assets engineering. Tomsk: Tomskij Politechničeskij Universitet, 2023, Roč. 334, č. 7, s. 214-225 [tlačená forma] [online]. ISSN 2500-1019. ISSN (online) 2413-1830. - SCO ; WOS CC, s. 214 - 225

2023 [01/20] / **NLD** - Bocus, Massimo - Neale, Samuel E. - Cnudde, Pieter - Van Speybroeck, Véronique. **Dynamic evolution of catalytic active sites within zeolite catalysis**. DOI 10.1016/B978-0-12-823144-9.00012-1 In: **Comprehensive Inorganic Chemistry III, Third Edition**. Amsterdam: Elsevier. Elsevier Science, 2023, s. 165-200. ISBN 9780128231531. - SCO, s. 165 - 200

2023 [01/20] / **USA** - Berger, Fabian - Rybicki, Marcin - Sauer, Joachim. **Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites** [elektronický dokument]. DOI 10.1021/acscatal.2c05493 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 3, s. 2011-2024 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 2011 - 2024

2023 [01/20] / **GBR** - Ghojavand, Sajjad - Dib, Eddy - Rey, Jérôme - Daouli, Ayoub - Clatworthy, Edwin B. - Bazin, Philippe - Ruaux, Valérie - Badawi, Michael - Mintova, Svetlana. **Interplay between alkali-metal cations and silanol sites in nanosized CHA zeolite and implications for CO2 adsorption** [elektronický dokument]. DOI 10.1038/s42004-023-00918-1 In: **Communications chemistry**. [London]: Springer Nature, 2023, Roč. 6, č. 1, art. no. 134 [online]. ISSN (online) 2399-3669. - SCO ; CCC ; WOS CC, s. art. no. 134

2023 [01/20] / **USA** - Daouli, Ayoub - Rey, Jérôme - Lahrar, El Hassane - Valtchev, Valentin - Badawi, Michael - Guillet-Nicolas, Rémy. **Ab Initio Screening of Divalent Cations for CH4, CO2, H2, and N2 Separations in Chabazite Zeolite** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c01882 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 45, s. 15962-15973 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 15962 - 15973

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s.

6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Wang, Mengen - Boscoboinik, Jorge Anibal - Lu, Deyu. **First-Principles Study of n-Butane Monomolecular Cracking and Dehydrogenation on Two-Dimensional-Zeolite Model Systems: Reaction Mechanisms and Effects of Spatial Confinement** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c01403 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 28, s. 13593-13600 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 13593 - 13600

2023 [01/20] / **GBR** - Cnudde, Pieter - Waroquier, Michel - Van Speybroeck, Veronique. **Universal descriptors for zeolite topology and acidity to predict the stability of butene cracking intermediates** [elektronický dokument]. DOI 10.1039/d3cy00642e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 16, s. 4857-4872 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4857 - 4872

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **GBR** - Hutton, Daniel J. - Göltl, Florian. **Free and internal energies for the adsorption of short alkanes into the zeolite SSZ-13 from ab initio molecular dynamics simulations** [elektronický dokument]. DOI 10.1039/d3cp02523c In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 39, s. 26604-26612 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 26604 - 26612

2023 [01/20] / **GBR** - Aziz, Muhammad Tariq - Naqvi, Syed Ali Raza - Janjua, Muhammad Ramzan Saeed Ashraf - Alam, Manawwer - Gill, Waqas Amber. **Exploring the adsorption behavior of molecular hydrogen on CHA-zeolite by comparing the performance of various force field methods** [elektronický dokument]. DOI 10.1039/d3ra04262f In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 44, s. 30937-30950 [online]. ISSN (online) 2046-2069. - SCO ; CCC ; WOS CC, s. 30937 - 30950

2023 [01/20] / **DEU** - Fischer, Michael. **Adsorption of Carbamazepine in All-Silica Zeolites Studied with Density Functional Theory Calculations**** [elektronický dokument]. DOI 10.1002/cphc.202300022 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2023, Roč. 24, č. 9, art. no. e202300022 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - van Stanten, Rutger A. **Mechanisms in Heterogeneous Catalysis** [textový dokument (print)] [elektronický dokument] . New Jersey: World Scientific Publishing, 2023. 1. vyd. ISBN [9781800614017, 9781800614000]. - SCO, s. 1 - 718

2022 [01/20] / **USA** - Rybicki, Marcin - Sillar, Kaido - Sauer, Joachim. **Dual-Site Model for Ab Initio Calculations of Gibbs Free Energies and Enthalpies of Adsorption: Methane in Zeolite Mobile Five (H-MFI)** [elektronický dokument]. DOI 10.1021/acs.jpclett.2c03302 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2022, Roč. 13, č. 50, s. 11595-11600 [online]. ISSN (online) 1948-7185. - SCO, s. 11595 - 11600

2022 [01/20] / **USA** - Lin, L.-C. **Computational Study of Alkane Adsorption in Bronsted Acid Zeolites for More Efficient Alkane Cracking** [elektronický dokument] In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2022, Roč. 38, č. 25, [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO, s. 7665 - 7677

2022 [01/20] / **USA** - Alaithan, Z.A. - Mallia, G. - Harrison, N.M. **Monomolecular Cracking of Propane: Effect of Zeolite Confinement and Acidity** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2022, Roč. 7, č. 9, [online]. ISSN (online) 2470-1343. - SCO, s. 7531 - 7540

2022 [01/20] / **USA** - Ma, S. - Liu, Z.-P. **The Role of Zeolite Framework in Zeolite Stability and Catalysis from Recent Atomic Simulation** [elektronický dokument] In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, č. 1-4, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 59 - 68

2021 [01/20] / **USA** - Galimberti, D.R. - Sauer, J. **Chemically Accurate Vibrational Free Energies of Adsorption from Density Functional Theory Molecular Dynamics: Alkanes in Zeolites** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 9, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 5849 - 5862

2021 [01/20] / **USA** - Gutierrez-Acebo, E. - Rey, J. - Bouchy, C. - Schuurman, Y. - Chizallet, C. **Ethylcyclohexane Hydroconversion in EU-1 Zeolite: DFT-based Microkinetic Modeling Reveals the Nature of the Kinetically Relevant Intermediates** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2021, Roč. 13, č. 15, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 3434 - 3442

2021 [01/20] / **USA** - Li, X. - Pei, C. - Gong, J. **Shale gas revolution: Catalytic conversion of C1-C3 light alkanes to value-added chemicals** [elektronický dokument] In: **Chem**. Cambridge, MA: Elsevier. Cell Press, 2021, Roč. 7, č. 7, [tlačená forma] [online]. ISSN 2451-9308. ISSN (online) 2451-9294. - SCO, s. 1755 - 1801

2021 [01/20] / **USA** - Berger, F. - Rybicki, M. - Sauer, J. **Adsorption and cracking of propane by zeolites of different pore size** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 395, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 117 - 128

2020 [01/12] / **USA** - Zhang, N. - Ma, J. - Li, R. - Jiao, H. **Hydrocracking of Fused Aromatic Hydrocarbons Catalyzed by Al-Substituted HZSM-5 - A Case Study of 9,10-Dihydroanthracene** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 16, [online]. ISSN (online) 2155-5435. - SCO, s. 9215 - 9226

2020 [01/12] / **USA** - Fecik, M. - Plessow, P.N. - Studt, F. **A systematic study of methylation from benzene to hexamethylbenzene in H-SSZ-13 using density functional theory and ab initio calculations** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 15, [online]. ISSN (online) 2155-5435. - SCO, s. 8916 - 8925

2020 [01/12] / **USA** - Nazarova, G. - Ivashkina, E. - Ivanchina, E. - Oreshina, A. - Vymyatnin, E. - Burumbaeva, G. **Integrated mathematical modeling of catalytic cracking and zeolite-containing catalyst oxidative regeneration** [elektronický dokument] In: **Petroleum science and technology**. New York: Taylor & Francis Group. Marcel Dekker, 2020, Roč. 38, č. 12, [tlačená forma] [online]. ISSN 1091-6466. ISSN (online) 1532-2459. - SCO, s. 754 - 762

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2020 [01/12] / Angyan, J. - Dobson, J. - Jansen, G. - Gould, T. **London Dispersion Forces in Molecules, Solids and Nano-structures: An Introduction to Physical Models and Computational Methods** In: **RSC Theoretical and Computational Chemistry Series**. London: Royal Society of Chemistry, 2020. - SCO, s. 1 - 434

2019 [01/12] / **USA** - Li, G.N. - Pidko, E.A. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano-

Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 134 - 156

2019 [01/12] / **USA** - Gutierrez-Acebo, E. - Rey, J. - Bouchy, C. - Schuurman, Y. - Chizallet, C. **In: ACS Catalysis**. Washington: American Chemical Society, 2019, Roč. 9, č. 3, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1692 - 1704

2019 [01/12] / **USA** - Ke, H.B. - Taylor, C.D. **In: Corrosion**: journal of science and engineering. Houston: NACE International, 2019, Roč. 75, č. 7, [tlačená forma]. ISSN 0010-9312. ISSN (online) 1938-159X. - SCIE ; WOS CC, s. 708 - 726

2019 [01/12] / **USA** - Ramirez, A. - Chowdhury, A.D. - Dokania, A. - Cnudde, P. - Caglapn, M. - Yarulina, I. - Abou-Hamad, E. - Gevers, L. - Ould-Chikh, S. - De Wispelaere, K. - van Speybroeck, V. - Gascon, J. **In: ACS Catalysis**. Washington: American Chemical Society, 2019, Roč. 9, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 6320 - 6334

2019 [01/12] / Fraux, G. - Chibani, S. - Coudert, F.X. **In: Philosophical Transactions of the Royal Society A-Mathematical Physical and Engineering Sciences**, 2019, Roč. 377, č. 2149. - SCIE ; WOS CC, s. Art. No. 20180220

2019 [01/12] / **USA** - Bailleul, S. - Rogge, S.M.J. - Vanduyfhuys, L. - Van Speybroeck, V. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 16, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 3993 - 4010

2019 [01/12] / **USA** - Klimes, J. - Tew, D.P. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 151, č. 23, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 234108

2018 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Vanduyfhuys, L. - Demuynck, R. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 10, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 189 - 228

2018 [01/12] / **USA** - Chen, L. - Falsig, H. - Janssens, T.V.W. - Gronbeck, H. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2018, Roč. 358, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 179 - 186

2018 [01/12] / Kadam, S.A. - Li, H.G. - Wormsbecher, R.F. - Travert, A. **In: Chemistry-A European Journal**, 2018, Roč. 24, č. 21. - SCIE ; WOS CC, s. 5489 - 5492

2018 [01/12] / van Santen, R.A. - Liu, C. **In: Modelling and Simulation in the Science of Micro- and Meso-Porous Materials**, 2018. - SCIE ; WOS CC, s. 151 - 188

2018 [01/12] / **GBR** - Hajek, J. - Caratelli, C. - Demuynck, R. - De Wispelaere, K. - Vanduyfhuys, L. - Waroquier, M. - Van Speybroeck, V. **In: Chemical Science**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 9, č. 10, [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCIE ; WOS CC, s. 2723 - 2732

2018 [01/12] / Fang, H.J. - Awati, R. - Boulfelfel, S.E. - Ravikovitch, P.I. - Sholl, D.S. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 24. - SCIE ; WOS CC, s. 12880 - 12891

2018 [01/12] / **GBR** - Santen, R.A. - Sengar, A. - Steur, E. **In: Faraday Discussions**. London: The Royal Society of Chemistry, 2018, Roč. 208, [tlačená forma] [online]. ISSN 1359-6640. ISSN (online) 1364-5498. - SCIE ; WOS CC, s. 35 -

52

2018 [01/12] / **GBR** - Grajciar, L. - Heard, C.J. - Bondarenko, A.A. - Polynski, M.V. - Meeprasert, J. - Pidko, E.A. - Nachtigall, P. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 47, č. 22, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 8307 - 8348

2018 [01/12] / **USA** - Rybicki, M. - Sauer, J. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2018, Roč. 140, č. 51, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 18151 - 18161

2017 [01/12] / Sun, L. - Deng, W.Q. **In: Wiley Interdisciplinary Reviews-Computational Molecular Science**, 2017, Roč. 7, č. 1. - SCIE ; WOS CC, s. Art. No. 1282

2017 [01/12] / Janda, A. - Vlaisavljevich, B. - Smit, B. - Lin, L.C. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 3. - SCIE ; WOS CC, s. 1618 - 1638

2017 [01/12] / **USA** - Van der Mynsbrugge, J. - Janda, A. - Sharada, S.M. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ACS Catalysis**. Washington: American Chemical Society, 2017, Roč. 7, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2685 - 2697

2017 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2017, Roč. 345, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 53 - 69

2016 [01/12] / **USA** - De Wispelaere, K. - Wondergem, C.S. - Ensing, B. - Hemelsoet, K. - Meijer, E.J. - Weckhuysen, B.M. - Van Speybroeck, V. - Ruiz-Martinez, J. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 3, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1991 - 2002

2016 [01/12] / De Wispelaere, K. - Bailleul, S. - Van Speybroeck, V. **In: Catalysis Science & Technology**, 2016, Roč. 6, č. 8. - SCIE ; WOS CC, s. 2686 - 2705

2016 [01/12] / **USA** - Janda, A. - Vlaisavljevich, B. - Lin, L.C. - Smit, B. - Bell, A.T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 14, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 4739 - 4756

2016 [01/12] / **USA** - Li, H.G. - Kadam, S.A. - Vimont, A. - Wormsbecher, R.F. - Travert, A. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 4536 - 4548

2016 [01/12] / **GBR** - Chibani, S. - Chebbi, M. - Lebegue, S. - Cantrel, L. - Badawi, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 36, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 25574 - 25581

2015 [01/12] / Tranca, D.C. - Zimmerman, P.M. - Gomes, J. - Lambrecht, D. - Keil, F.J. - Head-Gordon, M. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 52. - SCIE ; WOS CC, s. 28836 - 28853

2015 [01/12] / **USA** - Liu, C. - Li, G.N. - Hensen, E.J.M. - Pidko, E.A. **In: ACS Catalysis**. Washington: American Chemical Society, 2015, Roč. 5, č. 11, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 7024 - 7033

2015 [01/12] / **USA** - Erichsen, M.W. - De Wispelaere, K. - Hemelsoet, K. - Moors, S.L.C. - Deconinck, T. - Waroquier, M. - Svelle, S. - Van Speybroeck, V. - Olsbye, U. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2015, Roč.

328, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 186 - 196

2015 [01/12] / De Wispelaere, K. - Ensing, B. - Ghysels, A. - Meijer, E.J. - Van Speybroeck, V. **In: Chemistry-A European Journal**, 2015, Roč. 21, č. 26. - SCIE ; WOS CC, s. 9385 - 9396

2015 [01/12] / Janda, A. - Vlaisavljevich, B. - Lin, L.C. - Sharada, S.M. - Smit, B. - Head-Gordon, M. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 19. - SCIE ; WOS CC, s. 10427 - 10438

2015 [01/12] / Katada, N. - Sota, S. - Morishita, N. - Okumura, K. - Niwa, M. **In: Catalysis Science & Technology**, 2015, Roč. 5, č. 3. - SCIE ; WOS CC, s. 1864 - 1869

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2015 [01/12] / Yun, J.H. - Lobo, R.F. **In: Catalysis Science & Technology**, 2015, Roč. 5, č. 1. - SCIE ; WOS CC, s. 264 - 273

2014 [01/12] / **GBR** - Van Speybroeck, V. - De Wispelaere, K. - Van der Mynsbrugge, J. - Vandichel, M. - Hemelsoet, K. - Waroquier, M. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 43, č. 21, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7326 - 7357

2014 [01/12] / Jones, A.J. - Iglesia, E. **In: Angewandte Chemie-International Edition**, 2014, Roč. 53, č. 45. - SCIE ; WOS CC, s. 12177 - 12181

2014 [01/12] / **USA** - Jiang, T. - Goltl, F. - Bulo, R.E. - Sautet, P. **In: ACS Catalysis**. Washington: American Chemical Society, 2014, Roč. 4, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2351 - 2358

2014 [01/12] / **USA** - Shang, J. - Li, G. - Singh, R. - Xiao, P. - Danaci, D. - Liu, J.Z. - Webley, P.A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 8, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 084705

2014 [01/12] / **GBR** - Fang, H.J. - Demir, H. - Kamakoti, P. - Sholl, D.S. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2014, Roč. 2, č. 2, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 274 - 291

2014 [01/12] / **GBR** - Mace, A. - Laasonen, K. - Laaksonen, A. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 1, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 166 - 172

2013 [01/12] / **USA** - Moors, S.L.C. - De Wispelaere, K. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 11, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2556 - 2567

2013 [01/12] / Derouane, E.G. - Vedrine, J.C. - Pinto, R.R. - Borges, P.M. - Costa, L. - Lemos, M.A.N.D.A. - Lemos, F. - Ribeiro, F.R. **In: Catalysis Reviews-Science and Engineering**, 2013, Roč. 55, č. 4. - SCIE ; WOS CC, s. 454 - 515

2013 [01/12] / Patrylak, K.I. - Patrylak, L.K. - Repetskyi, I.A. **In: Theoretical and Experimental Chemistry**, 2013, Roč. 49, č. 3. - SCIE ; WOS CC, s. 143 - 157

2013 [01/12] / Sharada, S.M. - Zimmerman, P.M. - Bell, A.T. - Head-Gordon, M. **In: Journal of Physical Chemistry C**,

2013, Roč. 117, č. 24. - SCIE ; WOS CC, s. 12600 - 12611

2013 [01/12] / Hemelsoet, K. - Van der Mynsbrugge, J. - De Wispelaere, K. - Waroquier, M. - Van Speybroeck, V. **In: ChemPhysChem**, 2013, Roč. 14, č. 8. - SCIE ; WOS CC, s. 1526 - 1545

2013 [01/12] / **USA** - Moses, P.G. - Norskov, J.K. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 735 - 745

2013 [01/12] / Hansen, N. - Keil, F.J. **In: Chemie Ingenieur Technik**: Verfahrenstechnik, technische Chemie, Apparatewesen, Biotechnologie, 2013, Roč. 85, č. 4, [tlačená forma]. ISSN 0009-286X. ISSN (online) 1522-2640. - SCIE ; WOS CC, s. 413 - 419

2013 [01/12] / **GBR** - Fang, H.J. - Kamakoti, P. - Ravikovitch, P.I. - Aronson, M. - Paur, C. - Sholl, D.S. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 31, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 12882 - 12894

2013 [01/12] / **GBR** - Kling, D.P. - Machado, E.S.A. - Chagas, H.C. - dos Santos, A.P.A. - Rosenbach, N. - Carneiro, J.W. - Mota, C.J.A. **In: Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 49, č. 40, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCIE ; WOS CC, s. 4480 - 4482

2012 [01/12] / Fang, H.J. - Kamakoti, P. - Zang, J. - Cundy, S. - Paur, C. - Ravikovitch, P.I. - Sholl, D.S. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 19. - SCIE ; WOS CC, s. 10692 - 10701

2012 [01/12] / **USA** - Zimmerman, P.M. - Tranca, D.C. - Gomes, J. - Lambrecht, D.S. - Head-Gordon, M. - Bell, A.T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2012, Roč. 134, č. 47, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 19468 - 19476

2012 [01/12] / Tranca, D.C. - Hansen, N. - Swisher, J.A. - Smit, B. - Keil, F.J. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 44. - SCIE ; WOS CC, s. 23408 - 23417

2012 - spolu : **4**

ADC_033: / Tunega, Daniel (Autor) (34%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (33%) - Zaoral, Tomáš (Autor) (33%): **Assessment of ten DFT methods in predicting structures of sheet silicates: Importance of dispersion corrections**. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 137, č. 11 (2012), s. 14105-14105 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,157 - 2012
SJR: 1,832 - 2012
CiteScore: 5,3 - 2012
Nordic List: 1 - 2012

Ohlasy (115):

2025 [01/20] / **NLD** - Jia, J. - Zaoui, Ali - Sekkal, W. **Preventing crack propagation for self-healing potential in PVA-modified CSH composites** [elektronický dokument]. DOI 10.1016/j.conbuildmat.2025.142771 In: **Construction and Building Materials**: An international journal dedicated to the investigation and innovative use of materials in construction and repair. Amsterdam: Elsevier, 2025, Roč. 491, art. no. 142771 [tlačená forma] [online]. ISSN 0950-0618. ISSN (online) 1879-0526. - SCO ; WOS CC, s. art. no. 142771

2025 [01/20] / **GBR** - Christensen, Rasmus - Persson, Kristin A. - Smedskjaer, Morten M. **Structural origin of disorder-induced ion conduction in NaFePO4 cathode materials** [elektronický dokument]. DOI 10.1039/d5ta02295a In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2025, Roč. 13, č. 30, s. 24619-24632 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 24619 - 24631

2025 [01/20] / **CHE** - Polcowñuk Iriarte, Iván Aitor - Mocciaro, Anabella - Rendtorff, Nicolás Maximiliano - Richard, Diego. **Dehydroxylation of Kaolinite: Evaluation of Activation Energy by Thermogravimetric Analysis and Density Functional Theory Insights** [elektronický dokument]. DOI 10.3390/min15060607 In: **Minerals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 6, art. no. 607 [online]. ISSN (online) 2075-163X. - SCO ; CCC ; WOS CC, s. art. no. 607

2025 [01/20] / **USA** - Pedone, Alfonso - Bertani, Marco - Benassi, Matilde. **Revisiting Machine Learning Potentials for Silicate Glasses: The Missing Role of Dispersion Interactions** [elektronický dokument]. DOI 10.1021/acs.jctc.5c00218 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 9, s. 4769-4778 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 4769 - 4778

2025 [01/20] / **USA** - Shepelenko, Margarita - Livneh, Tsachi - Natalio, Filipe - Kronik, Leeor. **Infrared Absorption Spectrum of α-Moganite from First-Principles** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c04193 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 3, s. 1831-1840 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 1831 - 1840

2024 [01/20] / **NLD** - Zhang, Qi - Ye, Changwen - Zhou, Hao - Chen, Yuting - Ao, Fang - Luo, Yi - Yang, Weiqing - Ma, Menglin - Chen, Xianfei. **Active sites regulation and adsorption performance of Al-pillared bentonite for the removal of lead from aqueous phase** [elektronický dokument]. DOI 10.1016/j.jwpe.2024.106274 In: **Journal of Water Process Engineering**. Amsterdam: Elsevier, 2024, Roč. 67, art. no. 106274 [online]. ISSN (online) 2214-7144. - SCO ; CCC ; WOS CC, s. art. no. 106274

2024 [01/20] / **NLD** - Li, Yiqian - Li, Yinhao - Na, Liyuan - Xiao, Tianyu - Cui, Yingxin - Li, Peng - Lü, Zhe. **Sulfur poisoning and O2−-pumping regeneration of La0.75Sr0.25Cr0.5Mn0.5O3−δ-Ni-CeO2 anode** [elektronický dokument]. DOI 10.1016/j.jpowsour.2024.235061 In: **Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2024, Roč. 614, art. no. 235061 [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCO, s. art. no. 235061

2024 [01/20] / **GBR** - Ulian, Gianfranco - Valdrè, Giovanni. **Crystal structure and elastic and phonon properties of realgar versus pressure** [elektronický dokument]. DOI 10.1107/S1600576724000025 In: **Journal of applied crystallography**. Chester: International Union of Crystallography, 2024, Roč. 57, č. Pt 2, s. 220-231 [tlačená forma] [online]. ISSN 0021-8898. ISSN (online) 1600-5767. - SCO ; CCC ; WOS CC, s. 220 - 231

2024 [01/20] / **USA** - Bertani, Marco - Charpentier, Thibault - Faglioni, Francesco - Pedone, Alfonso. **Accurate and Transferable Machine Learning Potential for Molecular Dynamics Simulation of Sodium Silicate Glasses** [elektronický dokument]. DOI 10.1021/acs.jctc.3c01115 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 3, s. 1358-1370 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online)

1549-9626. - SCO ; CCC ; WOS CC, s. 1358 - 1370

2024 [01/20] / **CHE** - Desdion, Quentin - Bessac, Fabienne - Hoyau, Sophie. **Atrazine Desorption Mechanism from an Hydrated Calcium Montmorillonite—A DFT Molecular Dynamics Study** [elektronický dokument]. DOI 10.3390/ijms25031604 In: **International journal of molecular sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 25, č. 3, art. no. 1604 [online] [tlačená forma]. ISSN 1661-6596. ISSN (online) 1422-0067. - SCO ; CCC ; WOS CC, s. art. no. 1604

2024 [01/20] / **CHN** - Li, Tianyu - Chai, Zhaoyun - Yang, Zeqian - Xin, Zipeng - Sun, Haocheng - Yan, Ke. **Molecular Simulation of Surface Hydration Mechanism and Electric Field Weakening Adsorption Properties of Kaolinite**. DOI 10.11896/cldb.22050283 In: **Cailiao Daobao**. Chongqing: Cailiao Daobaoshe, 2024, Roč. 38, č. 1, art. no. 22050283 [tlačená forma] [online]. ISSN 1005-023X. - SCO, s.

2024 [01/20] / **USA** - Rao, Wenxiu - Liu, Xin - Lv, Guocheng - Liu, Meng - Wang, Lijuan - Niu, Jinan - Li, Zhaohui - Liao, Libing. **Correlation between Hinckley index and stacking order-disorder in kaolinite** [elektronický dokument]. DOI 10.2138/am-2022-8830 In: **The American mineralogist**: an international journal of earth and planetary materials. Washington: Mineralogical Society of America, 2024, Roč. 109, č. 1, s. 135-143 [tlačená forma] [online]. ISSN 0003-004X. ISSN (online) 1945-3027. - SCO ; CCC ; WOS CC, s. 135 - 143

2023 [01/20] / **NLD** - Yin, Yue - Huang, Caijuan - Luo, Xian - Xu, Benjun. **Iron behavior during the continuous phase transition of iron-doped titanium dioxide determined via high-temperature in-situ X-ray diffraction, rietveld refinement, and density functional theory studies** [elektronický dokument]. DOI 10.1016/j.jmrt.2023.01.159 In: **Journal of Materials Research and Technology**. Amsterdam: Elsevier, 2023, Roč. 23, s. 2426-2439 [tlačená forma] [online]. ISSN 2238-7854. ISSN (online) 2214-0697. - SCO ; CCC ; WOS CC, s. 2426 - 2439

2023 [01/20] / **USA** - Kong, Xiangtong - Garg, Shikha - Mortazavi, Mahshid - Ma, Jinxing - Waite, T. David. **Heterogenous Iron Oxide Assemblages for Use in Catalytic Ozonation: Reactivity, Kinetics, and Reaction Mechanism** [elektronický dokument]. DOI 10.1021/acs.est.2c07319 In: **Environmental science & technology**. Washington: American Chemical Society, 2023, Roč. 57, č. 47, s. 18636-18646 [tlačená forma] [online]. ISSN 0013-936X. ISSN (online) 1520-5851. - SCO ; CCC ; WOS CC, s. 18636 - 18646

2023 [01/20] / **CHE** - Ren, Shiwei - Wang, Zhuoer - Zhang, Wenqing - Ding, Yubing - Yi, Zhengran. **Donor-Acceptor-Based Organic Polymer Semiconductor Materials to Achieve High Hole Mobility in Organic Field-Effect Transistors** [elektronický dokument]. DOI 10.3390/polym15183713 In: **Polymers**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 15, č. 18, art. no. 3713 [online]. ISSN (online) 2073-4360. - SCO ; CCC ; WOS CC, s. art. no. 3713

2023 [01/20] / **CHE** - Ren, Shiwei - Zhang, Wenqing - Wang, Zhuoer - Yassar, Abderrahim - Liao, Zhiting - Yi, Zhengran. **Synergistic Use of All-Acceptor Strategies for the Preparation of an Organic Semiconductor and the Realization of High Electron Transport Properties in Organic Field-Effect Transistors** [elektronický dokument]. DOI 10.3390/polym15163392 In: **Polymers**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 15, č. 16, art. no. 3392 [online]. ISSN (online) 2073-4360. - SCO ; CCC ; WOS CC, s. art. no. 3392

2023 [01/20] / **GBR** - Hanein, Theodore - Nguyen, Hoang - Provis, John L. - Utton, Claire - Kunther, Wolfgang. **Thermodynamics of calcined clays used in cementitious binders: origin to service life considerations** [elektronický dokument]. DOI 10.1039/d3ta01896b In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2023, Roč. 11, č. 34, s. 17920-17937 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 17920 - 17937

2023 [01/20] / **USA** - Belzunces, Bastien - Hoyau, Sophie - Cuny, Jérôme - Bessac, Fabienne. **Desorption Mechanism of a Pesticide from a Hydrated Calcium Montmorillonite Unraveled by Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c01006 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage,

Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 27, s. 12953-12966 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; WOS CC, s. 12953 - 12966

2023 [01/20] / **NLD** - Li, Tianyu - Chai, Zhaoyun - Yang, Zeqian - Xin, Zipeng - Sun, Haocheng - Yan, Ke. **Insights into the influence mechanism of different interlayer cations on the hydration activity of montmorillonite surface: A DFT calculation** [elektronický dokument]. DOI 10.1016/j.clay.2023.106965 In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2023, Roč. 239, art. no. 106965 [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO ; CCC ; WOS CC, s. art. no. 106965

2023 [01/20] / **GBR** - Zhao, Jian - Wang, Yi Fei - Luan, Zhao Long - Cao, Yu - He, Man Chao. **Theoretical analysis of the effect of doping with Na(I), K(I), Mg(II), Ca(II) and Fe(II) on the electronic and mechanical properties of pyrophyllite** [elektronický dokument]. DOI 10.1180/clm.2023.17 In: **Clay Minerals**. London: Mineralogical Society, 2023, Roč. 58, č. 2, s. 113-120 [tlačená forma]. ISSN 0009-8558. ISSN (online) 1471-8030. - SCO ; CCC ; WOS CC, s. 113 - 120

2023 [01/20] / **GBR** - Su, Zhuoying - Qiu, Wenjuan - He, Yuming - Zeng, Ying - Xie, Dongming - Xiao, Xin - Nan, Junmin - Zuo, Xiaoxi. **A strontium ferrite modified separator for adsorption and catalytic conversion of polysulfides for excellent lithium-sulfur batteries** [elektronický dokument]. DOI 10.1039/d3dt01126g In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2023, Roč. 52, č. 26, s. 9032-9041 [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO ; CCC ; WOS CC, s. 9032 - 9041

2023 [01/20] / **USA** - Shepherd, Sam - Tribello, Gareth A. - Wilkins, David M. **A fully quantum-mechanical treatment for kaolinite** [elektronický dokument]. DOI 10.1063/5.0152361 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 20, art. no. 204704 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 204704

2022 [01/20] / **DEU** - Dong, M.-M. - Hao, Z.-W. - Niu, Y. - Wang, C.-K. - Fu, X.-X. **M3C2(OH)2 (M = Zr and Hf): An Ideal Electrode Material for sub-5 nm 2D Field-Effect Transistors** In: **Advanced Materials Interfaces**. Weinheim: John Wiley & Sons. Wiley-VCH, 2022, Roč. 9, č. 34, [online]. ISSN 2196-7350. - SCO, s. Art. No. 2201166

2022 [01/20] / **NLD** - Kobayashi, K. - Yamaguchi, A. - Okumura, M. **Machine learning potentials of kaolinite based on the potential energy surfaces of GGA and meta-GGA density functional theory** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2022, Roč. 228, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 106596

2022 [01/20] / **GBR** - Moreno-Rodriguez, D. - Jankovic, A. - Scholtzova, E. **Immobilisation of diuron herbicide employing smectites** In: **Materials Today Communications**, 2022, Roč. 31. - SCO, s. Art. No. 103252

2022 [01/20] / **NLD** - Richard, D. - Rendtorff, N.M. **Kaolin group minerals under pressure: The study of their structural and electronic properties by DFT methods** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2022, Roč. 219, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 106444

2022 [01/20] / **NLD** - Singh, J. - White, R.L. **Variable temperature infrared spectroscopy with a button sample holder and thermoelectric heating/cooling** [elektronický dokument] In: **Analytica chimica acta**. Amsterdam: Elsevier, 2022, Roč. 1198, [tlačená forma] [online]. ISSN 0003-2670. ISSN (online) 1873-4324. - SCO, s. Art. No. 339558

2022 [01/20] / **USA** - Kurapothula, P.K.J. - Shepherd, S. - Wilkins, D.M. **Hydrogen-bonding and nuclear quantum effects in clays** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2022, Roč. 156, č. 8, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No.

084702

2022 [01/20] / **USA** - Novakovic, L. - Sayre, D. - Schacher, D. - Dias, R.P. - Salamat, A. - Lawler, K.V. **Dispersion interactions in proposed covalent superhydride superconductors** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 105, č. 2, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 024512

2022 [01/20] / **NLD** - Richard, D. - Martinez, J.M. - Mizrahi, M. - Andrini, L. - Rendtorff, N.M. **Assessment of structural order indices in kaolinites: A multi-technique study including EXAFS** In: **Journal of Electron Spectroscopy and Related Phenomena**, 2022, Roč. 254. ISSN 03682048. - SCO, s. Art. No. 147128

2021 [01/20] / **DEU** - Matkovic, A. - Ludescher, L. - Peil, O.E. - Sharma, A. - Gradwohl, K.-P. - Kratzer, M. - Zimmermann, M. - Genser, J. - Knez, D. - Fisslthaler, E. - Gammer, C. - Lugstein, A. - Bakker, R.J. - Romaner, L. - Zahn, D.R.T. - Hofer, F. - Salvan, G. - Raith, J.G. - Teichert, C. **Iron-rich talc as air-stable platform for magnetic two-dimensional materials** [elektronický dokument] In: **NPJ 2D Materials and Applications**. Berlín: Nature Research, 2021, Roč. 5, č. 1. ISSN (online) 2397-7132. - SCO, s. Art. No. 94

2021 [01/20] / **USA** - Resende, G.C. - Ribeiro, G.A.S. - Silveira, O.J. - Lemos, J.S. - Rhodes, D. - Balicas, L. - Terrones, M. - Mazzoni, M.S.C. - Fantini, C. - Carvalho, B.R. - Pimenta, M.A. **Effects of dimensionality and excitation energy on the Raman tensors of triclinic ReSe2** [elektronický dokument] In: **Journal of Raman Spectroscopy**. New York: John Wiley & Sons, 2021, Roč. 52, č. 12, [tlačená forma] [online]. ISSN 0377-0486. ISSN (online) 1097-4555. - SCO, s. 2068 - 2080

2021 [01/20] / **NLD** - Richard, D. - Rendtorff, N.M. **Local Environments in Iron-Bearing Clay Minerals by DFT Approaches: The Case of Structural Fe in Kaolinite** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2021, Roč. 213, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 106251

2021 [01/20] / **DEU** - Balan, E. - Fritsch, E. - Radtke, G. - Paulatto, L. - Juillot, F. - Baron, F. - Petit, S. **First-principles modeling of the infrared spectrum of Fe- A nd Al-bearing lizardite** In: **European Journal of Mineralogy**: an international journal of mineralogy, petrology, geochemistry and related sciences. Stuttgart: E. Schweizerbart'sche Verlagsbuchhandlung, 2021, Roč. 33, č. 5, [tlačená forma]. ISSN 0935-1221. - SCO, s. 647 - 657

2021 [01/20] / **USA** - Wang, J. - Fu, L. - Yang, H. - Zuo, X. - Wu, D. **Energetics, Interlayer Molecular Structures, and Hydration Mechanisms of Dimethyl Sulfoxide (DMSO)-Kaolinite Nanoclay Guest-Host Interactions** In: **Journal of Physical Chemistry Letters**, 2021, Roč. 12, č. 40. - SCO, s. 9973 - 9981

2021 [01/20] / **GBR** - Diaz-Anichtchenko, D. - Turnbull, R. - Bandiello, E. - Anzellini, S. - Achary, S.N. - Errandonea, D. **Pressure-induced chemical decomposition of copper orthovanadate (Cu3V2O8)** [elektronický dokument] In: **Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2021, Roč. 9, č. 38, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO, s. 13402 - 13409

2021 [01/20] / **NLD** - Ulian, G. - Moro, D. - Valdre, G. **Water adsorption behaviour on (001) pyrophyllite surface from ab initio Density Functional Theory simulations** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2021, Roč. 212, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 106221

2021 [01/20] / **CHE** - Toraman, H.E. - Alexopoulos, K. - Oh, S.C. - Cheng, S. - Liu, D. - Vlachos, D.G. **Ethylene production by direct conversion of methane over isolated single active centers** [elektronický dokument] In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2021, Roč. 420, [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO, s. Art. No. 130493

2021 [01/20] / **USA** - Blasko, M. - Pasteka, L.F. - Urban, M. **DFT Functionals for Modeling of Polyethylene Chains Cross-Linked by Metal Atoms. DLPNO-CCSD(T) Benchmark Calculations** In: **Journal of Physical Chemistry A**, 2021, Roč. 125, č. 34. - SCO, s. 7382 - 7395

2021 [01/20] / **NLD** - Heimann, J.E. - Grimes, R.T. - Rosenzweig, Z. - Bennett, J.W. **A density functional theory (DFT) investigation of how small molecules and atmospheric pollutants relevant to art conservation adsorb on kaolinite** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2021, Roč. 206, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 106075

2021 [01/20] / **USA** - Song, L. - Liu, W. - Xin, F. - Li, Y. **Study of adhesion properties and mechanism of sodium silicate binder reinforced with silicate fume** [elektronický dokument] In: **International Journal of Adhesion and Adhesives**. New York: Elsevier. Elsevier Science, 2021, Roč. 106, [tlačená forma] [online]. ISSN 0143-7496. ISSN (online) 1879-0127. - SCO, s. Art. No. 102820

2021 [01/20] / **NLD** - Luo, Q. - Liu, W. - Zhuo, Q. - Han, Y. **Interaction mechanism of organic carboxylate with kaolinite and montmorillonite: A density functional theory study** [elektronický dokument] In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2021, Roč. 613, [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO, s. Art. No. 126047

2021 [01/20] / **GBR** - Noneman, H.F. - Hollingsworth, M.E. - Singh, J. - White, R.L. **A high sensitivity variable temperature infrared spectroscopy investigation of kaolinite structure changes** In: **Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy**, 2021, Roč. 247. - SCO, s. Art. No. 119113

2021 [01/20] / **NLD** - Schliemann, R. - Churakov, S.V. **Atomic scale mechanism of clay minerals dissolution revealed by ab initio simulations** In: **Geochimica et cosmochimica Acta**. [s.l.]: Published by Elsevier Ltd., 2021, Roč. 293. - SCO, s. 438 - 460

2021 [01/20] / **NLD** - Ulian, G. - Moro, D. - Valdre, G. **Electronic and optical properties of graphene/molybdenite bilayer composite** [elektronický dokument] In: **Composite Structures**. Amsterdam: Elsevier, 2021, Roč. 255, [tlačená forma] [online]. ISSN 0263-8223. ISSN (online) 1879-1085. - SCO, s. Art. No. 112978

2020 [01/12] / **NLD** - Shang, Z. - Zhang, X. **Theoretical study on the interactions between silica and the products of 3-mercaptopropyltriethoxysilane (MPTS) with different hydrolysis degrees** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 502, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; SCIE ; WOS CC, s. Art. No. 143853

2020 [01/12] / **USA** - Zheng, Q. - Jiang, J. - Chen, C. - Yu, J. - Li, X. - Tang, L. - Li, S. **Nanoengineering Microstructure of Hybrid C-S-H/Silicene Gel** In: **ACS Applied Materials and Interfaces**, 2020, Roč. 12, č. 15. - SCO, s. 17806 - 17814

2020 [01/12] / **CHE** - Xi, P. - Ma, R. - Liu, W. **Study on the crystal structure of coal kaolinite and non-coal kaolinite: Insights from experiments and DFT simulations** [elektronický dokument] In: **Symmetry**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 12, č. 7, [online]. ISSN (online) 2073-8994. - SCO, s. Art. No. 1125

2020 [01/12] / **NLD** - Li, T. - Huang, X. - Wang, Q. - Yang, G. **Adsorption of metal ions at kaolinite surfaces: Ion-specific effects, and impacts of charge source and hydroxide formation** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2020, Roč. 194, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 105706

2019 [01/12] / Azizi, D. - Larachi, F. **In: Journal of Physical Chemistry A**, 2019, Roč. 123, č. 4. - SCIE ; WOS CC, s. 889

- 905

2019 [01/12] / **NLD** - Richard, D. - Rendtorff, N.M. **In: Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2019, Roč. 169, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCIE ; WOS CC, s. 67 - 73

2019 [01/12] / **USA** - Fischer, M. - Kim, W.J. - Badawi, M. - Lebegue, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 150, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094102

2019 [01/12] / **USA** - Hernandez-Laguna, A. - del Valle, C.P. - Hernandez-Haro, N. - Ortega-Castro, J. - Munoz-Santiburcio, D. - Vidal, I. - Sanchez-Navas, A. - Escamilla-Roa, E. - Sainz-Diaz, C.I. **In: Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2019, Roč. 25, č. 11, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCIE ; WOS CC, s. Art. No. 341

2019 [01/12] / **DEU** - Gusmao, M.S.S. - Gopal, P. - Siloi, I. - Curtarolo, S. - Fornari, M. - Nardelli, M.B. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2019, Roč. 9, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 13698

2019 [01/12] / **NLD** - Zhao, H. - Qi, N. - Li, Y. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 466, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 607 - 614

2018 [01/12] / Churakov, S.V. - Liu, X.D. **In: Surface and Interface Chemistry of Clay Minerals**, 2018, Roč. 9. - SCIE ; WOS CC, s. 49 - 87

2018 [01/12] / **GBR** - Colmenero, F. - Timon, V. - Bonales, L.J. - Cobos, J. **In: Clay Minerals**. London: Mineralogical Society, 2018, Roč. 53, č. 3, [tlačená forma]. ISSN 0009-8558. ISSN (online) 1471-8030. - SCIE ; WOS CC, s. 377 - 392

2018 [01/12] / **USA** - Yaghoubi, A. - Masenelli-Varlot, K. - Boisron, O. - Ramesh, S. - Melinon, P. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2018, Roč. 30, č. 20, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 7234 - 7244

2018 [01/12] / **USA** - Akiyama, S. - Miyaji, A. - Hayashi, Y. - Hiza, M. - Sekiguchi, Y. - Koyama, T. - Shiga, A. - Baba, T. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2018, Roč. 359, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 184 - 197

2018 [01/12] / **NLD** - Yang, Z.Y. - Liu, W.L. - Zhang, H. - Jiang, X.L. - Min, F.F. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 436, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 58 - 65

2018 [01/12] / **USA** - Taborosi, A. - Szilagyi, R.K. - Zsirka, B. - Fonagy, O. - Horvath, E. - Kristof, J. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2018, Roč. 57, č. 12, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 7151 - 7167

2017 [01/12] / **USA** - Belzunces, B. - Hoyau, S. - Benoit, M. - Tarrat, N. - Bessac, F. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2017, Roč. 38, č. 3, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 133 - 143

2017 [01/12] / **USA** - Fischer, M. - Angel, R.J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 174111

2017 [01/12] / **USA** - Fu, L.J. - Yang, H.M. **In: Nanoscale research letters**. New York: Springer Nature, 2017, Roč. 12, [tlačená forma] [online]. ISSN 1931-7573. ISSN (online) 1556-276X. - SCIE ; WOS CC, s. Art. No. 411

2017 [01/12] / **DEU** - Hart, L.S. - Webb, J.L. - Dale, S. - Bending, S.J. - Mucha-Kruczynski, M. - Wolverson, D. - Chen, C.Y. - Avila, J. - Asensio, M.C. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2017, Roč. 7, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 5145

2017 [01/12] / Pouvreau, M. - Greathouse, J.A. - Cygan, R.T. - Kalinichev, A.G. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 27. - SCIE ; WOS CC, s. 14757 - 14771

2017 [01/12] / **CHE** - Fu, L.J. - Yang, H.M. - Tang, A.D. - Hu, Y.H. **In: Nano research**. Peking: Tshinghua Press, 2017, Roč. 10, č. 8, [tlačená forma] [online]. ISSN 1998-0124. ISSN (online) 1998-0000. - SCIE ; WOS CC, s. 2782 - 2799

2017 [01/12] / **NLD** - Kwon, K.D. - Sposito, G. **In: Chemical Geology**: an Official Journal of the European Association for Geochemistry: including Isotope Geoscience. Amsterdam: Elsevier, 2017, Roč. 464, [tlačená forma] [online]. ISSN 0009-2541. ISSN (online) 1872-6836. - SCIE ; WOS CC, s. 4 - 13

2017 [01/12] / **NLD** - Zhang, T. - Sun, H. - Wang, F.D. - Zhang, W.D. - Tang, S.W. - Ma, J.M. - Gong, H.W. - Zhang, J.P. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2017, Roč. 425, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 340 - 350

2017 [01/12] / **USA** - de Lima, F.D.C. - Miwa, R.H. - Miranda, C.R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 147, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 174704

2017 [01/12] / **GBR** - Sassi, M. - Okumura, M. - Machida, M. - Rosso, K.M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 39, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 27007 - 27014

2017 [01/12] / Greathouse, J.A. - Cygan, R.T. - Fredrich, J.T. - Jerauld, G.R. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 41. - SCIE ; WOS CC, s. 22773 - 22786

2017 [01/12] / **NLD** - Fonseca, C.G. - Vaiss, V.S. - Wypych, F. - Diniz, R. - Leitao, A.A. **In: Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2017, Roč. 143, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCIE ; WOS CC, s. 212 - 219

2016 [01/12] / **NLD** - Watrowski, R. - Castillo-Tong, D. C. - Schuster, E. - Fischer, M. B. - Speiser, P. - Zeillinger, R. **In: Tumor Biology**: Tumor Markers, Tumor Targeting and Translational Cancer Research. Houten: Springer Nature. Springer International Publishing AG, 2016, Roč. 37, č. 6, [tlačená forma] [online]. ISSN 1010-4283. ISSN (online) 1423-0380. - SCIE ; SCO ; WOS CC, s. 249 - 257

2016 [01/12] / **GBR** - Taborosi, A. - Szilagyi, R.K. **In: Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2016, Roč. 45, č. 6, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCIE ; WOS CC, s. 2523 - 2535

2016 [01/12] / **USA** - Kepp, K.P. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2016, Roč. 55, č. 6, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 2717 - 2727

2016 [01/12] / **NLD** - Li, H.T. - Kang, T.H. - Zhang, B. - Zhang, J.J. - Ren, J. **In: Computational Materials Science**. Amsterdam: Elsevier, 2016, Roč. 117, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 33 - 39

2016 [01/12] / Hernandez-Haro, N. - Munoz-Santiburcio, D. - Del Valle, C.P. - Ortega-Castro, J. - Sainz-Diaz, C.I. - Garrido, C.J. - Hernandez-Laguna, A. **In: American Mineralogist**, 2016, Roč. 101, č. 5. - SCIE ; WOS CC, s. 1207 - 1216

2016 [01/12] / **GBR** - Hayashi, Y. - Akiyama, S. - Miyaji, A. - Sekiguchi, Y. - Sakamoto, Y. - Shiga, A. - Koyama, T.R. - Motokura, K. - Baba, T. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 36, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 25191 - 25209

2016 [01/12] / **USA** - Guler-Kilic, S. - Kilic, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 16, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 165203

2016 [01/12] / Yao, X.X. - Wang, W.W. - Chen, W. - Liu, X.H. **In: Nanoscience**, 2016, Roč. 3. - SCIE ; WOS CC, s. 211 - 275

2016 [01/12] / **NLD** - Han, Y.H. - Liu, W.L. - Chen, J.H. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2016, Roč. 370, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 403 - 409

2016 [01/12] / Kwon, K.D. - Newton, A.G. **In: Geochimica et cosmochimica Acta**. [s.l.]: Published by Elsevier Ltd., 2016, Roč. 190. - SCIE ; WOS CC, s. 100 - 114

2016 [01/12] / **DEU** - Fischer, M. - Evers, F.O. - Formalik, F. - Olejniczak, A. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2016, Roč. 135, č. 12, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 257

2016 [01/12] / Zen, A. - Roch, L.M. - Cox, S.J. - Hu, X.L. - Sorella, S. - Alfe, D. - Michaelides, A. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 46. - SCIE ; WOS CC, s. 26402 - 26413

2015 [01/12] / Liu, X.D. - Cheng, J. - Sprik, M. - Lu, X.C. - Wang, R.C. **In: Geochimica et cosmochimica Acta**. [s.l.]: Published by Elsevier Ltd., 2015, Roč. 168. - SCIE ; WOS CC, s. 293 - 301

2015 [01/12] / **USA** - Demichelis, R. - Bruno, M. - Massaro, F.R. - Prencipe, M. - De La Pierre, M. - Nestola, F. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2015, Roč. 36, č. 19, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 1439 - 1445

2015 [01/12] / Kwon, K.D. - Refson, K. - Sposito, G. **In: American Mineralogist**, 2015, Roč. 100, č. 7. - SCIE ; WOS CC, s. 1509 - 1517

2015 [01/12] / **CHE** - Kremer, A. E. - Namer, B. - Bolier, R. - Fischer, M. J. - Elfrink, R. P. - Beuers, U. **In: Digestive Diseases**. Bazilej: Karger Publishers, 2015, Roč. 33, [online]. ISSN 0257-2753. ISSN (online) 1421-9875. - SCIE ; WOS CC, s. 325 - 336

2015 [01/12] / Sakuma, H. - Suehara, S. **In: Journal of Geophysical Research-Solid Earth**, 2015, Roč. 120, č. 4. - SCIE ; WOS CC, s. 2212 - 2219

2015 [01/12] / Bocquet, M.L. - Coasne, B. - Pellenq, R. - Ulm, F.J. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 12. - SCIE ; WOS CC, s. 6511 - 6517

2015 [01/12] / Liu, X.H. - George, J. - Maintz, S. - Dronskowski, R. **In: Angewandte Chemie-International Edition**, 2015, Roč. 54, č. 6. - SCIE ; WOS CC, s. 1954 - 1959

2015 [01/12] / **GBR** - Weck, P.F. - Kim, E. - Jove-Colon, C.F. **In: Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2015, Roč. 44, č. 28, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCIE ; WOS CC, s. 12550 - 12560

2015 [01/12] / **GBR** - Alvim, R.S. - Miranda, C.R. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 7, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 4952 - 4960

2015 [01/12] / **USA** - Greathouse, J.A. - Geatches, D.L. - Pike, D.Q. - Greenwell, H.C. - Johnston, C.T. - Wilcox, J. - Cygan, R.T. **In: Clays and Clay Minerals**. Bloomington: Clay Minerals Society, 2015, Roč. 63, č. 3-4, [tlačená forma] [online]. ISSN 0009-8604. ISSN (online) 1552-8367. - SCIE ; WOS CC, s. 185 - 198

2015 [01/12] / **DEU** - Ulian, G. - Valdre, G. **In: Physics and Chemistry of Minerals**. Berlín: Springer Nature, 2015, Roč. 42, č. 7, [tlačená forma]. ISSN 0342-1791. ISSN (online) 1432-2021. - SCIE ; WOS CC, s. 609 - 627

2015 [01/12] / **GBR** - Taborosi, A. - Szilagyi, R.K. **In: Clay Minerals**. London: Mineralogical Society, 2015, Roč. 50, č. 3, [tlačená forma]. ISSN 0009-8558. ISSN (online) 1471-8030. - SCIE ; WOS CC, s. 307 - 327

2015 [01/12] / Nagendran, S. - Periyasamy, G. - Kamath, P.V. **In: Zeitschrift fur Anorganische und Allgemeine Chemie**, 2015, Roč. 641, č. 14. - SCIE ; WOS CC, s. 2396 - 2403

2015 [01/12] / **NLD** - Montoya, A. - Haynes, B.S. **In: Computational Materials Science**. Amsterdam: Elsevier, 2015, Roč. 98, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 435 - 445

2014 [01/12] / **GBR** - Ramos-Sanchez, G. - Callejas-Tovar, A. - Scanlon, L.G. - Balbuena, P.B. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 2, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 743 - 752

2014 [01/12] / **GBR** - Taborosi, A. - Kurdia, R. - Szilagyi, R.K. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 47, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 25830 - 25839

2014 [01/12] / Deringer, V.L. - Stoffel, R.P. - Dronskowski, R. **In: Crystal Growth and Design**, 2014, Roč. 14, č. 2. - SCIE ; WOS CC, s. 871 - 878

2014 [01/12] / **NLD** - Shi, J. - Lou, Z.Y. - Yang, M.L. - Zhang, Y. - Liu, H.B. - Meng, Y.F. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2014, Roč. 624, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 37 - 43

2014 [01/12] / **USA** - He, J.G. - Hummer, K. - Franchini, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075409

2014 [01/12] / Pinto, H.P. - Michalkova, A. - Leszczynski, J. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 12. -

SCIE ; WOS CC, s. 6110 - 6121

2014 [01/12] / **USA** - Al-Hamdani, Y.S. - Alfe, D. - von Lilienfeld, O.A. - Michaelides, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 141, č. 18, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 18530

2014 [01/12] / **NLD** - Demichelis, R. - Raiteri, P. - Gale, J.D. **In: Journal of Crystal Growth**. Amsterdam: Elsevier, 2014, Roč. 401, [tlačená forma] [online]. ISSN 0022-0248. ISSN (online) 1873-5002. - SCIE ; WOS CC, s. 33 - 37

2014 [01/12] / Chaka, A.M. - Felmy, A.R. **In: Journal of Physical Chemistry A**, 2014, Roč. 118, č. 35. - SCIE ; WOS CC, s. 7469 - 7488

2013 [01/12] / **USA** - Ulian, G. - Tosoni, S. - Valdre, G. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 139, č. 20, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 204101

2013 [01/12] / **USA** - Szaleniec, M. - Drzewiecka-Matuszek, A. - Witko, M. - Hejduk, P. **In: Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2013, Roč. 19, č. 10, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCIE ; WOS CC, s. 4487 - 4501

2013 [01/12] / Demichelis, R. - Raiteri, P. - Gale, J.D. - Dovesi, R. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 34. - SCIE ; WOS CC, s. 17814 - 17823

2013 [01/12] / Deringer, V.L. - Dronskowski, R. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 29. - SCIE ; WOS CC, s. 15075 - 15089

2013 [01/12] / Irrera, S. - Roldan, A. - Portalone, G. - De Leeuw, N.H. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 8. - SCIE ; WOS CC, s. 3949 - 3957

2013 [01/12] / **GBR** - Ramos-Sanchez, G. - Balbuena, P.B. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 28, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 11950 - 11959

2013 [01/12] / Shapley, T.V. - Molinari, M. - Zhu, R.L. - Parker, S.C. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 47. - SCIE ; WOS CC, s. 24975 - 24984

ADC_034: / Benedek, R. (Autor) (25%) - Thackeray, M.M. (Autor) (25%) - Low, J. (Autor) (25%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (25%): **Simulation of Aqueous Dissolution of Lithium Manganate Spinel from First Principles**. – CCC ; SCO ; WOS CC.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 116, č. 6 (2012), s. 4050-4059 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,462 - 2012

SJR: 2,529 - 2012
CiteScore: 8 - 2012

Ohlasy (58):

2025 [01/20] / **NLD** - Niu, Yao - Wang, Jing - Wang, Peifeng - Xing, Haiyang - Zhang, Kai - Xu, Youlong. **Multi-doping induces truncated octahedral structure formation in lithium manganate cathode material** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.161552 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 681, art. no. 161552 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 161552

2024 [01/20] / **USA** - Shu, Yuming - Lei, Hanghang - Huang, Jiangnan - Pan, Qing - Lian, Huimin - Li, Yujin - Cao, Ziwei - Wang, Haoji - Hu, Xinyu - Zhang, Baichao - Du, Ke - Hu, Guorong - Cao, Yanbing - Zou, Guoqiang - Peng, Zhongdong - Deng, Wentao - Hou, Hongshuai - Chen, Di - Ji, Xiaobo. **Oxides Induced Preferential Growth of {110} Planes for Superior Performance Single-Crystal LiMn2O4 through Solid-State Process** [elektronický dokument]. DOI 10.1021/acs.jpclett.4c02093 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2024, Roč. 15, č. 34, s. 8628-8635 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 8628 - 8635

2024 [01/20] / **GBR** - Zhang, Chao - Wan, Jing Zhe - Gao, Liang - Cai, Zhi Peng - Ma, Chao - Wang, Kai Xue - Chen, Jie Sheng. **Extraordinary cycling performance of high-voltage spinel LiNi0.5Mn1.5O4 materials enabled by interfacial engineering via molecular self-assembly** [elektronický dokument]. DOI 10.1039/d4ta02334j In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2024, Roč. 12, č. 21, s. 12810-12817 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 12810 - 12817

2024 [01/20] / **USA** - Nesterova, Valentina - Korostelev, Vladislav - Klyukin, Konstantin. **Unveiling the Role of Termination Groups in Stabilizing MXenes in Contact with Water** [elektronický dokument]. DOI 10.1021/acs.jpclett.4c00045 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2024, Roč. 15, č. 13, s. 3698-3704 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 3698 - 3704

2022 [01/20] / **NLD** - Chen, J. - Meng, T. - Leng, E. - E, J. **Review on metal dissolution characteristics and harmful metals recovery from electronic wastes by supercritical water** [elektronický dokument] In: **Journal of Hazardous Materials**: Environmental Control, Risk Assessment, Impact and Management. Amsterdam: Elsevier, 2022, Roč. 424, [tlačená forma] [online]. ISSN 0304-3894. ISSN (online) 1873-3336. - SCO, s. Art. No. 127693

2021 [01/20] / **USA** - Eckhoff, M. - Behler, J. **Insights into lithium manganese oxide-water interfaces using machine learning potentials** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 155, č. 24, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 244703

2021 [01/20] / **CHN** - Liang, Q. - Guo, Y. - Guo, J. - Xiang, M. - Liu, X. - Bai, W. - Ning, P. **Preparation and High Temperature Electrochemical Performance of LiNi0.08Mn1.92O4 Cathode Material of Submicron Truncated Octahedron** In: **Acta Chimica Sinica**, 2021, Roč. 79, č. 12. - SCO, s. 1526 - 1533

2021 [01/20] / **GBR** - Liang, Q. - Wang, Z. - Bai, W. - Guo, J. - Xiang, M. - Liu, X. - Bai, H. **Stimulative formation of truncated octahedral LiMn2O4by Cr and Al co-doping for use in durable cycling Li-ion batteries** [elektronický dokument] In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2021, Roč. 50, č. 46, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO, s. 17052 - 17061

2021 [01/20] / **CHN** - Li, X. - Tian, G. **First-principles calculation of adsorption mechanism of hydrochloric acid on chalcopyrite surface** In: **Guocheng Gongcheng Xuebao/The Chinese Journal of Process Engineering**, 2021, Roč. 21, č. 7. - SCO, s. 836 - 846

2021 [01/20] / **NLD** - Lee, S. - Kim, H. - Lee, J.-H. - Kim, B.-K. - Shin, H. - Kim, J. - Park, S. **Nano-interface engineering in all-solid-state lithium metal batteries: Tailoring exposed crystal facets of epitaxially grown LiNi0.5Mn1.5O4 films** [elektronický dokument] In: **Nano Energy**. Amsterdam: Elsevier, 2021, Roč. 79, [tlačená forma] [online]. ISSN 2211-2855. ISSN (online) 2211-3282. - SCO, s. Art. No. 105480

2021 [01/20] / **DEU** - Huang, Y. - Dong, Y. - Li, S. - Lee, J. - Wang, C. - Zhu, Z. - Xue, W. - Li, Y. - Li, J. **Lithium Manganese Spinel Cathodes for Lithium-Ion Batteries** [elektronický dokument] In: **Advanced Energy Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2021, Roč. 11, č. 2, [tlačená forma] [online]. ISSN 1614-6832. ISSN (online) 1614-6840. - SCO, s. Art. No. 2000997

2020 [01/12] / **GBR** - Liu, Z. - Huang, Y. - Huang, Y. - Yang, Q. - Li, X. - Huang, Z. - Zhi, C. **Voltage issue of aqueous rechargeable metal-ion batteries** [elektronický dokument] In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 49, č. 1, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO, s. 180 - 232

2020 [01/12] / **USA** - Warburton, R.E. - Young, M.J. - Letourneau, S. - Elam, J.W. - Greeley, J. **Descriptor-Based Analysis of Atomic Layer Deposition Mechanisms on Spinel LiMn2O4 Lithium-Ion Battery Cathodes** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2020, Roč. 32, č. 5, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 1794 - 1806

2020 [01/12] / **GBR** - Wang, S. - Liu, H. - Xiang, M. - Guo, J. - Bai, W. - Bai, H. - Liu, X. - Su, C. **Improved electrochemical properties and kinetics of an LiMn2O4-based cathode co-modified: Via Cu doping with truncated octahedron morphology** [elektronický dokument] In: **New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2020, Roč. 44, č. 25, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCO, s. 10569 - 10577

2020 [01/12] / **NLD** - Amin, R. - Muralidharan, N. - Petla, R.K. - Ben Yahia, H. - Jassim Al-Hail, S.A. - Essehli, R. - Daniel, C. - Khaleel, M.A. - Belharouak, I. **Research advances on cobalt-free cathodes for Li-ion batteries - The high voltage LiMn1.5Ni0.5O4 as an example** [elektronický dokument] In: **Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2020, Roč. 467, [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCO, s. Art. No. 228318

2020 [01/12] / **GBR** - Kuenzel, M. - Kim, G.-T. - Zarrabeitia, M. - Lin, S.D. - Schuer, A.R. - Geiger, D. - Kaiser, U. - Bresser, D. - Passerini, S. **Crystal engineering of TMPOx-coated LiNi0.5Mn1.5O4 cathodes for high-performance lithium-ion batteries** [elektronický dokument] In: **Materials today**: science, technology, policy. Kidlington: Elsevier. Elsevier Science, 2020, Roč. 39, [tlačená forma] [online]. ISSN 1369-7021. ISSN (online) 1873-4103. ISSN (chybné) 1396-7021. - SCO, s. 127 - 136

2019 [01/12] / **USA** - Banerjee, A. - Ziv, B. - Shilina, Y. - Ziegelbauer, J.M. - Liu, H.S. - Harris, K.J. - Botton, G. - Goward, G.R. - Luski, S. - Aurbach, D. - Halalay, I.C. **In: Journal of the Electrochemical Society**. Pennington: The Electrochemical Society, 2019, Roč. 166, č. 3, 5369- [tlačená forma] [online]. ISSN 0013-4651. ISSN (online) 1945-7111. - SCIE ; WOS CC, s.

2019 [01/12] / Okuno, Y. - Ushirogata, K. - Sodeyama, K. - Shukri, G. - Tateyama, Y. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 4. - SCIE ; WOS CC, s. 2267 - 2277

2019 [01/12] / **USA** - Intan, N.N. - Klyukin, K. - Alexandrov, V. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2019, Roč. 11, č. 22, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 20110 - 20116

2019 [01/12] / **USA** - Ke, H.B. - Taylor, C.D. **In: Corrosion**: journal of science and engineering. Houston: NACE

International, 2019, Roč. 75, č. 7, [tlačená forma]. ISSN 0010-9312. ISSN (online) 1938-159X. - SCIE ; WOS CC, s. 708 - 726

2019 [01/12] / **USA** - Zhu, Z. - Peelaers, H. - Van de Walle, C.G. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2019, Roč. 31, č. 14, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 5224 - 5228

2019 [01/12] / Young, M.J. - Letourneau, S. - Warburton, R.E. - Dose, W.M. - Johnson, C. - Greeley, J. - Elam, J.W. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 39. - SCIE ; WOS CC, s. 23783 - 23790

2018 [01/12] / **NLD** - Zheng, X.Y. - Liu, W.J. - Qu, Q.T. - Shi, Q. - Zheng, H.H. - Huang, Y.H. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 455, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 349 - 356

2018 [01/12] / Klyukin, K. - Rosso, K.M. - Alexandrov, V. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 28. - SCIE ; WOS CC, s. 16086 - 16091

2018 [01/12] / Shen, Z.Z. - Kerisit, S.N. - Stack, A.G. - Rosso, K.M. **In: Journal of Physical Chemistry Letters**, 2018, Roč. 9, č. 7. - SCIE ; WOS CC, s. 1809 - 1814

2018 [01/12] / Zhan, C. - Wu, T.P. - Lu, J. - Amine, K. **In: Energy & Environmental Science**, 2018, Roč. 11, č. 2. - SCIE ; WOS CC, s. 243 - 257

2018 [01/12] / **NLD** - Ullah, A. - Majid, A. - Rani, N. **In: Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2018, Roč. 27, č. 1, [tlačená forma] [online]. ISSN 2095-4956. - SCIE ; WOS CC, s. 219 - 237

2018 [01/12] / **USA** - Kwon, Y. - Lee, Y. - Kim, S.O. - Kim, H.S. - Kim, K.J. - Byun, D. - Choi, W. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2018, Roč. 10, č. 35, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 29457 - 29466

2018 [01/12] / **NLD** - Nomura, F. - Liu, Y.B. - Tanabe, T. - Gunji, T. - Tsuda, T. - Ugawa, S. - Lee, H. - Ohsaka, T. - Matsumoto, F. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2018, Roč. 283, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 478 - 487

2018 [01/12] / **USA** - Yu, X.K. - Chen, X. - Buchholz, D.B. - Li, Q.Q. - Wu, J.S. - Fenter, P.A. - Bedzyk, M.J. - Dravid, V.P. - Barnett, S.A. **In: ACS applied nano materials**. Washington: American Chemical Society, 2018, Roč. 1, č. 2, [online]. ISSN (online) 2574-0970. - SCIE ; WOS CC, s. 642 - 653

2017 [01/12] / **USA** - Bhandari, A. - Bhattacharya, J. **In: Journal of the Electrochemical Society**. Pennington: The Electrochemical Society, 2017, Roč. 164, č. 2, 106- [tlačená forma] [online]. ISSN 0013-4651. ISSN (online) 1945-7111. - SCIE ; WOS CC, s.

2017 [01/12] / **NLD** - Yang, C.X. - Deng, Y.F. - Gao, M. - Yang, X.F. - Qin, X.S. - Chen, G.H. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2017, Roč. 225, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 198 - 206

2017 [01/12] / **USA** - Leung, K. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2017, Roč. 29, č. 6, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 2550 - 2562

2017 [01/12] / **DEU** - Kalluri, S. - Yoon, M. - Jo, M. - Liu, H.K. - Dou, S.X. - Cho, J. - Guo, Z.P. **In: Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2017, Roč. 29, č. 48, [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCIE ; WOS CC, s. Art. No. 1605807

2016 [01/12] / **USA** - Lee, Y.K. - Park, J. - Lu, W. **In: Journal of the Electrochemical Society**. Pennington: The Electrochemical Society, 2016, Roč. 163, č. 7, 1359- [tlačená forma] [online]. ISSN 0013-4651. ISSN (online) 1945-7111. - SCIE ; WOS CC, s.

2016 [01/12] / **GBR** - Lu, J. - Lee, K.S. **In: Materials Technology**: advanced Performance Materials. [s.l.]: Taylor & Francis Group, 2016, Roč. 31, č. 11. ISSN 1066-7857. ISSN (online) 1753-5557. - SCIE ; WOS CC, s. 628 - 641

2016 [01/12] / **NLD** - Fang, J.C. - Xu, Y.F. - Xu, G.L. - Shen, S.Y. - Li, J.T. - Huang, L. - Sun, S.G. **In: Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2016, Roč. 304, [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCIE ; WOS CC, s. 15 - 23

2016 [01/12] / **USA** - Ma, J. - Hu, P. - Cui, G.L. - Chen, L.Q. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2016, Roč. 28, č. 11, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 3578 - 3606

2016 [01/12] / **NLD** - Jin, W. - Yin, G.Q. - Wang, Z.G. - Fu, Y.Q. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2016, Roč. 385, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 72 - 79

2015 [01/12] / **GBR** - Gao, X.W. - Deng, Y.F. - Wexler, D. - Chen, G.H. - Chou, S.L. - Liu, H.K. - Shi, Z.C. - Wang, J.Z. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2015, Roč. 3, č. 1, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 404 - 411

2015 [01/12] / **NLD** - Alias, N. - Mohamad, A.A. **In: Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2015, Roč. 274, [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCIE ; WOS CC, s. 237 - 251

2015 [01/12] / **USA** - Fu, Y. - Jiang, H. - Hu, Y.J. - Dai, Y.H. - Zhang, L. - Li, C.Z. **In: Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2015, Roč. 54, č. 15, [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCIE ; WOS CC, s. 3800 - 3805

2015 [01/12] / Scivetti, I. - Teobaldi, G. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 37. - SCIE ; WOS CC, s. 21358 - 21368

2014 [01/12] / **GBR** - Lin, H.B. - Hu, J.N. - Rong, H.B. - Zhang, Y.M. - Mai, S.W. - Xing, L.D. - Xu, M.Q. - Li, X.P. - Li, W.S. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2014, Roč. 2, č. 24, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 9272 - 9279

2014 [01/12] / **NLD** - Han, Y.K. - Lee, K. - Kang, S. - Huh, Y.S. - Lee, H. **In: Computational Materials Science**. Amsterdam: Elsevier, 2014, Roč. 81, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 548 - 550

2014 [01/12] / Assadi, M.H.N. - Sahajwalla, V. **In: Industrial and Engineering Chemistry Research**, 2014, Roč. 53, č. 10. - SCIE ; WOS CC, s. 3861 - 3864

2014 [01/12] / **USA** - Kumar, N. - Leung, K. - Siegel, D.J. **In: Journal of the Electrochemical Society**. Pennington: The Electrochemical Society, 2014, Roč. 161, č. 8, 3059- [tlačená forma] [online]. ISSN 0013-4651. ISSN (online) 1945-7111. - SCIE ; WOS CC, s.

2014 [01/12] / **NLD** - Fu, Y. - Jiang, H. - Hu, Y.J. - Zhang, L. - Li, C.Z. **In: Journal of Power Sources**: the International Journal on the Science and Technology of Electrochemical Energy Systems. Amsterdam: Elsevier, 2014, Roč. 261, [tlačená forma] [online]. ISSN 0378-7753. ISSN (online) 1873-2755. - SCIE ; WOS CC, s. 306 - 310

2014 [01/12] / **NLD** - Bagci, S. - Tutuncu, H.M. - Duman, S. - Bulut, E. - Ozacar, M. - Srivastava, G.P. **In: Journal of Physics and Chemistry of Solids**: an International Journal. Amsterdam: Elsevier, 2014, Roč. 75, č. 4, [tlačená forma]. ISSN (online) 0022-3697. - SCIE ; WOS CC, s. 463 - 469

2014 [01/12] / **GBR** - Manthiram, A. - Chemelewski, K. - Lee, E.S. **In: Energy and Environmental Science**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 7, č. 4, [tlačená forma] [online]. ISSN 1754-5692. ISSN (online) 1754-5706. - SCIE ; WOS CC, s. 1339 - 1350

2014 [01/12] / **DEU** - Laszczynski, N. - von Zamory, J. - Loeffler, N. - Cho, G.B. - Kim, G.T. - Passerini, S. **In: ChemElectroChem**. Weinheim: John Wiley & Sons. Wiley-VCH, 2014, Roč. 1, č. 9, [online] [tlačená forma]. ISSN (online) 2196-0216. - SCIE ; WOS CC, s. 1537 - 1542

2013 [01/12] / **NLD** - Jiang, J.B. - Du, K. - Cao, Y.B. - Peng, Z.D. - Hu, G.R. - Duan, J.G. **In: Powder Technology**: an International Journal on the Science and Technology of Wet and Dry Particulate Systems. Amsterdam: Elsevier. Elsevier Science, 2013, Roč. 246, [tlačená forma] [online]. ISSN 0032-5910. ISSN (online) 1873-328X. - SCIE ; WOS CC, s. 723 - 727

2013 [01/12] / **USA** - Leung, K.Y. - De Castro, S.C.P. - Cabreiro, F. - Gustavsson, P. - Copp, A.J. - Greene, N.D.E. **In: Molecular and cellular biochemistry**. New York: Springer Nature. Springer, 2013, Roč. 378, č. 1-2, [tlačená forma] [online]. ISSN 0300-8177. ISSN (online) 1573-4919. - SCIE ; SCO ; WOS CC, s. 1539 - 1547

2013 [01/12] / **GBR** - Chemelewski, K.R. - Li, W. - Gutierrez, A. - Manthiram, A. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2013, Roč. 1, č. 48, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 15334 - 15341

2013 [01/12] / **GBR** - Wang, Y.J. - Hu, P. - Ma, X.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 40, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 17112 - 17117

2013 [01/12] / **GBR** - Chemelewski, K.R. - Shin, D.W. - Li, W. - Manthiram, A. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2013, Roč. 1, č. 10, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 3347 - 3354

2012 [01/12] / **USA** - Kim, J.S. - Kim, K. - Cho, W. - Shin, W.H. - Kanno, R. - Choi, J.W. **In: Nano letters**. Washington: American Chemical Society, 2012, Roč. 12, č. 12, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 6358 - 6365

2012 [01/12] / **USA** - Wu, J.-L. - Leung, K.-F. - Tong, S.-F. - Lam, C.-W. **In: Rapid Communications in Mass Spectrometry**. Hoboken: John Wiley & Sons, 2012, Roč. 26, č. 2, [tlačená forma] [online]. ISSN 0951-4198. ISSN (online) 1097-0231. - SCO, s. 9852 - 9861

ADC_035: / Bučko, Tomáš (Autor) [UKOPRCFZ] (25%) - Hafner, Jürgen (Autor) (25%) - Lebegue, Sebastien (Autor) (25%) - Ángyán, János G. (Autor) (25%): **Spin crossover transition of Fe(phen)(2)(NCS)(2): periodic dispersion-corrected density-functional study**. – CCC ; SCO ; WOS CC.
In: *Physical Chemistry Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Londýn (Veľká Británia) : The Royal Society of Chemistry, Cambridge (Veľká Británia) : The Royal Society of Chemistry. – ISSN 1463-9076. – ISSN (online) 1463-9084. – Roč. 14, č. 16 (2012), s. 5389-5396 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,168 - 2012
SJR: 1,921 - 2012
CiteScore: 5,7 - 2012

Ohlasy (58):
2025 [01/20] / **NLD** - Reinhardt, Peter. **János Ángyán—A European career**. DOI 10.1016/bs.aiq.2025.02.003 In: **Advances in Quantum Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2025. ISSN 00653276. - SCO, s.

2025 [01/20] / **USA** - Jaber El Lala, Iman - Sánchez-De-Armas, Rocío - Calzado, Carmen J. **Dinuclear Fe(II) Spin-Crossover Complex Deposited on the Au(111) Surface: Exploration Based on Quantum-Chemistry Calculations** [elektronický dokument]. DOI 10.1021/acs.inorgchem.4c05434 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2025, Roč. 64, č. 11, s. 5522-5531 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 5522 - 5531

2025 [01/20] / **NLD** - Lazaar, Koussai - Aouaini, Fatma - Alkallas, Fatemah H. - Alyousef, Haifa - Gueddida, Saber. **Exploring the two step spin transition of Fe(NCBH3)(4phpy)2(m-bpypz)2 with ab initio calculations** [elektronický dokument]. DOI 10.1016/j.jssc.2024.125167 In: **Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2025, Roč. 344, art. no. 125167 [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCO ; CCC ; WOS CC, s. art. no. 125167

2024 [01/20] / **GBR** - Radoń, Mariusz. **Predicting spin states of iron porphyrins with DFT methods including crystal packing effects and thermodynamic corrections** [elektronický dokument]. DOI 10.1039/d4cp01327a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2024, Roč. 26, č. 26, s. 18182-18195 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 18182 - 18195

2023 [01/20] / **GBR** - Radoń, Mariusz. **Benchmarks for transition metal spin-state energetics: why and how to employ experimental reference data?** [elektronický dokument]. DOI 10.1039/d3cp03537a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 45, s. 30800-30820 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 30800 - 30820

2023 [01/20] / **CHE** - Zhang, Yachao. **Surface-Induced Electronic and Vibrational Level Shifting of [Fe(py)2bpym(NCS)2] on Al(100)** [elektronický dokument]. DOI 10.3390/ma16186150 In: **Materials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 16, č. 18, art. no. 6150 [online]. ISSN (online) 1996-1944. - SCO ; CCC ; WOS CC, s. art. no. 6150

2023 [01/20] / **DEU** - Herz, Jakob - Meyer, Robert - Wolny, Juliusz A. - Schünemann, Volker - Urbassek, Herbert M. **Crystal effects in the vibrational spectra of one-dimensional molecular spin crossover crystals using molecular dynamics simulations** [elektronický dokument]. DOI 10.1007/s00339-023-06594-1 In: **Applied physics A**: materials science and processing. Berlín: Springer Nature. Springer International Publishing AG, 2023, Roč. 129, č. 5, art. no. 345 [tlačená forma] [online]. ISSN 0947-8396. ISSN (online) 1432-0630. - SCO ; CCC ; WOS CC, s. art. no. 345

2023 [01/20] / **CHN** - Li, Zhao Yang - Wu, Ying Ying - Li, Yao - Wang, Jin Hua - Sulaiman, Arshia - Javed, Mohammad Khurram - Zhang, Ya Chao - Li, Wei - Bu, Xian He. **Slow Phase Transition-Induced Scan Rate Dependence of Spin Crossover in a Two-Dimensional Supramolecular Fe(III) Complex**. DOI 10.31635/ccschem.022.202101721 In: **CCS Chemistry**. Beijing: Chinese chemical soc, c/o Dept int affairs, secretary of chem soc, 2023, Roč. 5, č. 2, s. 412-422. ISSN 2096-5745. - SCO ; WOS CC, s. 412 - 422

2023 [01/20] / **USA** - Lazaar, Koussai - Aouaini, Fatma - Gueddida, Saber. **Binuclear spin-crossover [Fe(bt)(NCS)2]2(bpm) complex: A study using first principles calculations** [elektronický dokument]. DOI 10.1063/5.0147313 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 14, art. no. 144307 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s.

2022 [01/20] / **USA** - Privault, G. - Mevellec, J.-Y. - Lorenc, M. - Humbert, B. - Janod, E. - Daro, N. - Chastanet, G. - Subedi, A. - Collet, E. **Symmetry-Resolved Study of Lattice Vibration and Libration Modes in [Fe(phen)2(NCS)2] Crystal** In: **Crystal Growth and Design**, 2022, Roč. 22, č. 8. - SCO, s. 5100 - 5109

2022 [01/20] / **NLD** - Avila, Y. - Scanda, K. - Mojica, R. - Rodriguez-Hernandez, J. - Cruz-Santiago, L.A. - Gonzalez, M. - Reguera, E. **Thermally-induced spin transition in Fe(4,4´-Azopyridine)[Fe(CN)5NO]** [elektronický dokument] In: **Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2022, Roč. 310, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCO, s. Art. No. 123054

2022 [01/20] / **NLD** - Mejia-Rodriguez, D. - Albavera-Mata, A. - Fonseca, E. - Chen, D.-T. - Cheng, H.-P. - Hennig, R.G. - Trickey, S.B. **Barriers to predictive high-throughput screening for spin-crossover** [elektronický dokument] In: **Computational Materials Science**. Amsterdam: Elsevier, 2022, Roč. 206, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO, s. Art. No. 111161

2021 [01/20] / **GBR** - Vidal, D. - Cirera, J. - Ribas-Arino, J. **Accurate calculation of spin-state energy gaps in Fe(iii) spin-crossover systems using density functional methods** [elektronický dokument] In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2021, Roč. 50, č. 47, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO, s. 17635 - 17642

2021 [01/20] / **USA** - Yang, F.-L. - Wu, W.-H. - Wang, Y.-Q. - Chen, X. - Liang, B.-B. - Mi, H.-L. - Zhang, G.-L. - Chen, X.-Y. - Shi, Y. **Abundant Solvatomorphism-Tuned Spin Crossover in a Dinuclear Fe(II) Compound: Computational Insights on Molecular Distortion and Packing Effects** In: **Crystal Growth and Design**, 2021, Roč. 21, č. 12. - SCO, s. 6671 - 6683

2021 [01/20] / **CHE** - Shakil, M. - Naz, A. - Zeba, I. - Gillani, S.S.A. - Rafique, M. - Ahmed, S. - Zafar, M. **Structural and Magnetic Behavior of MoS2 on Doping of Transition Metals: a DFT Study** [elektronický dokument] In: **Journal of Superconductivity and Novel Magnetism**. Cham: Springer Nature, 2021, Roč. 34, č. 12, [tlačená forma] [online]. ISSN 1557-1939. ISSN (online) 1557-1947. - SCO, s. 3441 - 3453

2021 [01/20] / **GBR** - Sanchez-De-Armas, R. - Montenegro-Pohlhammer, N. - Develioglu, A. - Burzuri, E. - Calzado, C.J. **Spin-crossover complexes in nanoscale devices: Main ingredients of the molecule-substrate interactions** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 13, č. 44, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 18702 - 18713

2021 [01/20] / **DEU** - Montenegro-Pohlhammer, N. - Sanchez-de-Armas, R. - Calzado, C.J. **Deposition of the Spin Crossover FeII-Pyrazolylborate Complex on Au(111) Surface at the Molecular Level** [elektronický dokument] In: **Chemistry - A European Journal**. Weinheim: John Wiley & Sons. Wiley-VCH, 2021, Roč. 27, č. 2, [tlačená forma] [online]. ISSN 0947-6539. ISSN (online) 1521-3765. - SCO, s. 712 - 723

2020 [01/12] / Aldaz, C.R. - Martinez, T.J. - Zimmerman, P.M. **The Mechanics of the Bicycle Pedal Photoisomerization**

in Crystalline cis,cis-1,4-Diphenyl-1,3-butadiene In: **Journal of Physical Chemistry A**, 2020, Roč. 124, č. 43. - SCO, s. 8897 - 8906

2020 [01/12] / **USA** - Ohlrich, M. - Powell, B.J. **Fast, accurate enthalpy differences in spin crossover crystals from DFT+U** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 104107

2020 [01/12] / Cirera, J. - Ruiz, E. **Assessment of the SCAN Functional for Spin-State Energies in Spin-Crossover Systems** In: **Journal of Physical Chemistry A**, 2020, Roč. 124, č. 24. - SCO, s. 5053 - 5058

2020 [01/12] / **GBR** - Chakraborty, A. - Chakraborty, A. - Ghosh, S. - Dasgupta, I. **Theoretical analysis of pressure induced spin crossover phenomenon in a di-nuclear Fe(II) molecular complex** In: **Journal of Physics Condensed Matter**, 2020, Roč. 32, č. 16. - SCO, s. Art. No. 165802

2020 [01/12] / **GBR** - Vela, S. - Vela, S. - Fumanal, M. - Cirera, J. - Ribas-Arino, J. **Thermal spin crossover in Fe(ii) and Fe(iii). Accurate spin state energetics at the solid state** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 9, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 4938 - 4945

2019 [01/12] / **GBR** - Radon, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 9, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 4854 - 4870

2019 [01/12] / **USA** - Steinbauer, J. - Biermann, S. - Bhandary, S. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 245418

2019 [01/12] / **DEU** - Molnar, G. - Mikolasek, M. - Ridier, K. - Fahs, A. - Nicolazzi, W. - Bousseksou, A. **In: Annalen der Physik**. Weinheim: John Wiley & Sons. Wiley-VCH, 2019, Roč. 531, č. 10, [tlačená forma]. ISSN 0003-3804. ISSN (online) 1521-3889. - SCIE ; WOS CC, s. Art. No. 1900076

2018 [01/12] / Wen, Z.Q. - Zhou, L.P. - Cheng, J.F. - Li, S.J. - You, W.L. - Wang, X.F. **In: Journal of Physics-Condensed Matter**, 2018, Roč. 30, č. 10. - SCIE ; WOS CC, s. Art. No. 105301

2018 [01/12] / **USA** - Vela, S. - Paulsen, H. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2018, Roč. 57, č. 15, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 9478 - 9488

2018 [01/12] / **FRA** - Wolny, J.A. - Schunemann, V. - Nemeth, Z. - Vanko, G. **In: Comptes Rendus Chimie**. [s.l.]: Elsevier, 2018, Roč. 21, č. 12, [tlačená forma] [online]. ISSN 1631-0748. ISSN (online) 1878-1543. - SCIE ; WOS CC, s. 1152 - 1169

2017 [01/12] / Kreutzburg, L. - Hubner, C.G. - Paulsen, H. **In: materials**, 2017, Roč. 10, č. 2. - SCIE ; WOS CC, s. nestr.

2017 [01/12] / **USA** - Fumanal, M. - Jimenez-Gravalos, F. - Ribas-Arino, J. - Vela, S. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2017, Roč. 56, č. 8, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 4474 - 4483

2017 [01/12] / Sirirak, J. - Sertphon, D. - Phonsri, W. - Harding, P. - Harding, D.J. **In: : International journal of quantum chemistry,** 2017, Roč. 117, č. 9. - SCIE ; WOS CC, s. Art. No. 25362

2016 [01/12] / **GBR** - Pointillart, F. - Liu, X. - Kepenekian, M. - Le Guennic, B. - Golhen, S. - Dorcet, V. - Roisnel, T. -

Cador, O. - You, Z. - Hauser, J. - Decurtins, S. - Ouahab, L. - Liu, S.X. **In: Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2016, Roč. 45, č. 28, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCIE ; WOS CC, s. 11267 - 11271

2016 [01/12] / Kang, S. - Shiota, Y. - Kariyazaki, A. - Kanegawa, S. - Yoshizawa, K. - Sato, O. **In: Chemistry-A European Journal**, 2016, Roč. 22, č. 2. - SCIE ; WOS CC, s. 532 - 538

2016 [01/12] / **JPN** - Thang, D.V. - Thanh, N.V. - Hien, N.T. - Sinh, N.H. - Tuan, N.A. **In: Materials Transactions**. Sendai: Japan Institute of Metals and Materials, 2016, Roč. 57, č. 3, [tlačená forma]. ISSN 1345-9678. ISSN (online) 1347-5320. - SCIE ; WOS CC, s. 302 - 304

2016 [01/12] / **CHE** - Vela, S. - Gourlaouen, C. - Fumanal, M. - Ribas-Arino, J. **In: Magnetochemistry**. Basel: Multidisciplinary Digital Publishing Institute, 2016, Roč. 2, č. 1, [online]. ISSN (online) 2312-7481. - SCIE ; WOS CC, s. Art. No. 6

2016 [01/12] / **CHE** - Paulsen, H. **In: Magnetochemistry**. Basel: Multidisciplinary Digital Publishing Institute, 2016, Roč. 2, č. 1, [online]. ISSN (online) 2312-7481. - SCIE ; WOS CC, s. Art. No. 14

2016 [01/12] / **GBR** - Li, R. - Tian, J.Z. - Zhuang, C.H. - Zhang, Y.C. - Geng, X.Y. - Zhu, L.N. - Sun, J.S. **In: Journal of experimental biology**. Londýn: Company of Biologists, 2016, Roč. 219, č. 8, [tlačená forma] [online]. ISSN 0022-0949. ISSN (online) 1477-9145. - SCIE ; SCO ; WOS CC, s. Art. No. 124704

2015 [01/12] / Zhang, Y.C. - Deng, M.S. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 37. - SCIE ; WOS CC, s. 21681 - 21687

2015 [01/12] / **USA** - Chen, J. - Millis, A.J. - Marianetti, C.A. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 241111

2015 [01/12] / **GBR** - Vela, S. - Fumanal, M. - Ribas-Arino, J. - Robert, V. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 16306 - 16314

2014 [01/12] / **USA** - Rudavskyi, A. - Sousa, C. - de Graaf, C. - Havenith, R.W.A. - Broer, R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 18, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 184318

2014 [01/12] / Moyret-Lalle, C. - Ruiz, E. - Puisieux, A. **In: World Journal of Critical Oncology**, 2014, Roč. 5, č. 3. - SCIE ; SCO ; WOS CC, s. 14 - 22

2014 [01/12] / **GBR** - Vela, S. - Novoa, J.J. - Ribas-Arino, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 27012 - 27024

2014 [01/12] / **GBR** - Borgogno, A. - Rastrelli, F. - Bagno, A. **In: Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2014, Roč. 43, č. 25, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCIE ; WOS CC, s. 9486 - 9496

2014 [01/12] / **USA** - Saha-Dasgupta, T. - Oppeneer, P.M. **In: MRS Bulletin**: a publication of the Materials Research Society. Pittsburgh: Materials Research Society, 2014, Roč. 39, č. 7, [tlačená forma]. ISSN 0883-7694. ISSN (online) 1938-1425. - SCIE ; WOS CC, s. 614 - 620

2014 [01/12] / **USA** - Zhang, Y.C. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 141, č. 21, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 214703

2014 [01/12] / Fumanal, M. - Vela, S. - Ribas-Arino, J. - Novoa, J.J. **In: Chemistry-An Asian Journal**, 2014, Roč. 9, č. 12. - SCIE ; WOS CC, s. 3612 - 3622

2014 [01/12] / Elijosiute, E. - Eicher-Lorka, O. - Griskonis, E. - Kuodis, Z. - Jankunaite, D. - Denafas, G. **In: Spectrochimica Acta part A-Molecular and Biomolecular Spectroscopy**, 2014, Roč. 129. - SCIE ; WOS CC, s. 43 - 51

2013 [01/12] / **USA** - Maldonado, P. - Kanungo, S. - Saha-Dasgupta, T. - Oppeneer, P.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 88, č. 2, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 020408

2013 [01/12] / **NLD** - Suffren, Y. - Rollet, F.G. - Levasseur-Grenon, O. - Reber, C. **In: Polyhedron**: The International Journal for Research in Inorganic Chemistry. Amsterdam: Elsevier, 2013, Roč. 52, [tlačená forma] [online]. ISSN 0277-5387. ISSN (online) 1873-3719. - SCIE ; WOS CC, s. 1081 - 1089

2013 [01/12] / Paulsen, H. - Schunemann, V. - Wolny, J.A. **In: European Journal of Inorganic Chemistry, Iss. 5-6, 2013**, 2013. - SCIE ; WOS CC, s. 628 - 641

2013 [01/12] / Bhattacharjee, A. - Roy, M. - Ksenofontov, V. - Kitchen, J.A. - Brooker, S. - Gutlich, P. **In: European Journal of Inorganic Chemistry, Iss. 5-6, 2013**, 2013. - SCIE ; WOS CC, s. 843 - 849

2013 [01/12] / **GBR** - Chattopadhyaya, M. - Alam, M.M. - Chakrabarti, S. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2013, Roč. 3, č. 43, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 19894 - 19898

2013 [01/12] / **GBR** - Rackwitz, S. - Klopper, W. - Schunemann, V. - Wolny, J.A. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 15450 - 15458

2013 [01/12] / **USA** - Gueddida, S. - Alouani, M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 87, č. 14, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 144413

2013 [01/12] / **GBR** - Gerasimova, T.P. - Katsyuba, S.A. **In: Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2013, Roč. 42, č. 5, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCIE ; WOS CC, s. 1787 - 1797

2013 [01/12] / Chis, V. - Droghetti, A. - Isai, R. - Morari, C. - Rungger, I. - Sanvito, S. **In: Processes in Isotopes and Molecules**, 2013, Roč. 1565. - SCIE ; WOS CC, s. 57 - 62

2012 [01/12] / **USA** - Tarafder, K. - Kanungo, S. - Oppeneer, P.M. - Saha-Dasgupta, T. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2012, Roč. 109, č. 7, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s. Art. No. 077203

ADC_036: / Göltl, Florian (Autor) (25%) - Grüneis, Andreas (Autor) (25%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (25%) - Hafner, Jürgen (Autor) (25%): **Van der Waals interactions between hydrocarbon molecules and zeolites: Periodic calculations at different levels of theory, from density functional theory to the random phase approximation and Moller-Plesset perturbation theory**. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 137, č. 11 (2012), s. 14111-14111 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,157 - 2012
SJR: 1,832 - 2012
CiteScore: 5,3 - 2012
Nordic List: 1 - 2012

Ohlasy (107):
2025 [01/20] / **DEU** - Huber, Philipp - Plessow, Philipp N. **Accurate and Efficient Description of Acidic Zeolites with Plane-Wave Density Functional Theory Using Range-Separated Hybrid Functionals** [elektronický dokument]. DOI 10.1002/cphc.202500147 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 15, art. no. e202500147 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **USA** - Plessow, Philipp N. **Anharmonic Adsorption Free Energies and Apparent Activation Barriers for Mobile Reactants Based on Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jctc.5c01100 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 17, s. 8518-8532 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 8518 - 8532

2025 [01/20] / **USA** - Mitro, Sujon Kumar - Brauer, Jakob - Fischer, Michael. **Benchmarking DFT Calculations for Adsorption Studies: Pharmaceuticals and Related Organic Molecules in Cation-Exchanged Zeolites** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c05270 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 46, s. 20722-20737 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 20722 - 20737

2025 [01/20] / **NLD** - Ammar, Wassim - Lemaitre, Laurent - Pérez-Pellitero, Javier - Méthivier, Alain - Manko, Maria - Larmier, Kim. **DFT and GCMC modeling study of the adsorption of glucose and xylose on metal-exchanged Faujasite zeolites** [elektronický dokument]. DOI 10.1016/j.seppur.2025.135182 In: **Separation and Purification Technology**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 379, art. no. 135182 [tlačená forma] [online]. ISSN 1383-5866. ISSN (online) 1873-3794. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 135182

2024 [01/20] / **GBR** - de Reviere, Arno - Verberckmoes, An - Sabbe, Maarten K. **Mechanistic origins for the enhanced ethanol dehydration kinetics in H-ZSM-5 by cofeeding n-butanol** [elektronický dokument]. DOI 10.1039/d4cy00532e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 15, s. 4319-4340 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4319 - 4340

2024 [01/20] / **CHE** - Samborska-Goik, Katarzyna - Pogrzeba, Marta. **A Critical Review of the Modelling Tools for the Reactive Transport of Organic Contaminants** [elektronický dokument]. DOI 10.3390/app14093675 In: **Applied sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 14, č. 9, art. no. 3675 [online]. ISSN (online) 2076-3417. -

SCO ; CCC ; WOS CC, s. art. no. 3675

2024 [01/20] / **USA** - Fischer, Michael - Brauer, Jakob. **Studying the adsorption of emerging organic contaminants in zeolites with dispersion-corrected density functional theory calculations: From numbers to recommendations** [elektronický dokument]. DOI 10.1002/open.202300273 In: **ChemistryOpen**. Hoboken: John Wiley & Sons. Wiley Blackwell, 2024, Roč. 13, č. 7, art. no. e202300273 [online]. ISSN (online) 2191-1363. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Contaldo, Gabriele - Ferri, Matteo - Negri, Chiara - Nova, Isabella - Maestri, Matteo - Tronconi, Enrico. **First-principles Assessment of the Role of Water in the Reduction Half Cycle of Low-Temperature NH3-SCR over Cu-CHA** [elektronický dokument]. DOI 10.1002/cctc.202300673 In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2023, Roč. 15, č. 20, art. no. e202300673 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **DEU** - Hellier, Adrien - Chizallet, Céline - Raybaud, Pascal. **PtOxCly(OH)z(H2O)n Complexes under Oxidative and Reductive Conditions: Impact of the Level of Theory on Thermodynamic Stabilities** [elektronický dokument]. DOI 10.1002/cphc.202200711 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2023, Roč. 24, č. 3, art. no. e202200711 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Schwalbe-Koda, Daniel - Gómez-Bombarelli, Rafael. **Generating, Managing, and Mining Big Data in Zeolite Simulations** [elektronický dokument]. DOI 10.1002/9781119819783.ch4 In: **AI-Guided Design and Property Prediction for Zeolites and Nanoporous Materials**. Hoboken: John Wiley & Sons, 2023, s. 81-111. ISBN 9781119819752. ISBN (online) 9781119819783. - SCO, s. 81 - 111

2023 [01/20] / **USA** - Daouli, Ayoub - Rey, Jérôme - Lahrar, El Hassane - Valtchev, Valentin - Badawi, Michael - Guillet-Nicolas, Rémy. **Ab Initio Screening of Divalent Cations for CH4, CO2, H2, and N2 Separations in Chabazite Zeolite** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c01882 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 45, s. 15962-15973 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 15962 - 15973

2023 [01/20] / **GBR** - Delachaux, F. - Hessou, E. P. - Vallières, C. - Monnier, H. - Badawi, M. **A dispersion-corrected DFT method for zeolite-based CO2/N2separation: Assessment and application** [elektronický dokument]. DOI 10.1016/j.jece.2022.109052 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2023, Roč. 11, č. 1, art. no. 109052 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s. art. no. 109052

2023 [01/20] / **GBR** - Cnudde, Pieter - Waroquier, Michel - Van Speybroeck, Veronique. **Universal descriptors for zeolite topology and acidity to predict the stability of butene cracking intermediates** [elektronický dokument]. DOI 10.1039/d3cy00642e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 16, s. 4857-4872 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4857 - 4872

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **GBR** - Zhour, Kazem - Daouli, Ayoub - Postnikov, Andrei - Hasnaoui, Abdellatif - Badawi, Michael. **Potential of nanostructured carbon materials for iodine detection in realistic environments revealed by first-principles calculations** [elektronický dokument]. DOI 10.1039/d3cp02205f In: **Physical Chemistry Chemical Physics**.

Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 39, s. 26461-26474 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 26461 - 26474

2022 [01/20] / **GBR** - Komissarov, L. - Verstraelen, T. **Zeo-1, a computational data set of zeolite structures** [elektronický dokument] In: **Scientific data**. London: Springer Nature. Nature Publishing Group, 2022, Roč. 9, č. 1, [online]. ISSN (online) 2052-4463. - SCO, s. Art. No. 61

2022 [01/20] / **USA** - Goldzak, T. - Wang, X. - Ye, H.-Z. - Berkelbach, T.C. **Accurate thermochemistry of covalent and ionic solids from spin-component-scaled MP2** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2022, Roč. 157, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 174112

2022 [01/20] / **USA** - Koninckx, E. - Kostetskyy, P. - Broadbelt, L.J. **Probing Heterodimer and Multiadsorbate Hydrocarbon Adsorption Trends in the MFI Framework** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 32. - SCO, s. 13894 - 13904

2022 [01/20] / **USA** - Hessou, E.P. - Badawi, M. - Valentin, L. - Atohoun, G. - Dzwigaj, S. - Calatayud, M. - Tielens, F. **Elucidation of the IR of Cu and Mn substituted intraframework SiBEA zeolites** [elektronický dokument] In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, č. 7-8, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 848 - 858

2022 [01/20] / **GBR** - Ayadi, T. - Badawi, M. - Cantrel, L. - Lebegue, S. **Rational approach for an optimized formulation of silver-exchanged zeolites for iodine capture from first-principles calculations** [elektronický dokument] In: **Molecular Systems Design and Engineering**. [s.l.]: The Royal Society of Chemistry, 2022, Roč. 7, č. 5, [online]. ISSN (online) 20589689. - SCO, s. 422 - 433

2022 [01/20] / **USA** - Ma, S. - Liu, Z.-P. **The Role of Zeolite Framework in Zeolite Stability and Catalysis from Recent Atomic Simulation** [elektronický dokument] In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, č. 1-4, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 59 - 68

2021 [01/20] / **CHE** - Capa-Cobos, L.F. - Jaramillo-Fierro, X. - Gonzalez, S. **Computational study of the adsorption of phosphates as wastewater pollutant molecules on faujasites** [elektronický dokument] In: **Processes**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 9, č. 10, [online]. ISSN (online) 2227-9717. - SCO, s. Art. No. 1821

2021 [01/20] / **CHE** - Hessou, E.P. - Bede, L.A. - Jabraoui, H. - Semmeq, A. - Badawi, M. - Valtchev, V. **Adsorption of toluene and water over cationic-exchanged y zeolites: A dft exploration** [elektronický dokument] In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 26, č. 18, [online]. ISSN (online) 1420-3049. - SCO, s. Art. No. 5486

2021 [01/20] / **USA** - Lange, M.F. - Berkelbach, T.C. **Improving MP2 bandgaps with low-scaling approximations to EOM-CCSD** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 155, č. 8, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 081101

2021 [01/20] / **USA** - Acharya, D. - Ulman, K. - Narasimhan, S. **Leveraging Polar Discontinuities to Tune the Binding of Methanol on BCN and Graphene-BN Lateral Heterostructures** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 27. - SCO, s. 15012 - 15024

2021 [01/20] / **USA** - Göltl, F. - Bhandari, S. - Mavrikakis, M. **Thermodynamics Perspective on the Stepwise Conversion of Methane to Methanol over Cu-Exchanged SSZ-13** [elektronický dokument] In: **ACS Catalysis**. Washington: American

Chemical Society, 2021, Roč. 11, č. 13, [online]. ISSN (online) 2155-5435. - SCO, s. 7719 - 7734

2021 [01/20] / **USA** - Schwalbe-Koda, D. - Gomez-Bombarelli, R. **Benchmarking binding energy calculations for organic structure-directing agents in pure-silica zeolites** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 174109

2020 [01/12] / **NLD** - Liu, J. - Yin, Y. - Fu, X.-Z. - Luo, J.-L. **Stability of C3-C6 carbonium ions inside zeolites: A first principles study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 503, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 144148

2020 [01/12] / **NLD** - Liu, M. - Vesely, O. - Eliasova, P. - Shamzhy, M. - Lyu, P. - Grajciar, L. **Identification of the most active sites for tetrahydropyranylation in zeolites: MFI as a test case** [elektronický dokument] In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 345, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; SCIE ; WOS CC, s. 165 - 174

2020 [01/12] / **USA** - Cnudde, P. - Demuynck, R. - Vandenbrande, S. - Waroquier, M. - Sastre, G. - Speybroeck, V.V. **Light Olefin Diffusion during the MTO Process on H-SAPO-34: A Complex Interplay of Molecular Factors** [elektronický dokument] In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2020, Roč. 142, č. 13, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 6007 - 6017

2020 [01/12] / **GBR** - Rehak, F.R. - Piccini, G. - Alessio, M. - Sauer, J. **Including dispersion in density functional theory for adsorption on flat oxide surfaces, in metal-organic frameworks and in acidic zeolites** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 7577 - 7585

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2020 [01/12] / Bhatt, M.D. - Lee, J.Y. **Advancement of Platinum (Pt)-Free (Non-Pt Precious Metals) and/or Metal-Free (Non-Precious-Metals) Electrocatalysts in Energy Applications: A Review and Perspectives** In: **Energy and Fuels**, 2020, Roč. 34, č. 6. - SCO, s. 6634 - 6695

2020 [01/12] / **USA** - Collinge, G. - Yuk, S.F. - Nguyen, M.-T. - Lee, M.-S. - Glezakou, V.-A. - Rousseau, R. **Effect of Collective Dynamics and Anharmonicity on Entropy in Heterogenous Catalysis: Building the Case for Advanced Molecular Simulations** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 16, [online]. ISSN (online) 2155-5435. - SCO, s. 9236 - 9260

2020 [01/12] / **DEU** - Chang, X. - Wan, Y. - Zhao, X. - Yuan, Z. - Zhao, X. - Li, Y. - Guo, S. - Yan, D. **Adsorptive separation of high purity tetramethylsilane on zeolites from low-boiling residues of dimethyldichlorosilane synthesis** [elektronický dokument] In: **Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2020, Roč. 254, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCO, s. Art. No. 123522

2020 [01/12] / **CHE** - Khalil, I. - Jabraoui, H. - Lebegue, S. - Kim, W.J. - Aguilera, L.-J. - Thomas, K. - Mauge, F. - Badawi, M. **Biofuel purification: Coupling experimental and theoretical investigations for efficient separation of phenol from aromatics by zeolites** [elektronický dokument] In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science,

2020, Roč. 402, [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO, s. Art. No. 126264

2019 [01/12] / **USA** - Boronat, M. - Corma, A. **In: ACS Catalysis**. Washington: American Chemical Society, 2019, Roč. 9, č. 2, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1539 - 1548

2019 [01/12] / **USA** - Fischer, M. - Kim, W.J. - Badawi, M. - Lebegue, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 150, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094102

2019 [01/12] / Hessou, E.R. - Jabraoui, H. - Houngue, M.T.A.K. - Mensah, J.B. - Pastore, M. - Badawi, M. **In: Zeitschrift fur Kristallographie-Crystalline Materials**, 2019, Roč. 234, č. 7-8. - SCIE ; WOS CC, s. 469 - 482

2019 [01/12] / **CHE** - Hessou, E.P. - Ponce-Vargas, M. - Mensah, J.B. - Tielens, F. - Santos, J.C. - Badawi, M. **In: Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 5, [online]. ISSN (online) 2079-4991. - SCIE ; WOS CC, s. Art. No. 715

2019 [01/12] / **NLD** - Berro, Y. - Gueddida, S. - Lebegue, S. - Pasc, A. - Canilho, N. - Kassir, M. - Hassan, F.E. - Badawi, M. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 494, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 721 - 730

2019 [01/12] / Jabraoui, H. - Khalil, I. - Lebegue, S. - Badawi, M. **In: Molecular Systems Design & Engineering**, 2019, Roč. 4, č. 4. - SCIE ; WOS CC, s. 882 - 892

2019 [01/12] / **CHE** - Noor, M.Z.B. - Chin, I.L.Y. - Irawan, S. **In: Journal of Petroleum Exploration and Production Technology**. Cham: Springer Nature, 2019, Roč. 9, č. 4, [tlačená forma] [online]. ISSN 2190-0558. ISSN (online) 2190-0566. - SCIE ; WOS CC, s. 2845 - 2851

2019 [01/12] / **USA** - Sauer, J. **In: Accounts of Chemical Research**. Washington: American Chemical Society, 2019, Roč. 52, č. 12, [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCIE ; WOS CC, s. 3502 - 3510

2019 [01/12] / **USA** - Klimes, J. - Tew, D.P. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 151, č. 23, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 234108

2018 [01/12] / **DEU** - Gatta, G.D. - Lotti, P. - Tabacchi, G. **In: Physics and Chemistry of Minerals**. Berlín: Springer Nature, 2018, Roč. 45, č. 2, [tlačená forma]. ISSN 0342-1791. ISSN (online) 1432-2021. - SCIE ; WOS CC, s. 115 - 138

2018 [01/12] / **USA** - Plessow, P.N. - Studt, F. **In: Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2018, Roč. 148, č. 4, [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCIE ; WOS CC, s. 1246 - 1253

2018 [01/12] / **USA** - Schafer, T. - Ramberger, B. - Kresse, G. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 148, č. 6, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 064103

2018 [01/12] / Fang, H.J. - Awati, R. - Boulfelfel, S.E. - Ravikovitch, P.I. - Sholl, D.S. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 24. - SCIE ; WOS CC, s. 12880 - 12891

2018 [01/12] / **GBR** - Alessio, M. - Bischoff, F.A. - Sauer, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 15, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. -

SCIE ; WOS CC, s. 9760 - 9769

2018 [01/12] / **GBR** - Maestri, M. - Iglesia, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 23, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 15725 - 15735

2018 [01/12] / **GBR** - Piccini, G. - Alessio, M. - Sauer, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 30, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 19964 - 19970

2018 [01/12] / **GBR** - Grajciar, L. - Heard, C.J. - Bondarenko, A.A. - Polynski, M.V. - Meeprasert, J. - Pidko, E.A. - Nachtigall, P. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 47, č. 22, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 8307 - 8348

2018 [01/12] / **DEU** - Hessou, E.P. - Kanhounnon, W.G. - Rocca, D. - Monnier, H. - Vallieres, C. - Lebegue, S. - Badawi, M. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2018, Roč. 137, č. 12, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 161

2017 [01/12] / **NLD** - Chebbi, M. - Chibani, S. - Paul, J.F. - Cantrel, L. - Badawi, M. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2017, Roč. 239, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 111 - 122

2017 [01/12] / John, M. - Alexopoulos, K. - Reyniers, M.F. - Marin, G.B. **In: Catalysis Science & Technology**, 2017, Roč. 7, č. 5. - SCIE ; WOS CC, s. 1055 - 1072

2017 [01/12] / **USA** - Schafer, T. - Ramberger, B. - Kresse, G. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 104101

2017 [01/12] / Arvidsson, A.A. - Zhdanov, V.P. - Carlsson, P.A. - Gronbeck, H. - Hellman, A. **In: Catalysis Science & Technology**, 2017, Roč. 7, č. 7. - SCIE ; WOS CC, s. 1470 - 1477

2017 [01/12] / **USA** - Kostetskyy, P. - Mpourmpakis, G. **In: Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2017, Roč. 56, č. 24, [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCIE ; WOS CC, s. 7062 - 7069

2017 [01/12] / **USA** - Dixit, A. - Claudot, J. - Lebegue, S. - Rocca, D. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2017, Roč. 13, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 5432 - 5442

2017 [01/12] / Rosales, C.B.S. - Rojas, M.I. - Avalle, L.B. **In: Journal of Electroanalytical Chemistry**, 2017, Roč. 799. ISSN 0022-0728. - SCIE ; WOS CC, s. 487 - 496

2017 [01/12] / Makoudi, Y. - Jeannoutot, J. - Palmino, F. - Cherioux, F. - Copie, G. - Krzeminski, C. - Cleri, F. - Grandidier, B. **In: Surface Science Reports**: a Review Journal, 2017, Roč. 72, č. 4, [tlačená forma]. ISSN 0167-5729. ISSN (online) 1879-274X. - SCIE ; WOS CC, s. 316 - 349

2016 [01/12] / **USA** - Boese, A.D. - Sauer, J. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2016, Roč. 37, č. 26, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 2374 - 2385

2016 [01/12] / **USA** - Silaghi, M.C. - Chizallet, C. - Sauer, J. - Raybaud, P. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2016, Roč. 339, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 242 - 255

2016 [01/12] / **USA** - Ambrosetti, A. - Silvestrelli, P.L. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. 183 - 197

2016 [01/12] / De Wispelaere, K. - Bailleul, S. - Van Speybroeck, V. **In: Catalysis Science & Technology**, 2016, Roč. 6, č. 8. - SCIE ; WOS CC, s. 2686 - 2705

2016 [01/12] / Para, M.L. - Perez, O.E.L. - Rojas, M.I. - Teijelo, M.L. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 8. - SCIE ; WOS CC, s. 4364 - 4372

2016 [01/12] / **USA** - John, M. - Alexopoulos, K. - Reyniers, M.F. - Marin, G.B. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 4081 - 4094

2016 [01/12] / **USA** - Hajek, J. - Van der Mynsbrugge, J. - De Wispelaere, K. - Cnudde, P. - Vanduyfhuys, L. - Waroquier, M. - Van Speybroeck, V. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2016, Roč. 340, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 227 - 235

2016 [01/12] / **DEU** - Fischer, M. - Evers, F.O. - Formalik, F. - Olejniczak, A. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2016, Roč. 135, č. 12, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 257

2016 [01/12] / **USA** - Wilhelm, J. - Seewald, P. - Del Ben, M. - Hutter, J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 5851 - 5859

2015 [01/12] / Piccini, G. - Alessio, M. - Sauer, J. - Zhi, Y.C. - Liu, Y. - Kolvenbach, R. - Jentys, A. - Lercher, J.A. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 11. - SCIE ; WOS CC, s. 6128 - 6137

2015 [01/12] / **USA** - Usvyat, D. - Maschio, L. - Schutz, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 143, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 102805

2015 [01/12] / **USA** - Tuma, C. - Sauer, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 143, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 102810

2015 [01/12] / **GBR** - Van Speybroeck, V. - Hemelsoet, K. - Joos, L. - Waroquier, M. - Bell, R.G. - Catlow, C.R.A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 44, č. 20, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7044 - 7111

2015 [01/12] / **USA** - Bao, J.L. - Yu, H.Y.S. - Duanmu, K. - Makeev, M.A. - Xu, X.F. - Truhlar, D.G. **In: ACS Catalysis**. Washington: American Chemical Society, 2015, Roč. 5, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2070 - 2080

2015 [01/12] / **USA** - Gillan, M.J. - Alfe, D. - Manby, F.R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 143, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. -

SCIE ; WOS CC, s. Art. No. 102812

2015 [01/12] / **USA** - John, M. - Alexopoulos, K. - Reyniers, M.F. - Marin, G.B. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2015, Roč. 330, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 28 - 45

2015 [01/12] / Zhang, Y.W. - Yu, J.Y. - Yeh, Y.H. - Gorte, R.J. - Rangarajan, S. - Mavrikakis, M. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 52. - SCIE ; WOS CC, s. 28970 - 28978

2015 [01/12] / Janesko, B.G. **Density Functionals: Thermochemistry. Book Series: Topics in Current Chemistry** [textový dokument (print)] . Berlin: Springer, 2015. 1 vyd. - BKCI-S ; WOS CC, s. 25 - 51

2015 [01/12] / Fjermestad, T. - Svelle, S. - Swang, O. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 4. - SCIE ; WOS CC, s. 2073 - 2085

2015 [01/12] / **USA** - Leydier, F. - Chizallet, C. - Costa, D. - Raybaud, P. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2015, Roč. 325, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 35 - 47

2014 [01/12] / **GBR** - Van Speybroeck, V. - De Wispelaere, K. - Van der Mynsbrugge, J. - Vandichel, M. - Hemelsoet, K. - Waroquier, M. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2014, Roč. 43, č. 21, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 7326 - 7357

2014 [01/12] / Stuckenschneider, K. - Merz, J. - Schembecker, G. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 11. - SCIE ; WOS CC, s. 5810 - 5819

2014 [01/12] / Goltl, F. - Houriez, C. - Guitou, M. - Chambaud, G. - Sautet, P. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 10. - SCIE ; WOS CC, s. 5374 - 5382

2014 [01/12] / **GBR** - Bohlen, M. - Bolton, K. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 12929 - 12939

2014 [01/12] / **USA** - Chiu, C.C. - Vayssilov, G.N. - Genest, A. - Borgna, A. - Rosch, N. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2014, Roč. 35, č. 10, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 809 - 819

2014 [01/12] / **USA** - Silvestrelli, P.L. - Ambrosetti, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124107

2014 [01/12] / **USA** - Piccini, G. - Sauer, J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2479 - 2487

2014 [01/12] / **USA** - Jiang, T. - Goltl, F. - Bulo, R.E. - Sautet, P. **In: ACS Catalysis**. Washington: American Chemical Society, 2014, Roč. 4, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. Art. No. 154105

2014 [01/12] / **USA** - Carter, D.J. - Rohl, A.L. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 3423 - 3437

2014 [01/12] / **GBR** - Fischer, M. - Bell, R.G. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 39, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 21062 - 21072

2014 [01/12] / Kropp, T. - Paier, J. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 41. - SCIE ; WOS CC, s. 23690 - 23700

2014 [01/12] / **USA** - Brogaard, R.Y. - Wang, C.M. - Studt, F. **In: ACS Catalysis**. Washington: American Chemical Society, 2014, Roč. 4, č. 12, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 4504 - 4509

2014 [01/12] / Jones, A.J. - Iglesia, E. **In: Angewandte Chemie-International Edition**, 2014, Roč. 53, č. 45. - SCIE ; WOS CC, s. 12177 - 12181

2014 [01/12] / **GBR** - Bromley, S.T. - Goumans, T.P.M. - Herbst, E. - Jones, A.P. - Slater, B. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 35, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 18623 - 18643

2013 [01/12] / **USA** - Rimola, A. - Costa, D. - Sodupe, M. - Lambert, J.F. - Ugliengo, P. **In: Chemical Reviews**. Washington: American Chemical Society, 2013, Roč. 113, č. 6, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 4216 - 4313

2013 [01/12] / Stuckenschneider, K. - Merz, J. - Hanke, F. - Rozyczko, P. - Milman, V. - Schembecker, G. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 37. - SCIE ; WOS CC, s. 18927 - 18935

2013 [01/12] / Del Ben, M. - Schonherr, M. - Hutter, J. - VandeVondele, J. **In: Journal of Physical Chemistry Letters**, 2013, Roč. 4, č. 21. - SCIE ; WOS CC, s. 3753 - 3759

2013 [01/12] / **USA** - Piccini, G. - Sauer, J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2013, Roč. 9, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 5038 - 5045

2013 [01/12] / **NLD** - Li, K. - Jiao, M.G. - Wang, Y. - Wu, Z.J. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2013, Roč. 617, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 149 - 155

2013 [01/12] / Derouane, E.G. - Vedrine, J.C. - Pinto, R.R. - Borges, P.M. - Costa, L. - Lemos, M.A.N.D.A. - Lemos, F. - Ribeiro, F.R. **In: Catalysis Reviews-Science and Engineering**, 2013, Roč. 55, č. 4. - SCIE ; WOS CC, s. 454 - 515

2013 [01/12] / **USA** - Paier, J. - Penschke, C. - Sauer, J. **In: Chemical Reviews**. Washington: American Chemical Society, 2013, Roč. 113, č. 6, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 3949 - 3985

2013 [01/12] / **USA** - Moses, P.G. - Norskov, J.K. **In: ACS Catalysis**. Washington: American Chemical Society, 2013, Roč. 3, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 735 - 745

2013 [01/12] / **GBR** - Boese, A.D. - Sauer, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 39, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 16481 - 16493

2013 [01/12] / Sharada, S.M. - Zimmerman, P.M. - Bell, A.T. - Head-Gordon, M. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 24. - SCIE ; WOS CC, s. 12600 - 12611

2012 [01/12] / Tranca, D.C. - Hansen, N. - Swisher, J.A. - Smit, B. - Keil, F.J. **In: Journal of Physical Chemistry C**, 2012, Roč. 116, č. 44. - SCIE ; WOS CC, s. 23408 - 23417

2013 - **spolu** : **4**

ADC_037: / Sklenák, Štěpán (Autor) (12%) - Andrikopoulos, Prokopis C. (Autor) (12%) - Whittleton, Sarah R. (Autor) (11%) - Jirglova, Hana (Autor) (11%) - Sazama, Petr (Autor) (11%) - Benco, Ľubomír (Autor) (11%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (10%) - Hafner, Juergen (Autor) (11%) - Sobalík, Zdeněk (Autor) (11%): **Effect of the Al Siting on the Structure of Co(II) and Cu(II) Cationic Sites in Ferrierite. A Periodic DFT Molecular Dynamics and FTIR Study**. – CCC ; SCO ; WOS CC.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 117, č. 8 (2013), s. 3958-3968 [tlačená forma] [online]
Počet všetkých autorov: 9
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,434 - 2013
SJR: 2,143 - 2013
CiteScore: 8,3 - 2013

Ohlasy (24):
2025 [01/20] / **DEU** - Shilina, M. I. - Gloriozov, I. P. **Predicting CO adsorption sites in Co-doped zeolite via density functional theory calculations** [elektronický dokument]. DOI 10.1016/j.matchemphys.2025.130893 In: **Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2025, Roč. 341, art. no. 130893 [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCO ; CCC ; WOS CC, s. art. no. 130893

2025 [01/20] / **DEU** - Rajeev, Anjana - Mohammed, Thasnim P. - George, Akhila - Sankaralingam, Muniyandi. **Direct Methane to Methanol Conversion: An Overview of Non-Syn Gas Catalytic Strategies** [elektronický dokument]. DOI 10.1002/tcr.202400186 In: **Chemical Record**. Weinheim: John Wiley & Sons. Wiley Periodicals, 2025, Roč. 25, č. 2, art. no. e202400186 [tlačená forma] [online]. ISSN 1527-8999. ISSN (online) 1528-0691. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Abdul Nasir, Jamal - Beale, Andrew M. - Catlow, C. Richard A. **Understanding deNOx mechanisms in transition metal exchanged zeolites** [elektronický dokument]. DOI 10.1039/d3cs00468f In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 53, č. 23, s. 11657-11691 [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO ; CCC ; WOS CC, s. 11657 - 11691

2022 [01/20] / **NLD** - Song, I. - Khivantsev, K. - Wu, Y. - Bowden, M. - Wang, Y. - Szanyi, J. **Unusual water-assisted NO adsorption over Pd/FER calcined at high temperatures: The effect of cation migration** In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2022, Roč. 318, [tlačená forma]. ISSN 0926-3373. - SCO, s. Art. No. 121810

2021 [01/20] / **PRK** - Kwak, S.J. - Kim, H.S. - Park, N. - Park, M.-J. - Lee, W.B. **Recent progress on Al distribution over zeolite frameworks: Linking theories and experiments** In: **Korean Journal of Chemical Engineering**, 2021, Roč. 38, č. 6. - SCO, s. 1117 - 1128

2021 [01/20] / **USA** - Olszowka, J.E. - Lemishka, M. - Mlekodaj, K. - Kubat, P. - Rutkowska-Zbik, D. - Dedecek, J. - Tabor, E. **Determination of Zn Speciation, Siting, and Distribution in Ferrierite Using Luminescence and FTIR Spectroscopy** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 17. - SCO, s. 9060 - 9073

2020 [01/12] / **USA** - Di Iorio, J.R. - Li, S. - Jones, C.B. - Nimlos, C.T. - Wang, Y. - Kunkes, E. - Vattipalli, V. - Prasad, S. - Moini, A. - Schneider, W.F. - Gounder, R. **Cooperative and Competitive Occlusion of Organic and Inorganic Structure-Directing Agents within Chabazite Zeolites Influences Their Aluminum Arrangement** [elektronický dokument] In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2020, Roč. 142, č. 10, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 4807 - 4819

2020 [01/12] / **USA** - Kvande, K. - Pappas, D.K. - Borfecchia, E. - Lomachenko, K.A. **Advanced X-ray Absorption Spectroscopy Analysis to Determine Structure-Activity Relationships for Cu-Zeolites in the Direct Conversion of Methane to Methanol** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano-Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2020, Roč. 12, č. 9, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 2385 - 2405

2020 [01/12] / **GBR** - Felvey, N.W. - Meloni, M.J. - Kronawitter, C.X. - Runnebaum, R.C. **Ethane dehydrogenation over Cr/ZSM-5: Characterization of active sites through probe molecule adsorption FTIR** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 10, č. 15, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 5069 - 5081

2019 [01/12] / **USA** - Pappas, D.K. - Borfecchia, E. - Dyballa, M. - Lomachenko, K.A. - Martini, A. - Berlier, G. - Arstad, B. - Lamberti, C. - Bordiga, S. - Olsbye, U. - Svelle, S. - Beato, P. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 621 - 627

2019 [01/12] / **GBR** - Li, H. - Paolucci, C. - Khurana, I. - Wilcox, L. - Goltl, F. - Albarracin-Caballero, J.D. - Shih, A.J. - Ribeiro, F.H. - Gounder, R. - Schneider, W.F. **In: Chemical Science**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 10, č. 8, [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCIE ; WOS CC, s. 2373 - 2384

2019 [01/12] / **USA** - Pappas, D.K. - Borfecchia, E. - Lomachenko, K.A. - Lazzarini, A. - Gutterod, E.S. - Dyballa, M. - Martini, A. - Berlier, G. - Bordiga, S. - Lamberti, C. - Arstad, B. - Olsbye, U. - Beato, P. - Svelle, S. **In: Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2019, Roč. 62, č. 7-11, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCIE ; WOS CC, s. 712 - 723

2018 [01/12] / **USA** - Knott, B.C. - Nimlos, C.T. - Robichaud, D.J. - Nimlos, M.R. - Kim, S. - Gounder, R. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 2, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 770 - 784

2017 [01/12] / **CHE** - He, M. - Zhang, J. - Liu, R. - Sun, X.L. - Chen, B.H. **In: Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2017, Roč. 7, č. 1, [online]. ISSN 2073-4344. - SCIE ; WOS CC, s. Art. No. 11

2017 [01/12] / **USA** - Le, H.V. - Parishan, S. - Saaltchik, A. - Gobel, C. - Schlesiger, C. - Malzer, W. - Trunschke, A. - Schomacker, R. - Thomas, A. **In: ACS Catalysis**. Washington: American Chemical Society, 2017, Roč. 7, č. 2, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1403 - 1412

2017 [01/12] / **NLD** - Castellanos, I. - Marie, O. **In: Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2017, Roč. 283, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCIE ; WOS CC, s. 54 - 65

2017 [01/12] / **USA** - Li, S.K. - Zhao, Z.C. - Zhao, R.R. - Zhou, D.H. - Zhang, W.P. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2017,

Roč. 9, č. 8, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 1494 - 1502

2017 [01/12] / **GBR** - Oda, A. - Ohkubo, T. - Yumura, T. - Kobayashi, H. - Kuroda, Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 36, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 25105 - 25114

2017 [01/12] / **HRV** - Maduna, K. - Zrncevic, S. **In: Hrvatske vode**. Záhreb: Hrvatske vode, 2017, Roč. 25, č. 101, [tlačená forma] [online]. ISSN 1330-1144. ISSN (online) 1849-0506. - SCIE ; WOS CC, s. 149 - 158

2016 [01/12] / **NLD** - Vilhena, F.D. - Serra, R.M. - Boix, A.V. - Ferreira, G.B. - Carneiro, J.W.D. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2016, Roč. 1091, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 115 - 121

2016 [01/12] / **GBR** - Stepniewski, A. - Radon, M. - Gora-Marek, K. - Broclawik, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 5, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 3716 - 3729

2015 [01/12] / Mao, Y. - Wang, H.F. - Hu, P. **In: : International journal of quantum chemistry,** 2015, Roč. 115, č. 10. - SCIE ; WOS CC, s. 618 - 630

2014 [01/12] / **USA** - Duan, T.W. - Yan, B. **In: Photochemistry and Photobiology**: an international journal. Hoboken: John Wiley & Sons. Wiley Blackwell, 2014, Roč. 90, č. 3, [tlačená forma]. ISSN 0031-8655. ISSN (online) 1751-1097. - SCIE ; WOS CC, s. 503 - 510

2014 [01/12] / **GBR** - Gora-Marek, K. - Stepniewski, A. - Radon, M. - Broclawik, E. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 43, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 24089 - 24098

ADC_038: / Bučko, Tomáš (Autor) [UKOPRCFZ] (70%) - Lebegue, Sebastien (Autor) (10%) - Hafner, Jürgen (Autor) (10%) - Ángyán, János G. (Autor) (10%): **Improved Density Dependent Correction for the Description of London Dispersion Forces**. – text. – CCC ; SCO ; WOS CC ; SCIE.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 9, č. 10 (2013), s. 4293-4299 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,558 - 2013
SJR: 2,437 - 2013
CiteScore: 8,1 - 2013

Ohlasy (176):
2025 [01/20] / **CHE** - Herbert, John M. - Gray, Montgomery - Liu, Kuan Yu - Carter-Fenk, Kevin. **Extended Symmetry-Adapted Perturbation Theory (XSAPT): A Cubic-Scaling Platform for Computing Accurate Intermolecular Interaction Energies and ab Initio Energy Decomposition Analysis** [elektronický dokument]. DOI 10.1007/430_2025_98 In: **Structure and Bonding Computational Methods for the Analysis of Non-Covalent Interactions**. Cham: Springer Nature, 2025, s. 137-222 [tlačená forma] [online]. ISBN 978-3-032-01542-6. ISBN (online) 978-3-032-01543-3. ISSN

00815993. ISSN (online) 16168550. - SCO, s. 137 - 222

2025 [01/20] / **USA** - Gao, Xiang - Ouyang, Wengen - Kronik, Leeor - Urbakh, Michael - Hod, Oded. **Anisotropic interlayer force fields for van der Waals interfaces: Development and applications** [elektronický dokument]. DOI 10.1063/5.0273079 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 4, art. no. 041001 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **NLD** - Chepkasov, Ilya V. - Baidyshev, Viktor S. - Kvashnin, Alexander G. **Polyaromatic hydrocarbons as prospective anode materials for metal ion battery** [elektronický dokument]. DOI 10.1016/j.est.2025.116831 In: **Journal of Energy Storage**. Amsterdam: Elsevier, 2025, Roč. 125, art. no. 116831 [tlačená forma] [online]. ISSN 2352-152X. ISSN (online) 2352-1538. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **USA** - Hasan, Mohammed Abdulabbas - Abdulhussein, Heider A. **Review: beyond the surface—exploring the complexities of 2D materials with density functional theory** [elektronický dokument]. DOI 10.1007/s10853-025-11190-0 In: **Journal of Materials Science**. Norwell: Springer Nature. Springer International Publishing AG, 2025, Roč. 60, č. 31, s. 13191-13235 [tlačená forma] [online]. ISSN 0022-2461. ISSN (online) 1573-4803. - SCO, s. 13191 - 13235

2025 [01/20] / **GBR** - Garrido Aldea, Jaime - Esteras, Dorye L. - Roche, Stephan - Garcia, Jose H. **Challenges and strategies for first-principles simulations of two-dimensional magnetic phenomena** [elektronický dokument]. DOI 10.1039/d4nr05503a In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 43, s. 24955-24989 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 24955 - 24989

2025 [01/20] / **GBR** - Rêgo, Celso R.C. - Wenzel, Wolfgang - Piotrowski, Maurício J. - Dias, Alexandre C. - Maciel de Oliveira Bastos, Carlos - de Araujo, Luis O. - Guedes-Sobrinho, Diego. **Digital workflow optimization of van der Waals methods for improved halide perovskite solar materials** [elektronický dokument]. DOI 10.1039/d4dd00312h In: **Digital Discovery**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 4, č. 4, s. 927-942. ISSN (online) 2635098X. - SCO ; WOS CC ; ESCI ; OA, s. 927 - 942

2025 [01/20] / **USA** - Pfeiffer, Florian - Krenz, Marvin - Sanna, Simone. **Theoretical Investigation and Simulated Imaging of Halogenated Tetracenes on Coinage Metal (111) Surfaces** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c06015 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 49, s. 21686-21695 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 21686 - 21695

2025 [01/20] / **DEU** - Chen, Xiaokai - Xuan, Xiaoyu - Guo, Wanlin - Zhang, Zhuhua. **Ferroelectricity in van der Waals multilayers via interfacial polarization engineering** [elektronický dokument]. DOI 10.1038/s41699-025-00531-x In: **NPJ 2D Materials and Applications**. Berlín: Nature Research, 2025, Roč. 9, č. 1, art. no. 10. ISSN (online) 2397-7132. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 10

2025 [01/20] / **GBR** - Núñez-Murillo, F. A. - López, L. A. - Mejía-Burgos, D. - Mazo-Zuluaga, J. - Mejía-López, J. **Single-layer CrI2as a magnetic semiconductor: a detailed first-principles study** [elektronický dokument]. DOI 10.1039/d5nr01077b In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 44, s. 25833-25845 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; WOS CC ; SCIE ; OA, s. 25833 - 25845

2025 [01/20] / **USA** - Lopes, Daniel S. - da Costa, Diego R. - Dias, Alexandre C. - Barcelos, Ingrid D. - Cadore, Alisson R. - Teldo, A. S.Pereira - de Sousa, Jeanlex S. **Tunable Electronic Properties of Multilayer Talc: Combined First-Principles and Experimental Insights** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c05824 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter.

Washington: American Chemical Society, 2025, Roč. 129, č. 45, s. 20404-20417 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 20404 - 20417

2025 [01/20] / **GBR** - Dickbreder, Tobias - Schneider, Florian - Klausfering, Lea - Dreier, Kim Noelle - Sabath, Franziska - Foster, Adam S. - Bechstein, Ralf - Kühnle, Angelika. **Water desorption from microcline (001): insights into the first water layer** [elektronický dokument]. DOI 10.1039/d5cp01796c In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 35, s. 18317-18325 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 18317 - 18325

2025 [01/20] / **GBR** - Zhou, Haojun - Chen, Yingquan - Ding, Mingyue - Zhong, Xiaoliang. **Formation mechanism of the (2 × 1) reconstruction of calcite (104)** [elektronický dokument]. DOI 10.1038/s41598-025-95955-2 In: **Scientific reports**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 15, č. 1, art. no. 11988 [online]. ISSN (online) 2045-2322. - SCO ; WOS CC ; SCIE ; OA, s. art. no. 11988

2025 [01/20] / **GBR** - Pashov, Dimitar - Larsen, Ross E. - Watson, Matthew D. - Acharya, Swagata - van Schilfgaarde, Mark. **TiSe2 is a band insulator created by lattice fluctuations, not an excitonic insulator** [elektronický dokument]. DOI 10.1038/s41524-025-01631-4 In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 11, č. 1, art. no. 152 [online]. ISSN (online) 2057-3960. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 152

2025 [01/20] / **GBR** - Wang, Lei - Liu, Xiaofeng - Li, Qunxiang - Yang, Jinlong - Hu, Wei. **Revealing the photocatalytic dissociation of water molecules on rutile TiO2 surface via hybrid functional based linear response time-dependent density functional theory** [elektronický dokument]. DOI 10.1039/d5sc02736e In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 36, s. 16876-16884 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 16876 - 16884

2025 [01/20] / **USA** - Heggemann, Jonas - Huang, Jie - Aeschlimann, Simon - Spiller, Simon - Foster, Adam S. - Rahe, Philipp. **Sidestepping Intermolecular Hydrogen Bonds: How Single Water Molecules Adsorb and Assemble on the Calcite(104)–(2 × 1) Surface** [elektronický dokument]. DOI 10.1021/acsnano.5c05845 In: **ACS Nano**. Washington: American Chemical Society, 2025, Roč. 19, č. 29, s. 26650-26658 [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO ; WOS CC ; SCIE ; OA, s. 26650 - 26658

2025 [01/20] / **USA** - Ikwa, Emmanuel - Rivallan, Mickael - Nardin, Thibaud - Hugon, Antoine - Loffreda, David. **How Morphological Descriptors Capture the Stability Order in Palladium Nanoparticles** [elektronický dokument]. DOI 10.1021/acs.jpclett.5c01188 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2025, Roč. 16, č. 25, s. 6513-6522 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC ; SCIE, s. 6513 - 6522

2025 [01/20] / **CHE** - Dubok, Aleksandr S. - Rychkov, Denis A. **What Is More Important When Calculating the Thermodynamic Properties of Organic Crystals, Density Functional, Supercell, or Energy Second-Order Derivative Method Choice?** [elektronický dokument]. DOI 10.3390/cryst15030274 In: **Crystals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 3, art. no. 274 [online]. ISSN (online) 2073-4352. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 274

2025 [01/20] / **USA** - Yadav, Shivam - Sekh, Sajid - Ptok, Andrzej. **Low temperature phase of AuSn4 induced by the van der Waals interactions** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.9.034202 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 9, č. 3, art. no. 034202 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. art. no. 034202

2025 [01/20] / **USA** - Li, Zhe - Xue, Feng - Tang, Xin Yi - Hong, Xiyu - Chen, Yang - Feng, Xiao - He, Ke. **Universally optimizable strategy for magnetic gaps towards high-temperature quantum anomalous Hall states via magnetic-insulator/topological-insulator building blocks** [elektronický dokument]. DOI 10.1103/PhysRevB.111.075106 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 111, č. 7, art. no.

075106 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 075106

2025 [01/20] / **USA** - Carneiro Queiroz da Silva, G. - Salazar, J. Marcos. **Emergence of an Icosahedral (H2)13 Cluster inside a Pure Silica Faujasite** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c08679 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 14, s. 7031-7039 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 7031 - 7039

2024 [01/20] / **USA** - González, José E. - Besse, Rafael - Lima, Matheus P. - Da Silva, Juarez L.F. **Decoding Van der Waals Impact on Chirality Transfer in Perovskite Structures: Density Functional Theory Insights** [elektronický dokument]. DOI 10.1021/acs.jcim.3c01895 In: **Journal of Chemical Information and Modeling**. Washington, D.C.: American Chemical Society, 2024, Roč. 64, č. 4, s. 1306-1318 [tlačená forma] [online]. ISSN 1549-9596. ISSN (online) 1549-960X. - SCO ; CCC ; WOS CC, s. 1306 - 1318

2024 [01/20] / **USA** - Brumovský, Miroslav - Tunega, Daniel. **Reductive Dechlorination of Chlorinated Ethenes at the Sulfidated Zero-Valent Iron Surface: A Mechanistic DFT Study** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c00865 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 10, s. 4180-4191 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 4180 - 4191

2024 [01/20] / **USA** - Samal, Pragnya Paramita - Krishnamurty, Sailaja. **First-Principles Simulation of Active Site Selectivity for CO2 and H2 Adsorption on Mg(OH)+/Mg2+ and Ca(OH)+/Ca2+ Zeolites** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c05835 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 51, s. 21659-21671 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 21659 - 21671

2024 [01/20] / **GBR** - Caicedo-Dávila, Sebastián - Cohen, Adi - Motti, Silvia G. - Isobe, Masahiko - McCall, Kyle M. - Grumet, Manuel - Kovalenko, Maksym V. - Yaffe, Omer - Herz, Laura M. - Fabini, Douglas H. - Egger, David A. **Disentangling the effects of structure and lone-pair electrons in the lattice dynamics of halide perovskites** [elektronický dokument]. DOI 10.1038/s41467-024-48581-x In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2024, Roč. 15, č. 1, art. no. 4184 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s. art. no. 4184

2024 [01/20] / **CHN** - Feng, Xin - Liang, Xuefeng - Li, Xinxia - Fang, Zhou - Wei, Weiqiang - Zhang, Lisheng - He, Yan - Li, Huifang. **Improving the response of 2D COFs to the surface doping strategies through rational design of their chemical structure** [elektronický dokument]. DOI 10.1007/s40843-024-3032-7 In: **Science China materials**. Beijing: Science China Press, 2024, Roč. 67, č. 10, s. 3272-3281 [tlačená forma] [online]. ISSN 2095-8226. ISSN (online) 2199-4501. - SCO ; CCC ; WOS CC, s. 3272 - 3281

2024 [01/20] / **USA** - Malik, Asif A. - Saeed, Zeinab M. - Ahmad, Ishtiyaq - Alkhidir, Tamador - Managutti, Praveen B. - Mohamed, Sharmarke - Dar, Aijaz A. **Polymorphism Steered Thermochromism in a Sulfonamide** [elektronický dokument]. DOI 10.1021/acsaom.4c00260 In: **ACS Applied Optical Materials**. Washington: American Chemical Society, 2024, Roč. 2, č. 8, s. 1709-1720 [online]. ISSN (online) 27719855. - SCO ; WOS CC, s. 1709 - 1720

2024 [01/20] / **USA** - Zhang, Pan - Ding, Yuelong - Cui, Wenwen - Hao, Jian - Shi, Jingming - Li, Yinwei. **Unveiling unconventional CH4-Xe compounds and their thermodynamic properties at extreme conditions** [elektronický dokument]. DOI 10.1063/5.0218769 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2024, Roč. 161, č. 1, art. no. 014501 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. -

SCO ; CCC ; WOS CC, s. art. no. 014501

2024 [01/20] / **DEU** - Almehairbi, Mubarak - Joshi, Vikram C. - Irfan, Ahamad - Saeed, Zeinab M. - Alkhidir, Tamador - Abdelhaq, Aya M. - Managutti, Praveen B. - Dhokale, Bhausaheb - Jadhav, Thaksen - Calvin Sun, Changquan - Mohamed, Sharmarke. **Surface Engineering of the Mechanical Properties of Molecular Crystals via an Atomistic Model for Computing the Facet Stress Response of Solids** [elektronický dokument]. DOI 10.1002/chem.202400779 In: **Chemistry - A European Journal**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 30, č. 38, art. no. e202400779 [tlačená forma] [online]. ISSN 0947-6539. ISSN (online) 1521-3765. - SCO ; WOS CC, s.

2024 [01/20] / **USA** - Shi, Benjamin X. - Wales, David J. - Michaelides, Angelos - Myung, Chang Woo. **Going for Gold(-Standard): Attaining Coupled Cluster Accuracy in Oxide-Supported Nanoclusters** [elektronický dokument]. DOI 10.1021/acs.jctc.4c00379 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 12, s. 5306-5316 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 5306 - 5316

2024 [01/20] / **DEU** - Liu, Modan - Elsing, David - Esmaeilpour, Meysam - Kozlowska, Mariana - Wenzel, Wolfgang - Wöll, Christof. **Layer-By-Layer Assembly of Asymmetric Linkers into Non-Centrosymmetric Metal Organic Frameworks: A Thorough Theoretical Treatment** [elektronický dokument]. DOI 10.1002/adfm.202302516 In: **Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 34, č. 20, art. no. 2302516 [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Guedes-Sobrinho, Diego - Caldeira Rêgo, Celso R. - Da Silva, Gabriel Reynald - Da Silva, Henrique R. - Wenzel, W. - Piotrowski, Maurício J. - Cavalheiro Dias, Alexandre. **Theoretical Exploration of Structural and Excitonic Properties in Black Phosphorus: From First-Principles to a Semi-Empirical Approach** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c08414 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 17, s. 7242-7251 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 7242 - 7251

2024 [01/20] / **USA** - Villot, Corentin - Lao, Ka Un. **Ab initio dispersion potentials based on physics-based functional forms with machine learning** [elektronický dokument]. DOI 10.1063/5.0204064 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2024, Roč. 160, č. 18, art. no. 184103 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 184103

2024 [01/20] / **USA** - Wang, Lei - Liu, Xiaofeng - Wan, Lingyun - Gao, Yunzhi - Wang, Xiaoning - Liu, Jie - Tan, Shijing - Guo, Qing - Zhao, Wenhui - Hu, Wei - Li, Qunxiang - Yang, Jinlong. **Excitonic Effects of the Excited-State Photocatalytic Reaction at the Molecule/Metal Oxide Interface** [elektronický dokument]. DOI 10.1021/acs.jpclett.3c03075 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2024, Roč. 15, č. 7, s. 2096-2104 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 2096 - 2104

2024 [01/20] / **DEU** - Koller, Thaddäus J. - Jin, Siyu - Krol, Viktoria - Ambach, Sebastian J. - Ranieri, Umbertoluca - Khandarkhaeva, Saiana - Spender, James - McWilliams, Stewart - Trybel, Florian - Giordano, Nico - Poreba, Tomasz - Mezouar, Mohamed - Kuang, Xiaoyu - Lu, Cheng - Dubrovinsky, Leonid - Dubrovinskaia, Natalia - Hermann, Andreas - Schnick, Wolfgang - Laniel, Dominique. **Simple Molecules under High-Pressure and High-Temperature Conditions: Synthesis and Characterization of α- and β-C(NH)2 with Fully sp3-Hybridized Carbon** [elektronický dokument]. DOI 10.1002/anie.202318214 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 63, č. 7, art. no. e202318214 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Novotný, Michal - Dubecký, Matúš - Karlický, František. **Toward accurate modeling of structure and energetics of bulk hexagonal boron nitride** [elektronický dokument]. DOI 10.1002/jcc.27222 In: **Journal of**

computational chemistry. Hoboken: John Wiley & Sons, 2024, Roč. 45, č. 2, s. 115-121 [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO ; CCC ; WOS CC, s. 115 - 121

2023 [01/20] / **USA** - Seidl, Stefan A. - Zhu, Xiangzhou - Reuveni, Guy - Aharon, Sigalit - Gehrmann, Christian - Caicedo-Dávila, Sebastián - Yaffe, Omer - Egger, David A. **Anharmonic fluctuations govern the band gap of halide perovskites** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.7.L092401 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 7, č. 9, art. no. L092401 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC, s. art. no. L092401

2023 [01/20] / **GBR** - Dickbreder, Tobias - Sabath, Franziska - Reischl, Bernhard - Nilsson, Rasmus V.E. - Foster, Adam S. - Bechstein, Ralf - Kühnle, Angelika. **Atomic structure and water arrangement on K-feldspar microcline (001)** [elektronický dokument]. DOI 10.1039/d3nr05585j In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 16, č. 7, s. 3462-3473 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC, s. 3462 - 3473

2023 [01/20] / **CHE** - Dehmani, Younes - Lainé, Juliette - Daouli, Ayoub - Sellaoui, Lotfi - Bonilla-Petriciolet, Adrián - Lamhasni, Taibi - Abouarnadasse, Sadik - Badawi, Michael. **Unravelling the adsorption mechanism of phenol on zinc oxide at various coverages via statistical physics, artificial neural network modeling and ab initio molecular dynamics** [elektronický dokument]. DOI 10.1016/j.cej.2022.139171 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2023, č. 452, art. no. 139171 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 139171

2023 [01/20] / **USA** - Heggemann, Jonas - Ranawat, Yashasvi S. - Krejčí, Ondřej - Foster, Adam S. - Rahe, Philipp. **Differences in Molecular Adsorption Emanating from the (2 × 1) Reconstruction of Calcite(104)** [elektronický dokument]. DOI 10.1021/acs.jpclett.2c03243 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 7, s. 1983-1989 [online]. ISSN (online) 1948-7185. - SCO ; WOS CC, s. 1983 - 1989

2023 [01/20] / **GBR** - Kazemi, Seyedeh Alieh - Imani Yengejeh, Sadegh - Ogunkunle, Samuel Akinlolu - Zhang, Lei - Wen, William - Wee-Chung Liew, Alan - Wang, Yun. **Vacancy impacts on electronic and mechanical properties of MX2 (M = Mo, W and X = S, Se) monolayers** [elektronický dokument]. DOI 10.1039/d3ra00205e In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 10, s. 6498-6506 [online]. ISSN (online) 2046-2069. - SCO ; CCC ; WOS CC, s. 6498 - 6506

2023 [01/20] / **GBR** - Karamanis, Ioannis - Daouli, Ayoub - Monnier, Hubert - Dziurla, Marie Antoinette - Maurin, Guillaume - Badawi, Michael. **A systematic DFT screening of cationic faujasite-type zeolites for the adsorption of NO, NO2 and H2O** [elektronický dokument]. DOI 10.1039/d3me00044c In: **Molecular Systems Design and Engineering**. [s.l.]: The Royal Society of Chemistry, 2023, Roč. 8, č. 9, s. 1165-1181 [online]. ISSN (online) 20589689. - SCO ; CCC ; WOS CC, s. 1165 - 1181

2023 [01/20] / **GBR** - Li, Chong - Wang, Fei - Cui, Bin - Pan, Zhifeng - Jia, Yu. **Localized magnetic moment induced by boron adatoms chemisorbed on graphene** [elektronický dokument]. DOI 10.1088/1361-648X/accdad In: **Journal of Physics**: Condensed Matter. Bristol: Institute of Physics. IOP Publishing, 2023, Roč. 35, č. 29, art. no. 295801 [tlačená forma] [online]. ISSN 0953-8984. ISSN (online) 1361-648X. - SCO ; CCC ; WOS CC, s. art. no. 295801

2023 [01/20] / **GBR** - Chepkasov, Ilya V. - Krasheninnikov, Arkady V. **Tetracene crystals as promising anode material for alkali metal ion batteries** [elektronický dokument]. DOI 10.1016/j.carbon.2023.118190 In: **Carbon**: an International Journal Founded in Conjunction with the American Carbon Society. Oxford: Elsevier, 2023, Roč. 213, art. no. 118190 [tlačená forma] [online]. ISSN 0008-6223. ISSN (online) 1873-3891. - SCO ; CCC ; WOS CC, s. art. no. 118190

2023 [01/20] / **USA** - Yourdkhani, Sirous - Klimeš, Jiří. **Using Noncovalent Interactions to Test the Precision of Projector-Augmented Wave Data Sets** [elektronický dokument]. DOI 10.1021/acs.jctc.3c00930 In: **Journal of Chemical**

Theory and Computation. Washington: American Chemical Society, 2023, Roč. 19, č. 23, s. 8871-8885 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 8871 - 8885

2023 [01/20] / **USA** - Menachekanian, Sevan - Mora Perez, Carlos - Pennathur, Anuj K. - Voegtle, Mattew J. - Blauth, Drew - Prezhdo, Oleg V. - Dawlaty, Jahan M. **Phenol as a Tethering Group to Gold Surfaces: Stark Response and Comparison to Benzenethiol** [elektronický dokument]. DOI 10.1021/acs.jpclett.3c02058 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 37, s. 8353-8359 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 8353 - 8359

2023 [01/20] / **USA** - Zhao, Qiyi - Ren, Yani - Li, Lu - He, Chuan - Che, Junling - Jia, Rongkai - Xu, Yonggang - Zhu, Lipeng - Xu, Xinlong. **Flexibility and anisotropy of MX3 (M = Zr, Hf; X = S, Se): New semiconductors with high photovoltaic performance** [elektronický dokument]. DOI 10.1063/5.0164156 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2023, Roč. 134, č. 12, art. no. 124302 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC, s. art. no. 124302

2023 [01/20] / **USA** - Al-Hamdani, Yasmine S. - Zen, Andrea - Alfè, Dario. **Unraveling H2 chemisorption and physisorption on metal decorated graphene using quantum Monte Carlo** [elektronický dokument]. DOI 10.1063/5.0174232 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 20, art. no. 204708 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 204708

2023 [01/20] / **GBR** - Ghojavand, Sajjad - Dib, Eddy - Rey, Jérôme - Daouli, Ayoub - Clatworthy, Edwin B. - Bazin, Philippe - Ruaux, Valérie - Badawi, Michael - Mintova, Svetlana. **Interplay between alkali-metal cations and silanol sites in nanosized CHA zeolite and implications for CO2 adsorption** [elektronický dokument]. DOI 10.1038/s42004-023-00918-1 In: **Communications chemistry**. [London]: Springer Nature, 2023, Roč. 6, č. 1, art. no. 134 [online]. ISSN (online) 2399-3669. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **DEU** - Cohen, Bat El - Alafi, Ron - Beinglass, Jonathan - Shpatz Dayan, Adva - Goldberg, Oren - Gold, Shachar - Balberg, Isaac - Kronik, Leeor - Etgar, Lioz - Millo, Oded - Azulay, Doron. **In-gap States and Carrier Recombination in Quasi-2D Perovskite Films** [elektronický dokument]. DOI 10.1002/solr.202300813 In: **Solar RRL**. Weinheim : John Wiley & Sons. Wiley-VCH, 2023, Roč. 7, č. 24, art. no. 2300813 [online]. ISSN (online) 2367-198X. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Mostaghimi, Mersad - Pacheco Hernandez, Helmy - Jiang, Yunzhe - Wenzel, Wolfgang - Heinke, Lars - Kozlowska, Mariana. **On–off conduction photoswitching in modelled spiropyran-based metal-organic frameworks** [elektronický dokument]. DOI 10.1038/s42004-023-01072-4 In: **Communications chemistry**. [London]: Springer Nature, 2023, Roč. 6, č. 1, art. no. 275 [online]. ISSN (online) 2399-3669. - SCO ; CCC ; WOS CC, s. art. no. 275

2023 [01/20] / **CHE** - Valenti, Sofia - Cazorla, Claudio - Romanini, Michela - Tamarit, Josep Lluís - Macovez, Roberto. **Eutectic Mixture Formation and Relaxation Dynamics of Coamorphous Mixtures of Two Benzodiazepine Drugs** [elektronický dokument]. DOI 10.3390/pharmaceutics15010196 In: **Pharmaceutics**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 15, č. 1, art. no. 196 [online]. ISSN (online) 1999-4923. - SCO ; WOS CC, s.

2023 [01/20] / **GBR** - Ulian, Gianfranco - Valdrè, Giovanni. **Structural, elastic, electronic, optical and vibrational properties of single-layered, bilayered and bulk molybdenite MoS2-2H** [elektronický dokument]. DOI 10.1107/S1600576723002571 In: **Journal of applied crystallography**. Chester: International Union of Crystallography, 2023, Roč. 56, č. 3, s. 611-623 [tlačená forma] [online]. ISSN 0021-8898. ISSN (online) 1600-5767. - SCO ; CCC ; WOS CC, s. 611 - 623

2023 [01/20] / **USA** - Poier, Pier Paolo - Adjoua, Olivier - Lagardère, Louis - Piquemal, Jean Philip. **Generalized Many-Body Dispersion Correction through Random-Phase Approximation for Chemically Accurate Density Functional**

Theory [elektronický dokument]. DOI 10.1021/acs.jpclett.2c03722 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 6, s. 1609-1617 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 1609 - 1617

2023 [01/20] / **USA** - Daouli, Ayoub - Rey, Jérôme - Lahrar, El Hassane - Valtchev, Valentin - Badawi, Michael - Guillet-Nicolas, Rémy. **Ab Initio Screening of Divalent Cations for CH4, CO2, H2, and N2 Separations in Chabazite Zeolite** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c01882 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 45, s. 15962-15973 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 15962 - 15973

2023 [01/20] / **USA** - Chepkasov, Ilya V. - Baidyshev, Viktor S. - Kvashnin, Alexander G. **Structure-driven tuning of O and CO adsorption on AuCu nanoparticles: A density functional theory study** [elektronický dokument]. DOI 10.1103/PhysRevB.108.205414 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 108, č. 20, art. no. 205414 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Delachaux, F. - Hessou, E. P. - Vallières, C. - Monnier, H. - Badawi, M. **A dispersion-corrected DFT method for zeolite-based CO2/N2separation: Assessment and application** [elektronický dokument]. DOI 10.1016/j.jece.2022.109052 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2023, Roč. 11, č. 1, art. no. 109052 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s.

2023 [01/20] / **GBR** - Manz, Thomas A. **Density-Derived Electrostatic and Chemical Methods** [elektronický dokument]. DOI 10.1016/B978-0-12-821978-2.00072-6 In: **Comprehensive Computational Chemistry**. Oxford: Elsevier, 2023, s. 362-405 [tlačená forma] [online]. ISBN 978-0-12-821978-2. ISBN (online) 978-0-12-823256-9. ISBN (chybné) 978-0-12-823256-9. - SCO, s. 362 - 405

2023 [01/20] / **USA** - Bryenton, Kyle R. - Johnson, Erin R. **Many-body dispersion in model systems and the sensitivity of self-consistent screening** [elektronický dokument]. DOI 10.1063/5.0142465 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 20, art. no. 204110 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **DEU** - Zhang, Chaoyang - Huang, Jing - Bu, Rupeng. **Intrinsic Structures and Properties of Energetic Materials** [textový dokument (print)] . Berlín: Springer Nature, 2023. 1. vyd. ISBN 9789819926992. - SCO, s.

2022 [01/20] / **GBR** - Guha, S. - Kabiraj, A. - Mahapatra, S. **High-throughput design of functional-engineered MXene transistors with low-resistive contacts** [elektronický dokument] In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2022, Roč. 8, č. 1, [online]. ISSN (online) 2057-3960. - SCO, s. Art. No. 202

2022 [01/20] / **USA** - Ma, C. - Li, Q.M. - Gao, W. **Regulating Rolling and Sliding of Carbon Nanotubes on Graphite Through Doping and Charging** In: **Tribology Letters**, 2022, Roč. 70, č. 4. - SCO, s. Art. No. 112

2022 [01/20] / **USA** - Wang, C. - Mueller, T. - Assary, R.S. **Ionic Dynamics of the Charge Carrier in Layered Solid Materials for Mg Rechargeable Batteries** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 19, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 8769 - 8776

2022 [01/20] / **NLD** - Yang, Q. - He, R. - Bai, P. - Xie, J. - Wang, H. **Research on binary gases sensing based on octadecyltrimethoxysilane functionalized silica** [elektronický dokument] In: **Inorganica Chimica Acta**: a Monthly Journal with an International Panel of Referees: the International Inorganic Chemistry Journal. Amsterdam: Elsevier. Elsevier Science, 2022, Roč. 540, [tlačená forma] [online]. ISSN 0020-1693. ISSN (online) 1873-3255. - SCO, s. Art. No. 121041

2022 [01/20] / **USA** - Chepkasov, I.V. - Smet, J.H. - Krasheninnikov, A.V. **Single- and Multilayers of Alkali Metal Atoms inside Graphene/MoS2Heterostructures: A Systematic First-Principles Study** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 37. - SCO, s. 15558 - 15564

2022 [01/20] / **USA** - Liu, G. - Wei, S.-H. - Zhang, C. **Verification of the Accuracy and Efficiency of Dispersion-Corrected Density Functional Theory Methods to Describe the Lattice Structure and Energy of Energetic Cocrystals** In: **Crystal Growth and Design**, 2022, Roč. 22, č. 9. - SCO, s. 5307 - 5321

2022 [01/20] / **USA** - Ramakers, S. - Marusczyk, A. - Amsler, M. - Eckl, T. - Mrovec, M. - Hammerschmidt, T. - Drautz, R. **Effects of thermal, elastic, and surface properties on the stability of SiC polytypes** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 106, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 075201

2022 [01/20] / **GBR** - Bartaquim, E.O. - Bezerra, R.C. - Bittencourt, A.F.B. - Da, Silva J.L.F. **Computational investigation of van der Waals corrections in the adsorption properties of molecules on the Cu(111) surface** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 34, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 20294 - 20302

2022 [01/20] / **USA** - De Rezende, A. - Malmali, M. - Dral, P.O. - Lischka, H. - Tunega, D. - Aquino, A.J.A. **Machine Learning for Designing Mixed Metal Halides for Efficient Ammonia Separation and Storage** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 29. - SCO, s. 12184 - 12196

2022 [01/20] / **GBR** - Daouli, A. - Hessou, E.P. - Monnier, H. - Dziurla, M.-A. - Hasnaoui, A. - Maurin, G. - Badawi, M. **Adsorption of NO, NO2 and H2O in divalent cation faujasite type zeolites: a density functional theory screening approach** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 15565 - 15578

2022 [01/20] / **USA** - Zhang, P. - Shi, J. - Cui, W. - Liu, C. - Ding, S. - Yang, K. - Hao, J. - Li, Y. **Formation of N H3-Xe compound at the extreme condition of planetary interiors** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 105, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 214109

2022 [01/20] / **CHE** - Jin, X. - Lee, K.-G. - Lee, T. - Lee, G. - Mi Oh, S. - Soon, A. - Hwang, S.-J. **Composition-controlled ultrathin holey TiO1-xNx nanosheets as powerful hybridization matrices for highly mass-efficient electrocatalysts** [elektronický dokument] In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2022, Roč. 437, [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO, s. Art. No. 135415

2022 [01/20] / **USA** - Gray, M. - Herbert, J.M. **Comprehensive Basis-Set Testing of Extended Symmetry-Adapted Perturbation Theory and Assessment of Mixed-Basis Combinations to Reduce Cost** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 4, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 2308 - 2330

2022 [01/20] / **CHE** - Mostaghimi, M. - Rego, C.R.C. - Haldar, R. - Woll, C. - Wenzel, W. - Kozlowska, M. **Automated Virtual Design of Organic Semiconductors Based on Metal-Organic Frameworks** [elektronický dokument] In: **Frontiers in Materials**. Lausanne: Frontiers Media, 2022, Roč. 9, [online]. ISSN (online) 2296-8016. - SCO, s. Art. No. 840644

2022 [01/20] / **USA** - Piotrowski, M.J. - Orenha, R.P. - Parreira, R.L.T. - Guedes-Sobrinho, D. **Assessment of the van der Waals, Hubbard U parameter and spin-orbit coupling corrections on the 2D/3D structures from metal gold congeners clusters** [elektronický dokument] In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons,

2022, Roč. 43, č. 4, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO, s. 230 - 243

2022 [01/20] / **DEU** - Kazemi, S.A. - Yengejeh, S.I. - Wang, V. - Wen, W. - Wang, Y. **Theoretical understanding of electronic and mechanical properties of 1T´ transition metal dichalcogenide crystals** [elektronický dokument] In: **Beilstein Journal of Nanotechnology**. Frankfurt nad Mohanom: Beilstein-Institut zur Förderung der Chemischen Wissenschaften, 2022, Roč. 13, [online]. ISSN (online) 2190-4286. - SCO, s. 160 - 171

2022 [01/20] / **USA** - Jin, X. - Lee, T. - Tamakloe, W. - Patil, S.B. - Soon, A. - Kang, Y.-M. - Hwang, S.-J. **In Situ Defect Engineering Route to Optimize the Cationic Redox Activity of Layered Double Hydroxide Nanosheet via Strong Electronic Coupling with Holey Substrate** [elektronický dokument] In: **Advanced Science**. Hoboken: John Wiley & Sons. Wiley Blackwell, 2022, Roč. 9, č. 1, [online]. ISSN (online) 2198-3844. - SCO, s. Art. No. 2103368

2021 [01/20] / **USA** - Alzate-Carvajal, N. - Park, J. - Pykal, M. - Lazar, P. - Rautela, R. - Scarfe, S. - Scarfe, L. - Menard, J.-M. - Otyepka, M. - Luican-Mayer, A. **Graphene Field Effect Transistors: A Sensitive Platform for Detecting Sarin** In: **ACS Applied Materials and Interfaces**, 2021, Roč. 13, č. 51. - SCO, s. 61751 - 61757

2021 [01/20] / **USA** - Wang, F. - Mathur, N. - Janes, A.N. - Sheng, H. - He, P. - Zheng, X. - Yu, P. - DeRuiter, A.J. - Schmidt, J.R. - He, J. - Jin, S. **Defect-mediated ferromagnetism in correlated two-dimensional transition metal phosphorus trisulfides** [elektronický dokument] In: **Science advances**. Washington: American Association for the Advancement of Science, 2021, Roč. 7, č. 43, [online]. ISSN (online) 2375-2548. - SCO, s. Art. No. eabj4086

2021 [01/20] / **GBR** - Oliveira, M. - Hunenberger, P.H. **Systematic optimization of a fragment-based force field against experimental pure-liquid properties considering large compound families: Application to oxygen and nitrogen compounds** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 33, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 17774 - 17793

2021 [01/20] / **CHE** - Hessou, E.P. - Bede, L.A. - Jabraoui, H. - Semmeq, A. - Badawi, M. - Valtchev, V. **Adsorption of toluene and water over cationic-exchanged y zeolites: A dft exploration** [elektronický dokument] In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 26, č. 18, [online]. ISSN (online) 1420-3049. - SCO, s. Art. No. 5486

2021 [01/20] / **USA** - Li, Y. - Liu, C. - Zhao, G.-D. - Hu, T. - Ren, W. **Two-dimensional multiferroics in a breathing kagome lattice** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 104, č. 6, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. L060405

2021 [01/20] / **USA** - Cockayne, E. - Wong-Ng, W. - Chen, Y.-S. - Culp, J.T. - Allen, A.J. **Density Functional Theory Study of the Structure of the Pillared Hofmann Compound Ni(3-Methyl-4,4¸-bipyridine)[Ni(CN)4] (Ni-BpyMe or PICNIC-21)** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 29. - SCO, s. 15882 - 15889

2021 [01/20] / **USA** - Henkel, P. - Mollenhauer, D. **Uncertainty of exchange-correlation functionals in density functional theory calculations for lithium-based solid electrolytes on the case study of lithium phosphorus oxynitride** [elektronický dokument] In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2021, Roč. 42, č. 18, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO, s. 1283 - 1295

2021 [01/20] / **USA** - Price, A.J.A. - Bryenton, K.R. - Johnson, E.R. **Requirements for an accurate dispersion-corrected density functional** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 23, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 230902

2021 [01/20] / **USA** - Welsh, I.D. - Crittenden, D.L. **New atoms-in-molecules dispersion models for use in ab initio**

derived force fields [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 0037157

2021 [01/20] / **NLD** - Hessou, E.P. - Jabraoui, H. - Khalil, I. - Dziurla, M.-A. - Badawi, M. **Ab initio screening of zeolite Y formulations for efficient adsorption of thiophene in presence of benzene** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 541, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 148515

2021 [01/20] / **NLD** - Shao, P. - Pei, J. - Tang, H. - Yu, S. - Yang, L. - Shi, H. - Yu, K. - Zhang, K. - Luo, X. **Defect-rich porous carbon with anti-interference capability for adsorption of bisphenol A via long-range hydrophobic interaction synergized with short-range dispersion force** [elektronický dokument] In: **Journal of Hazardous Materials**: Environmental Control, Risk Assessment, Impact and Management. Amsterdam: Elsevier, 2021, Roč. 403, [tlačená forma] [online]. ISSN 0304-3894. ISSN (online) 1873-3336. - SCO, s. Art. No. 123705

2021 [01/20] / **NLD** - Barhoumi, M. - Said, M. **Electronic and optical properties of bismuth oxyhalides from ab initio calculations** In: **Materials Science and Engineering B: Solid-State Materials for Advanced Technology**, 2021, Roč. 264. - SCO, s. Art. No. 114921

2020 [01/12] / **GBR** - Santos, I.C. - Gama, V. - Rabaca, S. - Veiros, L.F. - Nogueira, F. - Paixao, J.A. - Almeida, M. **Structural diversity in conducting bilayer salts (CNB-EDT-TTF)4A** In: **CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 48, [tlačená forma] [online]. ISSN 1466-8033. - SCO, s. 8313 - 8321

2020 [01/12] / **USA** - Li, Z. - Huang, J. - Ye, L. - Lv, Y. - Zhou, Z. - Shen, Y. - He, Y. - Jiang, L. **Encapsulation of Highly Volatile Fragrances in y Zeolites for Sustained Release: Experimental and Theoretical Studies** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 49, [online]. ISSN (online) 2470-1343. - SCO, s. 31925 - 31935

2020 [01/12] / **NLD** - Berro, Y. - Badawi, M. - El Haj Hassan, F. - Kassir, M. - Tielens, F. **Water-silanol interactions on the amorphous silica surface: A dispersion-corrected DFT investigation** [elektronický dokument] In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2020, Roč. 320, [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. Art. No. 114496

2020 [01/12] / **USA** - Duan, X. - Liu, Z. - Hanrahan, B.M. - Zhu, W. - Liu, S. **Designing xenes with two-dimensional triangular lattice** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 12, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 124003

2020 [01/12] / **USA** - Kashefolgheta, S. - Oliveira, M.P. - Rieder, S.R. - Horta, B.A.C. - Acree, W.E. - Hunenberger, P.H. **Evaluating Classical Force Fields against Experimental Cross-Solvation Free Energies** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 7556 - 7580

2020 [01/12] / **USA** - Oliveira, M.P. - Andrey, M. - Rieder, S.R. - Kern, L. - Hahn, D.F. - Riniker, S. - Horta, B.A.C. - Hunenberger, P.H. **Systematic Optimization of a Fragment-Based Force Field against Experimental Pure-Liquid Properties Considering Large Compound Families: Application to Saturated Haloalkanes** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 7525 - 7555

2020 [01/12] / **DEU** - Holtgrewe, K. - Mahatha, S.K. - Sheverdyaeva, P.M. - Moras, P. - Flammini, R. - Colonna, S. - Ronci,

F. - Papagno, M. - Barla, A. - Petaccia, L. - Aliev, Z.S. - Babanly, M.B. - Chulkov, E.V. - Sanna, S. - Hogan, C. - Carbone, C. **Topologization of beta-antimonene on Bi2Se3 via proximity effects** In: **Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2020, Roč. 10, č. 1, [tlačená forma]. ISSN 1437-7624. - SCO, s. Art. No. 14619

2020 [01/12] / **USA** - Geilhufe, R.M. - Olsthoorn, B. **Identification of strongly interacting organic semimetals** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 20, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 205134

2020 [01/12] / Towler, C.N.A. - Kendrick, J. - Burnett, A.D. **Understanding the Effect of Dispersion Corrections on the Calculated Spectra of** In: **International Conference on Infrared, Millimeter, and Terahertz Waves, IRMMW-THz**. Washington: IEEE Computer Society, 2020. - SCO, s. Art. No. 9370997

2020 [01/12] / **GBR** - Liu, J. - Kang, J. - Chen, S. - White, J.J. - Yin, H. - Liu, P. - Zhao, H. - Wang, Y. **Effects of compositional engineering and surface passivation on the properties of halide perovskites: a theoretical understanding** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 35, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 19718 - 19724

2020 [01/12] / **GBR** - Ghosh, S. - Makeev, M.A. - Macaggi, M.L. - Qi, Z. - Wang, H. - Rajput, N.N. - Martha, S.K. - Pol, V.G. **Dipotassium terephthalate as promising potassium storing anode with DFT calculations** [elektronický dokument] In: **Materials Today Energy**. London: Elsevier, 2020, Roč. 17, [online]. ISSN (online) 2468-6069. - SCO, s. Art. No. 100454

2020 [01/12] / **USA** - Otero-De-La-Roza, A. - Johnson, E.R. **Application of XDM to ionic solids: The importance of dispersion for bulk moduli and crystal geometries** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 054121

2020 [01/12] / Yuan, D. - Zhang, Y. - Ho, W. - Wu, R. **Effects of van der Waals Dispersion Interactions in Density Functional Studies of Adsorption, Catalysis, and Tribology on Metals** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 31. - SCO, s. 16926 - 16942

2020 [01/12] / **DEU** - Barhoumi, M. - Said, M. **Correction of band-gap energy and dielectric function of BiOX bulk with GW and BSE** [elektronický dokument] In: **Optik**: international journal for light and electron optics. Jena: Elsevier. Urban & Fischer, 2020, Roč. 216, [tlačená forma] [online]. ISSN 0030-4026. ISSN (online) 1618-1336. - SCO, s. Art. No. 164631

2020 [01/12] / **USA** - Morales-Garcia, A. - Illas, F. **Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 7, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 73601

2020 [01/12] / **GBR** - Caldeweyher, E. - Mewes, J.-M. - Ehlert, S. - Grimme, S. **Extension and evaluation of the D4 London-dispersion model for periodic systems** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 16, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 8499 - 8512

2020 [01/12] / **GBR** - Rehak, F.R. - Piccini, G. - Alessio, M. - Sauer, J. **Including dispersion in density functional theory**

for adsorption on flat oxide surfaces, in metal-organic frameworks and in acidic zeolites [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 7577 - 7585

2020 [01/12] / **NLD** - Song, Y. - Sun, Z. - Fan, Z. - Cai, W. - Shao, Y. - Sheng, G. - Wang, M. - Song, L. - Liu, Z. - Zhang, Q. - Sun, J. **Rational design of porous nitrogen-doped Ti3C2 MXene as a multifunctional electrocatalyst for Li-S chemistry** [elektronický dokument] In: **Nano Energy**. Amsterdam: Elsevier, 2020, Roč. 70, [tlačená forma] [online]. ISSN 2211-2855. ISSN (online) 2211-3282. - SCO, s. Art. No. 104555

2020 [01/12] / Sethio, D. - Martins, J.B.L. - Lawson Daku, L.M. - Hagemann, H. - Kraka, E. **Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr, Ba, Pb and X = Cl, Br, I)** In: **Journal of Physical Chemistry A**, 2020, Roč. 124, č. 8. - SCO, s. 1619 - 1633

2020 [01/12] / **GBR** - Demirci, S. - Gurel, H.H. - Jahangirov, S. - Ciraci, S. **Temperature, strain and charge mediated multiple and dynamical phase changes of selenium and tellurium** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 12, č. 5, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 3249 - 3258

2020 [01/12] / Shepelenko, M. - Feldman, Y. - Leiserowitz, L. - Kronik, L. **Order and Disorder in Calcium Oxalate Monohydrate: Insights from First-Principles Calculations** In: **Crystal Growth and Design**, 2020, Roč. 20, č. 2. - SCO, s. 858 - 865

2020 [01/12] / **USA** - Rodriguez-Zamora, P. - Salazar-Angeles, B. - Buendia, F. - Cordero-Silis, C. - Fabila, J. - Bazan-Diaz, L. - Fernandez-Diaz, L.M. - Paz-Borbon, L.O. - Diaz, G. - Garzon, I.L. **Revisiting the conformational adsorption of L- and D-cysteine on Au nanoparticles by Raman spectroscopy** [elektronický dokument] In: **Journal of Raman Spectroscopy**. New York: John Wiley & Sons, 2020, Roč. 51, č. 2, [tlačená forma] [online]. ISSN 0377-0486. ISSN (online) 1097-4555. - SCO, s. 243 - 255

2020 [01/12] / **GBR** - Peraca, C.S.T. - Nagurniak, G.R. - Orenha, R.P. - Parreira, R.L.T. - Piotrowski, M.J. **A theoretical indicator of transition-metal nanoclusters applied in the carbon nanotube nucleation process: A DFT study** [elektronický dokument] In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2020, Roč. 49, č. 2, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO, s. 492 - 503

2020 [01/12] / Angyan, J. - Dobson, J. - Jansen, G. - Gould, T. **London Dispersion Forces in Molecules, Solids and Nano-structures: An Introduction to Physical Models and Computational Methods** In: **RSC Theoretical and Computational Chemistry Series**. London: Royal Society of Chemistry, 2020. - SCO, s. 1 - 434

2020 [01/12] / Xie, J. - Zhang, L. - Xing, H.Y. - Bai, P.H. - Liu, B. - Wang, C.J. - Lei, K. - Wang, H. - Peng, S. - Yang, S. **In: Sensors and Actuators B-Chemical**, 2020, Roč. 305. - SCIE ; WOS CC, s. Art. No. 127479

2019 [01/12] / **USA** - Klimes, J. - Tew, D.P. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 151, č. 23, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 234108

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 57, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 33310 - 33336

2019 [01/12] / **USA** - Garcia-Muelas, R. - Rellan-Pineiro, M. - Li, Q. - Lopez, N. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 357 - 367

2019 [01/12] / **DEU** - Shahbaz, M. - Szalewicz, K. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2019, Roč. 138, č. 2, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 25

2019 [01/12] / **USA** - Beck, H. - Gehrmann, C. - Egger, D.A. **In: APL materials**. Melville: ACA and AIP Publishing, 2019, Roč. 7, č. 2, [online]. ISSN (online) 2166-532X. - SCIE ; WOS CC, s. Art. No. 021108

2019 [01/12] / **USA** - Dues, C. - Schmidt, W.G. - Sanna, S. **In: ACS Omega**. Washington: American Chemical Society, 2019, Roč. 4, č. 2, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 3850 - 3859

2019 [01/12] / **CHE** - Allen, A.J. - Wong-Ng, W. - Cockayne, E. - Culp, J.T. - Matranga, C. **In: Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 3, [online]. ISSN (online) 2079-4991. - SCIE ; WOS CC, s. Art. No. 354

2019 [01/12] / **USA** - Cai, T.Y. - Johnson, J.K. - Wu, Y. - Chen, X.P. **In: ACS applied materials and interfaces**. Washington: American Chemical Society, 2019, Roč. 11, č. 9, [tlačená forma] [online]. ISSN 1944-8244. ISSN (online) 1944-8252. - SCIE ; WOS CC, s. 9033 - 9041

2019 [01/12] / **GBR** - Kiruthika, S. - Fjellvag, H. - Ravindran, P. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2019, Roč. 7, č. 11, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 6228 - 6240

2019 [01/12] / Xu, L.Q. - Liu, S.Q. - Yang, J. - Shi, B.W. - Pan, Y.Y. - Zhang, X.Y. - Li, H. - Yan, J.H. - Li, J.Z. - Yang, J.B. - Lu, J. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 14. - SCIE ; WOS CC, s. 8923 - 8931

2019 [01/12] / **USA** - Tran, F. - Kalantari, L. - Traore, B. - Rocquefelte, X. - Blaha, P. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 6, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. - Cole, D.J. - Limas, N.G. - Fiszbein, B. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 34, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 19297 - 19324

2019 [01/12] / **CHE** - Hessou, E.P. - Ponce-Vargas, M. - Mensah, J.B. - Tielens, F. - Santos, J.C. - Badawi, M. **In: Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 5, [online]. ISSN (online) 2079-4991. - SCIE ; WOS CC, s. Art. No. 715

2019 [01/12] / Hessou, E.R. - Jabraoui, H. - Houngue, M.T.A.K. - Mensah, J.B. - Pastore, M. - Badawi, M. **In: Zeitschrift fur Kristallographie-Crystalline Materials**, 2019, Roč. 234, č. 7-8. - SCIE ; WOS CC, s. 469 - 482

2019 [01/12] / **GBR** - Stohr, M. - Van Voorhis, T. - Tkatchenko, A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 48, č. 15, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 4118 - 4154

2019 [01/12] / Caicedo-Davila, S. - Funk, H. - Lovrincic, R. - Muller, C. - Sendner, M. - Cojocaru-Miredin, O. - Lehmann, F. - Gunder, R. - Franz, A. - Levcenco, S. - Cohen, A.V. - Kronik, L. - Haas, B. - Koch, C.T. - Abou-Ras, D. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 29. - SCIE ; WOS CC, s. 17666 - 17677

2019 [01/12] / Salazar, J.M. - Badawi, M. - Radola, B. - Macaud, M. - Simon, J.M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 38. - SCIE ; WOS CC, s. 23455 - 23463

2019 [01/12] / Cohen, A.V. - Egger, D.A. - Rappe, A.M. - Kronik, L. **In: Journal of Physical Chemistry Letters**, 2019,

Roč. 10, č. 16. - SCIE ; WOS CC, s. 4490 - 4498

2019 [01/12] / **USA** - Chen, D.C. - Tang, J. - Zhang, X.X. - Li, Y. - Liu, H.J. **In: IEEE sensors journal**. New York: Institute of Electrical and Electronics Engineers. IEEE Sensors Council, 2019, Roč. 19, č. 1, [tlačená forma] [online]. ISSN 1530-437X. ISSN 2379-9153. ISSN (online) 1558-1748. - SCIE ; WOS CC, s. 39 - 46

2018 [01/12] / **USA** - Liu, P.F. - Bo, T. - Xu, J.P. - Yin, W. - Zhang, J.R. - Wang, F.W. - Eriksson, O. - Wang, B.T. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. UNSP

2018 [01/12] / **USA** - Sun, M.L. - Chou, J.P. - Shi, L.H. - Gao, J.F. - Hu, A. - Tang, W.C. - Zhang, G. **In: ACS Omega**. Washington: American Chemical Society, 2018, Roč. 3, č. 6, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 5971 - 5979

2018 [01/12] / Chen, D.C. - Zhang, X.X. - Tang, J. - Fang, J.N. - Li, Y. - Liu, H.J. **In: Applied Physics A-Materials Science & Processing**, 2018, Roč. 124, č. 6. - SCIE ; WOS CC, s. Art. No. 404

2018 [01/12] / **GBR** - Marcondes, M.L. - Wentzcovitch, R.M. - Assali, L.V.C. **In: Solid State Communications**: an International Journal. Oxford: Elsevier, 2018, Roč. 273, [tlačená forma] [online]. ISSN 0038-1098. ISSN (online) 1879-2766. - SCIE ; WOS CC, s. 11 - 16

2018 [01/12] / **GBR** - Zhao, Q.Y. - Guo, Y.H. - Zhou, Y.X. - Yao, Z.H. - Ren, Z.Y. - Bai, J.T. - Xu, X.L. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 10, č. 7, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 3547 - 3555

2018 [01/12] / **USA** - Loboda, O.A. - Dolgonos, G.A. - Boese, A.D. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. 708 - 713

2018 [01/12] / Hessou, E. - Jabraoui, H. - Chebbi, M. - Chibani, S. - Cantrel, L. - Badawi, M. **Evaluation of the Inhibiting Effect of Organic Compounds on the Adsorption of Iodine Compounds in Cation-Exchanged Zeolites: A DFT Study** In: **Recent Advances in Environmental Science From the Euro-Mediterranean and Surrounding Regions**. Cham: Springer, 2018. - BKCI-S ; WOS CC, s. 107 - 109

2018 [01/12] / **USA** - Bedoya-Martinez, N. - Giunchi, A. - Salzillo, T. - Venuti, E. - Della Valle, R.G. - Zojer, E. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4380 - 4390

2018 [01/12] / **USA** - Srour, J. - Badawi, M. - Hassan, F.E. - Postnikov, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 054106

2018 [01/12] / **USA** - Li, M.S. - Reimers, J.R. - Dobson, J.F. - Gould, T. **In: Proceedings of the National Academy of Sciences of the United States of America**. Washington: National Academy of Sciences of the United States of America, 2018, Roč. 115, č. 44, 10295- [tlačená forma] [online]. ISSN 0027-8424. ISSN (online) 1091-6490. - SCIE ; WOS CC, s.

2018 [01/12] / Hijazi, H. - Cantrel, L. - Paul, J.F. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 46. - SCIE ; WOS CC, s. 26401 - 26408

2018 [01/12] / **USA** - Wen, M.J. - Carr, S. - Fang, S. - Kaxiras, E. - Tadmor, E.B. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 23, [tlačená forma] [online]. ISSN 2469-9950.

ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235404

2018 [01/12] / **GBR** - Piotrowski, M.J. - Nagurniak, G.R. - da Silva, E.H. - Parreira, R.L.T. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 46, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 29480 - 29492

2018 [01/12] / Dolgonos, G.A. - Loboda, O.A. - Boese, A.D. **In: Journal of Physical Chemistry A**, 2018, Roč. 122, č. 2. - SCIE ; WOS CC, s. 708 - 713

2017 [01/12] / **NLD** - Chebbi, M. - Chibani, S. - Paul, J.F. - Cantrel, L. - Badawi, M. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2017, Roč. 239, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 111 - 122

2017 [01/12] / **NLD** - Lebedeva, I.V. - Lebedev, A.V. - Popov, A.M. - Knizhnik, A.A. **In: Computational Materials Science**. Amsterdam: Elsevier, 2017, Roč. 128, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 45 - 58

2017 [01/12] / **USA** - Hermann, J. - DiStasio, R.A. - Tkatchenko, A. **In: Chemical Reviews**. Washington: American Chemical Society, 2017, Roč. 117, č. 6, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 4714 - 4758

2017 [01/12] / **USA** - Boese, A.D. - Sauer, J. **In: Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2017, Roč. 17, č. 4, [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCIE ; WOS CC, s. 1636 - 1646

2017 [01/12] / **USA** - Fischer, M. - Angel, R.J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 174111

2017 [01/12] / **USA** - Caldeweyher, E. - Bannwarth, C. - Grimme, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 147, č. 3, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 034112

2017 [01/12] / Bedoya-Martinez, N. - Schrode, B. - Jones, A.O.F. - Salzillo, T. - Ruzie, C. - Demitri, N. - Geerts, Y.H. - Venuti, E. - Della Valle, R.G. - Zojer, E. - Resel, R. **In: Journal of Physical Chemistry Letters**, 2017, Roč. 8, č. 15. - SCIE ; WOS CC, s. 3690 - 3695

2017 [01/12] / Zhao, Q.Y. - Guo, Y.H. - Zhou, Y.X. - Xu, X. - Ren, Z.Y. - Bai, J.T. - Xu, X.L. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 42. - SCIE ; WOS CC, s. 23744 - 23751

2017 [01/12] / **DEU** - Zhao, Q.Y. - Guo, Y.H. - Si, K.Y. - Ren, Z.Y. - Bai, J.T. - Xu, X.L. **In: Physica Status Solidi B-Basic Solid State Physics**. Weinheim: John Wiley & Sons. Wiley-VCH, 2017, Roč. 254, č. 9, [tlačená forma] [online]. ISSN 0370-1972. ISSN (online) 1521-3951. - SCIE ; WOS CC, s. Art. No. 1700033

2017 [01/12] / **USA** - Tsatsoulis, T. - Hummel, F. - Usvyat, D. - Schutz, M. - Booth, G.H. - Binnie, S.S. - Gillan, M.J. - Alfe, D. - Michaelides, A. - Gruneis, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 20, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 204108

2016 [01/12] / **GBR** - Limas, N.G. - Manz, T.A. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 6, č. 51, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 45727 - 45747

2016 [01/12] / **DEU** - Suarez, J.A. - Plata, J.J. - Marquez, A.M. - Sanz, J.F. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2016, Roč. 135, č. 3, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 70

2016 [01/12] / **USA** - Cole, D.J. - Vilseck, J.Z. - Tirado-Rives, J. - Payne, M.C. - Jorgensen, W.L. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 5, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2312 - 2323

2016 [01/12] / **USA** - Grimme, S. - Hansen, A. - Brandenburg, J.G. - Bannwarth, C. **In: Chemical Reviews**. Washington: American Chemical Society, 2016, Roč. 116, č. 9, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 5105 - 5154

2016 [01/12] / **USA** - Li, J.R. - Rinke, P. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045201

2016 [01/12] / **USA** - Verstraelen, T. - Vandenbrande, S. - Heidar-Zadeh, F. - Vanduyfhuys, L. - Van Speybroeck, V. - Waroquier, M. - Ayers, P.W. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 3894 - 3912

2016 [01/12] / **USA** - Klimes, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094506

2016 [01/12] / Deringer, V.L. - Csanyi, G. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 38. - SCIE ; WOS CC, s. 21552 - 21560

2016 [01/12] / **USA** - Woods, L.M. - Dalvit, D.A.R. - Tkatchenko, A. - Rodriguez-Lopez, P. - Rodriguez, A.W. - Podgornik, R. **In: Reviews of modern physics**. Melville: American Institute of Physics. American Physical Society, 2016, Roč. 88, č. 4, [tlačená forma] [online]. ISSN 0034-6861. ISSN (online) 1539-0756. - SCIE ; WOS CC, s. Art. No. 045003

2016 [01/12] / **DEU** - Granas, O. - Vinichenko, D. - Kaxiras, E. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2016, Roč. 6, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 36108

2016 [01/12] / Piotrowski, M.J. - Ungureanu, C.G. - Tereshchuk, P. - Batista, K.E.A. - Chaves, A.S. - Guedes-Sobrinho, D. - Da Silva, J.L.F. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 50. - SCIE ; WOS CC, s. 28844 - 28856

2016 [01/12] / **DEU** - Heidar-Zadeh, F. - Fias, S. - Vohringer-Martinez, E. - Verstraelen, T. - Ayers, P.W. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2016, Roč. 136, č. 1, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 19

2015 [01/12] / Rego, C.R.C. - Oliveira, L.N. - Tereshchuk, P. - Da Silva, J.L.F. **In: Journal of Physics-Condensed Matter**, 2015, Roč. 27, č. 41. - SCIE ; WOS CC, s. Art. No. 415502

2015 [01/12] / Yanagisawa, S. - Okuma, K. - Inaoka, T. - Hamada, I. **In: Journal of Electron Spectroscopy and Related Phenomena**, 2015, Roč. 204. ISSN 03682048. - SCIE ; WOS CC, s. 159 - 167

2015 [01/12] / **NLD** - Sun, T. - Wang, Y. - Zhang, H.M. - Liu, P.R. - Zhao, H.J. **In: Journal of colloid and interface science**. Amsterdam: Elsevier, 2015, Roč. 454, [tlačená forma] [online]. ISSN 0021-9797. ISSN (online) 1095-7103. - SCIE ; WOS CC, s. 180 - 186

2015 [01/12] / **USA** - Guevara-Garcia, A. - Ireta, J. - Galvan, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 142, č. 1, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 014504

2014 [01/12] / **USA** - Kronik, L. - Tkatchenko, A. **In: Accounts of Chemical Research**. Washington: American Chemical Society, 2014, Roč. 47, č. 11, [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCIE ; WOS CC, s. 3208 - 3216

2014 [01/12] / Moellmann, J. - Grimme, S. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 14. - SCIE ; WOS CC, s. 7615 - 7621

2014 [01/12] / Egger, D.A. - Kronik, L. **In: Journal of Physical Chemistry Letters**, 2014, Roč. 5, č. 15. - SCIE ; WOS CC, s. 2728 - 2733

2013 [01/12] / **GBR** - Ling, S. - Watkins, M.B. - Shluger, A.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 45, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; SCO ; WOS CC, s. 19615 - 19624

ADC_039: / Bučko, Tomáš (Autor) [UKOPRCFZ] (70%) - Lebegue, Sebastien (Autor) (10%) - Hafner, Jürgen (Autor) (10%) - Ángyán, János G. (Autor) (10%): **Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids**. – text, tab., obr. – DOI 10.1103/PhysRevB.87.064110. – CCC ; WOS CC ; SCIE ; SCO.
In: *Physical Review B, Condensed matter and materials physics* [textový dokument (print)] [elektronický dokument] . – College Park (USA) : American Institute of Physics. American Physical Society. – ISSN 1098-0121. – ISSN (online) 1550-235X. – Roč. 87, č. 6 (2013), s. 4110-4110 [tlačená forma] [online] [CD-ROM]
Počet všetkých autorov: 4
[článok]
Lit.: 113
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 3.664 - 2013
SNIP: 1,334 - 2013
SJR: 2,813 - 2013
CiteScore: 6,9 - 2013
Kvartil Q:
2013, JIF - Physics, condensed matter - Q1

Ohlasy (316):
2025 [01/20] / **USA** - Muhli, Heikki - Ala-Nissila, Tapio - Caro, Miguel A. **Atom-wise formulation of the many-body dispersion problem for linear-scaling van der Waals corrections** [elektronický dokument]. DOI 10.1103/PhysRevB.111.054103 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 111, č. 5, art. no. 054103 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **NLD** - Lin, Zhonghai - Liu, Mengdi - Wang, Pingjian - Zeng, Ruiyang. **Properties of PeDAPbI4 Dion-**

Jacobson phase perovskite regulated by ligand with amino and hydroxy [elektronický dokument]. DOI 10.1016/j.jssc.2025.125388 In: **Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2025, Roč. 348, art. no. 125388 [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 125388

2025 [01/20] / **USA** - Tasci, Cankut - Cunha, Leonardo A. - Flick, Johannes. **Photon Many-Body Dispersion: Exchange-Correlation Functional for Strongly Coupled Light-Matter Systems** [elektronický dokument]. DOI 10.1103/PhysRevLett.134.073002 In: **Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 134, č. 7, art. no. 073002 [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 073002

2025 [01/20] / **USA** - Ibragimova, Rina - Kuklin, Mikhail S. - Zarrouk, Tigany - Caro, Miguel A. **Unifying the Description of Hydrocarbons and Hydrogenated Carbon Materials with a Chemically Reactive Machine Learning Interatomic Potential** [elektronický dokument]. DOI 10.1021/acs.chemmater.4c02905 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2025, Roč. 37, č. 3, s. 1094-1110 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 1094 - 1110

2025 [01/20] / **CHN** - Zhang, Feng - Zhang, Chenyang - Wu, Linlin - Sun, Wei - Zhang, Hongliang - Chen, Jianhua - Pei, Yong - Li, Songjiang. **Depression mechanism of sulfite ions on sphalerite and Pb2+ activated sphalerite in the flotation separation of galena from sphalerite** [elektronický dokument]. DOI 10.1007/s12613-024-2936-2 In: **International journal of minerals metallurgy and materials**. Peking: University of Science and Technology, 2025, Roč. 32, č. 2, s. 335-345 [tlačená forma] [online]. ISSN 1674-4799. ISSN (online) 1869-103X. - SCO ; WOS CC ; SCIE, s. 335 - 345

2025 [01/20] / **CHN** - Wang, Yi Qing - Lin, Zhi - Li, Ming Tao - Shen, Shao Hua. **Theoretical Insights into the Atomic and Electronic Structures of Polyperyleneimide: On the Origin of Photocatalytic Oxygen Evolution Activity** [elektronický dokument]. DOI 10.61558/2993-074X.3523 In: **Journal of Electrochemistry**. Xiamen City: Chinese Society of Electrochemistry, 2025, Roč. 31, č. 5, art. no. 2418002. ISSN 1006-3471. ISSN (online) 2993-074X. - SCO ; WOS CC ; ESCI ; OA, s.

2025 [01/20] / **GBR** - Rêgo, Celso R.C. - Wenzel, Wolfgang - Piotrowski, Maurício J. - Dias, Alexandre C. - Maciel de Oliveira Bastos, Carlos - de Araujo, Luis O. - Guedes-Sobrinho, Diego. **Digital workflow optimization of van der Waals methods for improved halide perovskite solar materials** [elektronický dokument]. DOI 10.1039/d4dd00312h In: **Digital Discovery**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 4, č. 4, s. 927-942. ISSN (online) 2635098X. - SCO ; WOS CC ; ESCI ; OA, s. 927 - 942

2025 [01/20] / **USA** - Lausch, K. Nikolas - El Haouari, Redouan - Trzewik, Daniel - Behler, Jörg. **Impact of the damping function in dispersion-corrected density functional theory on the properties of liquid water** [elektronický dokument]. DOI 10.1063/5.0275244 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 3, art. no. 034101 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 034101

2025 [01/20] / **GBR** - Deng, Xinxin - Dai, Suwei - Zhang, Zili - Luo, Bingcheng. **Geometric optimisation and structural properties of organic−inorganic halide perovskites from van der Waals density functional theory calculations** [elektronický dokument]. DOI 10.1080/00268976.2024.2403670 In: **Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2025, Roč. 123, č. 11, art. no. e2403670 [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **USA** - Ladygin, V. V. - Knoop, F. - Bernal-Choban, C. M. - Granroth, G. E. - Fultz, B. **Anharmonic phonons, thermal expansion, and nuclear quantum effects in Zn** [elektronický dokument]. DOI 10.1103/pr3j-jwd5 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 9, č. 12, art. no. 125001 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 125001

2025 [01/20] / **GBR** - Yang, Feihong - Pan, Yong - Jain, I. P. **Defect engineering of MoS2/borophene/WS2sandwich heterostructures enhanced the HER catalytic activity and improved water splitting efficiency** [elektronický dokument]. DOI 10.1039/d5ta06215b In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2025, Roč. 13, č. 43, s. 37508-37519 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 37508 - 37519

2025 [01/20] / **USA** - Milner, Scott T. **Calculating Nonbonded Potentials for Classical Simulations of Atoms in Molecules and Metal Surfaces** [elektronický dokument]. DOI 10.1021/acs.jctc.5c01017 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 20, s. 10413-10423 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 10413 - 10423

2025 [01/20] / **USA** - Ifliand, Maria - Houben, Lothar - Shepelenko, Margarita - Feldman, Yishay - Kossoy, Anna Eden - Friedman, Ofir - Hildebrand, Mariana - Addadi, Lia - Leiserowitz, Leslie - Kronik, Leeor. **Discovering the Crystal Structure of Biogenic Xanthine Crystals** [elektronický dokument]. DOI 10.1021/acs.cgd.5c00619 In: **Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2025, Roč. 25, č. 18, s. 7524-7536 [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 7524 - 7536

2025 [01/20] / **USA** - Wu, Junhong - Hu, Min - Wan, Dongyi - Cao, Zhengqin - Wei, Gang - Li, Long - Wu, Xiaoyu. **Adsorption and Gas Sensing Properties of SF6/N2Decomposition Components (NF3,SO2) on Pt-Doped MoSe2Monolayer: A DFT Study** [elektronický dokument]. DOI 10.1021/acsomega.5c03697 In: **ACS Omega**. Washington: American Chemical Society, 2025, Roč. 10, č. 36, s. 41124-41135 [online]. ISSN (online) 2470-1343. - SCO ; OA, s. 41124 - 41235

2025 [01/20] / **CHE** - Tan, Juanjuan - Huang, Shuying - Dong, Jianhong - Fan, Jiaming - Hou, Dejian - Lin, Shaomin. **Ir- and Pt-Doped InTe Monolayers as Potential Sensors for SF6 Decomposition Products: A DFT Investigation** [elektronický dokument]. DOI 10.3390/ma18174022 In: **Materials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 18, č. 17, art. no. 4022 [online]. ISSN (online) 1996-1944. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 4022

2025 [01/20] / **GBR** - Poddar, Suvankar - Das, Pulok - Bhattacharjee, Souvik - Chattopadhyay, Kalyan Kumar. **Inversion symmetry-broken CuBO2 delafossite through anionic site doping for improved piezoelectric composites with PVDF and its application in nanogenerators and optoelectronic neuromorphic computing** [elektronický dokument]. DOI 10.1039/d5ta02437d In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2025, Roč. 13, č. 34, s. 28451-28470 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC ; SCIE, s. 28451 - 28470

2025 [01/20] / **NLD** - Mukherjee, Supratik - Vaitheeswaran, G. **Investigation of the Structural, Vibrational, Electronic, and optical properties of energetic Nitrogen-Rich azidotetrazolates XCN7 (X = N2H5, NH4, K, Cs)** [elektronický dokument]. DOI 10.1016/j.chemphys.2024.112537 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2025, Roč. 590, art. no. 112537 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 112537

2025 [01/20] / **GBR** - Hu, Chen - Yang, Chao - Li, Bo - Peng, Bangzhu. **Removal of ochratoxin A from wine by adsorption-photocatalytic synergy of tubular TiO2/SiO2/g-C3N4: Mechanistic insights and degradation pathways** [elektronický dokument]. DOI 10.1016/j.foodchem.2025.142758 In: **Food chemistry**. Londýn: Elsevier, 2025, Roč. 471, art. no. 142758 [tlačená forma] [online]. ISSN 0308-8146. ISSN (online) 1873-7072. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 142758

2025 [01/20] / **NLD** - Li, Wan - Atikah Zulkafli, Nur Miza - Mamat, Mohamad Hafiz - Yaakob, Muhamad Kamil. **Revisiting the effects of spin-orbit coupling and dispersion correction on the structural and electronic properties of APbI3 (A=MA, FA) halide perovskite** [elektronický dokument]. DOI 10.1016/j.physb.2025.417075 In: **Physica B**:

Condensed Matter. Amsterdam: Elsevier, 2025, Roč. 704, art. no. 417075 [tlačená forma] [online]. ISSN 0921-4526. ISSN (online) 1873-2135. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 417075

2025 [01/20] / **GBR** - Yang, Feihong - Pan, Yong - Jain, I. P. **Single atom enhanced the catalytic activity of borophene catalysts for hydrogen evolution reaction** [elektronický dokument]. DOI 10.1016/j.ijhydene.2025.05.339 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 140, s. 223-232 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC ; SCIE, s. 223 - 232

2025 [01/20] / **NLD** - Xie, Shuhong - Zhan, Weixing - Zhang, Hanyu. **Theoretical investigation of Ni, Cu, Nb-doped HfS2 monolayers for sensing biomarkers relevant to early health status** [elektronický dokument]. DOI 10.1016/j.surfin.2025.106956 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2025, Roč. 72, art. no. 106956 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 106956

2025 [01/20] / **NLD** - Zhong, Minglian - Xiong, Huihui - Zeng, Ganhua - Zhang, Xiaofu. **Potential of TM-decorated PtSe2 monolayers for identifying VOCs biomarkers indicative of early-stage lung cancer** [elektronický dokument]. DOI 10.1016/j.surfin.2025.107476 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2025, Roč. 73, art. no. 107476 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 107476

2025 [01/20] / **NLD** - Chen, Xudong - Liu, Wengang - Zhang, Jing - Chen, Mengqiang - Liu, Wenbao - Sun, Yaguang - Shen, Yanbai - Zhao, Qiang. **Selective depression mechanism of N,N-bis(phosphonomethyl)sulfamic acid on dolomite in magnesite flotation: Integrated experimental and computational approach** [elektronický dokument]. DOI 10.1016/j.seppur.2025.133109 In: **Separation and Purification Technology**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 368, art. no. 133109 [tlačená forma] [online]. ISSN 1383-5866. ISSN (online) 1873-3794. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 133109

2025 [01/20] / **GBR** - Li, Shanshan - Zheng, Qingrong. **Effect of incorporation of graphene oxide on the purification and separation performance of MOFs for by-product hydrogen: By GCMC simulations, DFT calculations and experiments** [elektronický dokument]. DOI 10.1016/j.ijhydene.2025.152068 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 186, art. no. 152068 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 152068

2025 [01/20] / **CHE** - Wang, Linxia - Liu, Guangbei - Li, Hu - Fu, Yongxu - Kang, Qingbo - Zheng, Zejian - Li, Jiangke - Wu, Minghui - Gao, Shan - Yan, Xiaobing - Wang, Weichao. **δ-BS monolayer with high theoretical specific capacity for sodium-ion and calcium-ion batteries** [elektronický dokument]. DOI 10.1016/j.jallcom.2025.184695 In: **Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2025, Roč. 1045, art. no. 184695 [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCO ; WOS CC ; SCIE, s. art. no. 184695

2025 [01/20] / **NLD** - Xie, Wuming - Xiong, Huihui. **Exploring Ni, Rh, and Pd-modified single-layer hafnium disulfide as potential sensing materials for chronic obstructive pulmonary disease biomarkers: Insights from density functional theory study** [elektronický dokument]. DOI 10.1016/j.colsurfa.2025.138258 In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2025, Roč. 727, art. no. 138258 [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 138258

2025 [01/20] / **NLD** - Zhu, Jiaxin - Pan, Yong. **Janus monolayer MXY(M=Mo, W; X, Y=S, Se and Te)/β-Ga2O3 van der Waals heterojunctions with type I/II: A self powered UV to IR broad spectrum photodetector**. DOI 10.1016/j.mtnano.2025.100683 In: **Materials Today Nano**. Amsterdam: Elsevier, 2025, Roč. 32, art. no. 100683. ISSN 2588-8420 (online). - SCO ; WOS CC ; SCIE, s. art. no. 100683

2025 [01/20] / **USA** - Carneiro Queiroz da Silva, G. - Salazar, J. Marcos. **Emergence of an Icosahedral (H2)13 Cluster inside a Pure Silica Faujasite** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c08679 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 14, s. 7031-7039 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 7031 - 7039

2025 [01/20] / **USA** - Sulaiman, Nura M. - Weikun, Liu - Yunhan, Zhen - Douxing, Pan. **Lennard-Jones Potential Parameters and Cut-Off Modifications for Layered Transition Metal Dichalcogenides** [elektronický dokument]. DOI 10.1115/1.4068957 In: **Journal of applied mechanics**. NewYork: American Society of Mechanical Engineers, 2025, Roč. 92, č. 10, art. no. 101010 [tlačená forma]. ISSN 0021-8936. ISSN (online) 1528-9036. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 101010

2025 [01/20] / **USA** - Jinghan, Li - Yutian, Li - Sulaiman, Nura M. - Douxing, Pan. **Lennard-Jones interfacial parameters and cut-off modifications for layered buckled honeycomb bi-elemental crystals** [elektronický dokument]. DOI 10.1063/5.0277888 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2025, Roč. 138, č. 7, art. no. 075303 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 075303

2024 [01/20] / **USA** - Pan, Douxing - Li, Jinghan - Voon, Lok C.Lew Yan - Wei, Peijun. **Determination of Lennard-Jones potential parameters for interfacial interaction in elemental layered crystals** [elektronický dokument]. DOI 10.1063/5.0213582 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2024, Roč. 135, č. 20, art. no. 204301 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **CHE** - Zeng, Tingting - Ma, Donglin - Gui, Yingang. **Gas-Sensing Performance of Metal Oxide Heterojunction Materials for SF6 Decomposition Gases: A DFT Study** [elektronický dokument]. DOI 10.3390/ijms25158009 In: **International journal of molecular sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 25, č. 15, art. no. 8009, s. [online] [tlačená forma]. ISSN 1661-6596. ISSN (online) 1422-0067. - WOS CC ; SCO ; SCIE ; CCC, s.

2024 [01/20] / **DEU** - Mukherjee, Supratik - Vaitheeswaran, G. **Beyond Traditional Perovskites: Xenon's Influence on the Vibrational and Electronic Properties of K4Xe3O12** [elektronický dokument]. DOI 10.1002/adts.202400545 In: **Advanced theory and simulations**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 7, č. 12, art. no. 2400545 [online]. ISSN (online) 2513-0390. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Xia, Wei - Zhou, Zhijie - Sheng, Liangzheng - Chen, Lihang - Shen, Fuxing - Zheng, Fang - Zhang, Zhiguo - Yang, Qiwei - Ren, Qilong - Bao, Zongbi. **Bioinspired recognition in metal-organic frameworks enabling precise sieving separation of fluorinated propylene and propane mixtures** [elektronický dokument]. DOI 10.1038/s41467-024-53024-8 In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2024, Roč. 15, č. 1, art. no. 8716 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s. art. no. 8716

2024 [01/20] / **NLD** - Mukherjee, Supratik - Jharapla, Prathap Kumar - Vaitheeswaran, G. **Electronic structure, phonons, and optical properties of nitrogen-enriched 5-aminotetrazolium nitrate (5-ATN)**. DOI 10.1016/j.cocom.2024.e00967 In: **Computational condensed matter**. Amsterdam: Elsevier, 2024, Roč. 41, art. no. e00967 [tlačená forma]. ISSN 2352-2143. - SCO ; WOS CC, s. art. no. e00967

2024 [01/20] / **USA** - Xing, Zhe - Orlov, Dmytro - Schröder, Elsebeth. **Tailored pseudopotentials for magnesium surface core level shift calculations** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.8.123801 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2024, Roč. 8, č. 12, art. no. 123801 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC, s. art. no. 123801

2024 [01/20] / **NLD** - Xiong, Huihui - Zhang, Shulin - Ma, Yingying - Zhang, Yifu - Huang, Haojie - Li, Junhui - Sun, Chengcheng - Zhong, Xiaocong. **First-principles study of WS2 monolayer decorated with noble metals (Pt, Rh, Ir) as the promising candidates to detect nitrogenous poisonous gases** [elektronický dokument]. DOI 10.1016/j.surfin.2024.105363 In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2024, Roč. 55, art. no. 105363 [online]. ISSN (online) 2468-0230. - SCO ; CCC ; WOS CC, s. art. no. 105363

2024 [01/20] / **NLD** - Ma, Yingying - Yang, Minjia - Deng, Gengfeng - Xiong, Huihui. **Theoretical insights into gas-sensitive properties of B, Ga and In doped WS2 monolayer towards oxygen-containing toxic gases** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.160725 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2024, Roč. 670, art. no. 160725 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 160725

2024 [01/20] / **NLD** - Pan, Wenfeng - Li, Shulei - Zhu, Yangge - Gao, Lihui - Ma, Zilong - Cao, Yijun - Du, Shijie. **Hydration mechanism of molybdenite affected by surface oxidation: New insights from DFT and MD simulations** [elektronický dokument]. DOI 10.1016/j.colsurfa.2024.134599 In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2024, Roč. 698, art. no. 134599 [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO ; CCC ; WOS CC, s. art. no. 134599

2024 [01/20] / **NLD** - Yang, Minjia - Xiong, Huihui - Ma, Yingying - Yang, Liang. **Theoretical investigation of Ag and Au modified CSiN monolayer as a potential gas sensor for air decomposition components detection** [elektronický dokument]. DOI 10.1016/j.molliq.2024.125648 In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2024, Roč. 410, art. no. 125648 [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO ; CCC ; WOS CC, s. art. no. 125648

2024 [01/20] / **USA** - Kim, Hyun Tak - Park, Jaehyun - Mun, Jinhong - Shin, Hyeon Oh - Roh, Deok Ho - Kwon, Junhyeok - Kim, Sungtae - Kim, Sang Joon - Lee, Geunsik - Kang, Seok Ju - Kwon, Tae Hyuk. **Selective Electroreduction of CO2 to C2+ Alcohols Using Graphitic Frustrated Lewis Pair Catalyst** [elektronický dokument]. DOI 10.1021/acscatal.3c04275 In: **ACS Catalysis**. Washington: American Chemical Society, 2024, Roč. 14, č. 13, s. 10392-10402 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 10392 - 10402

2024 [01/20] / **USA** - Zhang, Haoming - Zhou, Wen - Jiang, Jiaming - Zeng, Wen - Zhou, Qu. **First-Principles Investigation of Transition Metal (Co, Rh, and Ir)-Modified WS2 Monolayer Membranes: Adsorption and Detection of SF6 Decomposition Gases** [elektronický dokument]. DOI 10.1021/acsanm.4c01791 In: **ACS applied nano materials**. Washington: American Chemical Society, 2024, Roč. 7, č. 11, s. 13379-13391 [online]. ISSN (online) 2574-0970. - SCO ; CCC ; WOS CC, s. 13379 - 13391

2024 [01/20] / **SGP** - Tse, Geoffrey. **First principle calculations: The electronic, optical, mechanical, and vibrational properties of TiS3** [elektronický dokument]. DOI 10.1142/S0217979224501455 In: **International Journal of Modern Physics B**: Condensed Matter Physics; Statistical Physics; Atomic, Molecular and Optical Physics. Singapur: World Scientific Publishing, 2024, Roč. 38, č. 10, art. no. 2450145 [tlačená forma] [online]. ISSN 0217-9792. ISSN (online) 1793-6578. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Guo, Jiayi - Hu, Danni - Bai, Chenqi - Xu, Lina - Xiao, Hongping - Shi, Qian - Li, Xinhua - Chen, Xi'an - Ma, Yingjin - Fang, Guoyong. **Structural and electrochemical properties of Tan+1Cn MXene anode materials for metal-ion batteries** [elektronický dokument]. DOI 10.1039/d3qi02335d In: **Inorganic Chemistry Frontiers**. London: The Royal Society of Chemistry, 2024, Roč. 11, č. 10, s. 2945-2956 [tlačená forma] [online]. ISSN 2052-1545. ISSN (online) 2052-1553. - SCO ; CCC ; WOS CC, s. 2945 - 2956

2024 [01/20] / **NLD** - Chen, Jun - Shang, Huanhuan - Ling, Yunjia - Shu, Qingdong - Sun, Yu - Min, Fanfei. **Microscopic mechanism of CO2 adsorption on M2+ (M = Fe, Ca, Mg)-doped kaolinite (0 0 1) surface: DFT calculations**

[elektronický dokument]. DOI 10.1016/j.chemphys.2024.112212 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2024, Roč. 579, art. no. 112212 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO, s. art. no. 112212

2024 [01/20] / **USA** - Rezapour, M. Reza - Biel, Blanca. **Using Graphdiyne Nanoribbons for Molecular Electronics Spectroscopy and Nucleobase Identification: A Theoretical Investigation** [elektronický dokument]. DOI 10.1021/acsaelm.3c01607 In: **ACS Applied Electronic Materials**. Washington: American Chemical Society, 2024, Roč. 6, č. 2, s. 1244-1251 [online]. ISSN (online) 2637-6113. - SCO ; CCC ; WOS CC, s. 1244 - 1251

2024 [01/20] / **NLD** - Huang, Hong - Mu, Jinglin - Liang, Manfen - Qi, Ruirui - Wu, Mei - Xu, Leilei - Xu, Haimei - Zhao, Jinping - Zhou, Jin - Miao, Zhichao. **One-pot synthesis of MoO3-ZrO2 solid acid catalyst for solvent-free solketal production from glycerol** [elektronický dokument]. DOI 10.1016/j.mcat.2023.113682 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2024, Roč. 552, art. no. 113682 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO ; CCC ; WOS CC, s. art. no. 113682

2024 [01/20] / **USA** - Samal, Pragnya Paramita - Krishnamurty, Sailaja. **First-Principles Simulation of Active Site Selectivity for CO2 and H2 Adsorption on Mg(OH)+/Mg2+ and Ca(OH)+/Ca2+ Zeolites** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c05835 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 51, s. 21659-21671 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 21659 - 21671

2024 [01/20] / **USA** - Cossu, F. - Nafday, D. - Palotás, K. - Biderang, M. - Kim, H. S. - Akbari, A. - Di Marco, I. **Stacking of charge-density waves in 2 H-NbSe2 bilayers**. DOI 10.1103/PhysRevResearch.6.043111 In: **Physical Review Research**. New York: American Institute of Physics. American Physical Society, 2024, Roč. 6, č. 4, art. no. 043111 [online]. ISSN 2643-1564. - SCO ; WOS CC, s. art. no. 043111

2023 [01/20] / **GBR** - Ghojavand, Sajjad - Dib, Eddy - Rey, Jérôme - Daouli, Ayoub - Clatworthy, Edwin B. - Bazin, Philippe - Ruaux, Valérie - Badawi, Michael - Mintova, Svetlana. **Interplay between alkali-metal cations and silanol sites in nanosized CHA zeolite and implications for CO2 adsorption** [elektronický dokument]. DOI 10.1038/s42004-023-00918-1 In: **Communications chemistry**. [London]: Springer Nature, 2023, Roč. 6, č. 1, art. no. 134 [online]. ISSN (online) 2399-3669. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Daouli, Ayoub - Rey, Jérôme - Lahrar, El Hassane - Valtchev, Valentin - Badawi, Michael - Guillet-Nicolas, Rémy. **Ab Initio Screening of Divalent Cations for CH4, CO2, H2, and N2 Separations in Chabazite Zeolite** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c01882 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 45, s. 15962-15973 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 15962 - 15973

2023 [01/20] / **CHE** - Grančič, Peter - Böhm, Leonard - Gerzabek, Martin H. - Tunega, Daniel. **On the Nature of Hydrophobic Organic Compound Adsorption to Smectite Minerals Using the Example of Hexachlorobenzene-Montmorillonite Interactions** [elektronický dokument]. DOI 10.3390/min13020280 In: **Minerals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 2, art. no. 280 [online]. ISSN (online) 2075-163X. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **NLD** - Rangarajan, Srinivas - Mavrikakis, Manos. **A comparative analysis of different van der Waals treatments for molecular adsorption on the basal plane of 2H-MoS2** [elektronický dokument]. DOI 10.1016/j.susc.2022.122226 In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2023, Roč. 729, art. no. 122226 [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Delachaux, F. - Hessou, E. P. - Vallières, C. - Monnier, H. - Badawi, M. **A dispersion-corrected**

DFT method for zeolite-based CO2/N2separation: Assessment and application [elektronický dokument]. DOI 10.1016/j.jece.2022.109052 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2023, Roč. 11, č. 1, art. no. 109052 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s.

2023 [01/20] / **NLD** - Srikaew, Manmanut - Wongnongwa, Yutthana - Jungsuitiwong, Siriporn - Kaiyasuan, Chokchai - Promarak, Vinich - Saengsuwan, Sayant. **Improvement of adsorption performance and selectivity of GO-COOH towards MB dye through effective carboxylation approach: Combined experimental and DFT studies** [elektronický dokument]. DOI 10.1016/j.colsurfa.2023.131920 In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2023, Roč. 673, art. no. 131920 [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO ; CCC ; WOS CC, s. art. no. 131920

2023 [01/20] / **USA** - Yourdkhani, Sirous - Klimeš, Jiří. **Using Noncovalent Interactions to Test the Precision of Projector-Augmented Wave Data Sets** [elektronický dokument]. DOI 10.1021/acs.jctc.3c00930 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2023, Roč. 19, č. 23, s. 8871-8885 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 8871 - 8885

2023 [01/20] / **USA** - Ma, Lei - Li, Meng Na - Zhang, Li Li. **Electronic and optical properties of GaN/MoSe2 and its vacancy heterojunctions studied by first-principles** [elektronický dokument]. DOI 10.1063/5.0123621 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2023, Roč. 133, č. 4, art. no. 045307 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC, s. art. no. 045307

2023 [01/20] / **DEU** - Wang, Jiali - Lu, Jiajun - Zhao, Xiuwen - Hu, Guichao - Yuan, Xiaobo - Ren, Junfeng. **Two-dimensional Janus AsXY (X = Se, Te; Y = Br, I) monolayers for photocatalytic water splitting** [elektronický dokument]. DOI 10.1140/epjb/s10051-023-00486-2 In: **The European Physical Journal B**: Condensed Matter and Complex Systems. Berlin: Springer Nature. Springer Science+Business Media, 2023, Roč. 96, č. 2, art. no. 17 [tlačená forma] [online]. ISSN 1434-6028. ISSN (online) 1434-6036. - SCO ; CCC ; WOS CC, s. art. no. 17

2023 [01/20] / **USA** - Felix, João P.C.S. - Batista, Krys E.A. - Morais, Wesley O. - Nagurniak, Glaucio R. - Orenha, Renato P. - Rêgo, Celso R.C. - Guedes-Sobrinho, Diego - Parreira, Renato L.T. - Ferrer, Mateus M. - Piotrowski, Maurício J. **Molecular adsorption on coinage metal subnanoclusters: A DFT+D3 investigation** [elektronický dokument]. DOI 10.1002/jcc.27063 In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2023, Roč. 44, č. 10, s. 1040-1051 [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO ; CCC ; WOS CC, s. 1040 - 1051

2023 [01/20] / **NLD** - Ling, Yunjia - Chen, Jun - Min, Fanfei - Cheng, Yali - Chu, Xinxia - Shang, Huanhuan - Wang, Tianyue. **Influence mechanism of Fe(II/III) doping on the adsorption of methylamine salts on kaolinite surfaces elucidated through DFT calculations** [elektronický dokument]. DOI 10.1016/j.molliq.2023.123082 In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2023, Roč. 390, art. no. 123082 [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO ; CCC ; WOS CC, s. art. no. 123082

2023 [01/20] / **DEU** - Zhang, Feng - Sun, Wei - Zhang, Hongliang - Chen, Daixiong - Li, Songjiang - Chen, Jianhua - Zhang, Chenyang. **Selective Adsorption Mechanism of Zinc Ions on the Surfaces of Galena and Sphalerite in the Flotation Separation of Pb-Zn** [elektronický dokument]. DOI 10.1007/s11837-023-06098-6 In: **JOM**: The Journal of The Minerals, Metals & Materials Society (TMS). Berlín: Springer Nature. Springer International Publishing AG, 2023, Roč. 75, č. 11, s. 4808-4818 [tlačená forma] [online]. ISSN 1047-4838. ISSN (online) 1543-1851. - SCO ; CCC ; WOS CC, s. 4808 - 4818

2023 [01/20] / **NLD** - Das, Bikram Kumar - Banerjee, Anibrata - Das, Arnab - Chattopadhyay, Kalyan Kumar. **Graphyne supported Co13, Fe13 and Ni13 nano-cluster as efficient electrocatalysts for nitrogen reduction reaction: A first principles study** [elektronický dokument]. DOI 10.1016/j.cattod.2022.09.012 In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2023, Roč. 423, art. no. 113906 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; CCC

; WOS CC, s. art. no. 113906

2023 [01/20] / **NLD** - Li, Qijun - Zhang, Xing - Dong, Shizhi - Li, Yanshuai - Zhao, Hewei - Xie, Hongbo - Wang, Zeliang - Zhou, Cai. **Effects of doping and modulation on hydrogen evolution reaction of Pt@MoS2 single-atom catalysts: A first-principles study** [elektronický dokument]. DOI 10.1016/j.mcat.2023.113485 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2023, Roč. 549, art. no. 113485 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO ; CCC ; WOS CC, s. art. no. 113485

2023 [01/20] / **CHE** - Zhang, Chenyang - Zhang, Feng - Liu, Siyuan - Fan, Dong - Rao, Xin - Chen, Jianhua - Wen, Jing - Zhu, Yangge - Sun, Wei. **Computational Insights into the Adsorption Mechanism of Zn Ion on the Surface (110) of Sphalerite from the Perspective of Hydration** [elektronický dokument]. DOI 10.3390/min13091113 In: **Minerals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 9, art. no. 1113 [online]. ISSN (online) 2075-163X. - SCO ; CCC ; WOS CC, s. art. no. 1113

2023 [01/20] / **CHE** - Napiórkowska, Ewa - Milcarz, Katarzyna - Szeleszczuk, Łukasz. **Review of Applications of Density Functional Theory (DFT) Quantum Mechanical Calculations to Study the High-Pressure Polymorphs of Organic Crystalline Materials** [elektronický dokument]. DOI 10.3390/ijms241814155 In: **International journal of molecular sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 24, č. 18, art. no. 14155 [online] [tlačená forma]. ISSN 1661-6596. ISSN (online) 1422-0067. - SCO ; CCC ; WOS CC, s. art. no. 14155

2023 [01/20] / **GBR** - Malibekova, Alma - Guliants, Vadim. **Rational design of selective functionalized silica adsorbents for Hg(ii) removal from FGD wastewater. A combined experimental and theoretical study** [elektronický dokument]. DOI 10.1039/d3cp02694a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 34, s. 23286-23295 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; WOS CC, s. 23286 - 23295

2023 [01/20] / **USA** - Li, Qinzhen - Tan, Yesen - Huang, Baoyu - Yang, Sha - Chai, Jinsong - Wang, Xiaoping - Pei, Yong - Zhu, Manzhou. **Mechanistic Study of the Hydride Migration-Induced Reversible Isomerization in Au22(SR)15H Isomers** [elektronický dokument]. DOI 10.1021/jacs.3c02768 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2023, Roč. 145, č. 29, s. 15859-15868 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC, s. 15859 - 15868

2023 [01/20] / **NLD** - Liu, Yujie - Ren, Ming - Song, Bo - Dong, Ming. **A DFT study of toxic gases (NH3, C2H2, NO) adsorption and detection on metal oxides (CuO, Ag2O, In2O3) modified MoTe2 monolayer** [elektronický dokument]. DOI 10.1016/j.apsusc.2023.156858 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, č. 622, art. no. 156858 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 156858

2023 [01/20] / **NLD** - Ezika, Anthony Chidi - Sadiku, Emmanuel Rotimi - Adekoya, Gbolahan Joseph - Ray, Suprakas Sinha - Hamam, Yskandar. **Quantum Mechanical Study of the Dielectric Response of V2C-ZnO/PPy Ternary Nanocomposite for Energy Storage Application** [elektronický dokument]. DOI 10.1007/s10904-023-02578-z In: **Journal of Inorganic and Organometallic Polymers and Materials**. Amsterdam: Springer Nature, 2023, Roč. 33, č. 6, s. 1569-1575 [tlačená forma] [online]. ISSN 1574-1443. ISSN (online) 1574-1451. - SCO ; CCC ; WOS CC, s. 1569 - 1575

2023 [01/20] / **CHN** - Ling, Yunjia - Chen, Jun - Sun, Yu - Chu, Xinxia - Lu, Fangqin - Min, Fanfei. **DFT calculations on the adsorption of dodecylamine on surface of Fe2+ doped kaolinite**. DOI 10.13247/j.cnki.jcumt.20220123 In: **Zhongguo Kuangye Daxue Xuebao/Journal of China University of Mining and Technology**. Jiangsu: China University of Mining and Technology, 2023, Roč. 52, č. 3, s. 596-606. ISSN 1000-1964. - SCO, s. 596 - 606

2023 [01/20] / **DEU** - Zhang, Chaoyang - Huang, Jing - Bu, Rupeng. **Intrinsic Structures and Properties of Energetic Materials** [textový dokument (print)] . Berlín: Springer Nature, 2023. 1. vyd. ISBN 9789819926992. - SCO, s. 1 - 458

2022 [01/20] / **USA** - Lu, S. - Zhang, S. - Hu, X. **Ab Initio Study of High-Capacity Hydrogen Storage in Lithium-Shrouded Honeycomb Borophene Oxide Nanosheet** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 49. - SCO, s. 20762 - 20772

2022 [01/20] / **USA** - Setiawan, H. - Sakamoto, M. - Fujisaki, T. - Lyth, S.M. - Shiratori, Y. **Development of a sustainable nitrogen-doped biochar desulfurizer for solid oxide fuel cell systems** In: **Biomass and Bioenergy**, 2022, Roč. 167. - SCO, s. Art. No. 106631

2022 [01/20] / **USA** - Fang, F. - Zheng, Y. - Chen, J. - Liu, C. - Min, F. **DFT Study on the Adsorption of Monomeric Hydroxyl Aluminum on Fe(II)/Mg Replacement Kaolinite (001) Surfaces** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2022, Roč. 7, č. 44, [online]. ISSN (online) 2470-1343. - SCO, s. 39662 - 39670

2022 [01/20] / **NLD** - Murono, T. - Hongo, K. - Nakano, K. - Maezono, R. **Ab-initio-based interface modeling and statistical analysis for estimate of the water contact angle on a metallic Cu(111) surface** [elektronický dokument] In: **Surfaces and Interfaces**. Amsterdam: Elsevier, 2022, Roč. 34, [online]. ISSN (online) 2468-0230. - SCO, s. Art. No. 102342

2022 [01/20] / **CHN** - Wang, N. - Xu, H.-F. - Yang, Q.-Y. - Zhang, M.-L. - Lin, Z.-J. **First-principles study of strain-tunable charge carrier transport properties and optical properties of CrI3 monolayer** In: **Wuli Xuebao/Acta Physica Sinica**, 2022, Roč. 71, č. 20. - SCO, s. Art. No. 207102

2022 [01/20] / **GBR** - Kim, U. - Mun, J. - Koo, D. - Seo, J. - Choi, Y. - Lee, G. - Park, H. **Catalytic centers with multiple oxidation states: a strategy for breaking the overpotential ceiling from the linear scaling relation in oxygen evolution** [elektronický dokument] In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2022, Roč. 10, č. 43, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 23079 - 23086

2022 [01/20] / **GBR** - Holland, J. - Bhandari, A. - Kramer, D. - Milman, V. - Hanke, F. - Skylaris, C.-K. **Ab initio study of lithium intercalation into a graphite nanoparticle** [elektronický dokument] In: **Materials advances**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 3, č. 23, [online]. ISSN (online) 2633-5409. - SCO, s. 8469 - 8484

2022 [01/20] / **USA** - Liu, G. - Wei, S.-H. - Zhang, C. **Verification of the Accuracy and Efficiency of Dispersion-Corrected Density Functional Theory Methods to Describe the Lattice Structure and Energy of Energetic Cocrystals** In: **Crystal Growth and Design**, 2022, Roč. 22, č. 9. - SCO, s. 5307 - 5321

2022 [01/20] / **NLD** - Gu, M. - Lee, D.-Y. - Mun, J. - Kim, D. - Cho, H.-I. - Kim, B. - Kim, W. - Lee, G. - Kim, B.-S. - Kim, H.-I. **Solar-to-hydrogen peroxide conversion of photocatalytic carbon dots with anthraquinone: Unveiling the dual role of surface functionalities** In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2022, Roč. 312, [tlačená forma]. ISSN 0926-3373. - SCO, s. Art. No. 121379

2022 [01/20] / **CHE** - Huang, B. - Zhao, X. - Pei, Y. **Three-stage alloying of [Ag44(p-MBA)30]4- cluster with [Au2(p-NTP)2Cl]-** [elektronický dokument] In: **Nano research**. Peking: Tshinghua Press, 2022, Roč. 15, č. 8, [tlačená forma] [online]. ISSN 1998-0124. ISSN (online) 1998-0000. - SCO, s. 7742 - 7751

2022 [01/20] / **USA** - De Rezende, A. - Malmali, M. - Dral, P.O. - Lischka, H. - Tunega, D. - Aquino, A.J.A. **Machine Learning for Designing Mixed Metal Halides for Efficient Ammonia Separation and Storage** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 29. - SCO, s. 12184 - 12196

2022 [01/20] / **USA** - Noh, W.Y. - Mun, J. - Lee, Y. - Kim, E.M. - Kim, Y.K. - Kim, K.Y. - Jeong, H.Y. - Lee, J.H. - Song, H.-K. - Lee, G. - Lee, J.S. **Molecularly Engineered Carbon Platform to Anchor Edge-Hosted Single-Atomic M-N/C (M**

= Fe, Co, Ni, Cu) Electrocatalysts of Outstanding Durability [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 13, [online]. ISSN (online) 2155-5435. - SCO, s. 7994 - 8006

2022 [01/20] / **GBR** - Daouli, A. - Hessou, E.P. - Monnier, H. - Dziurla, M.-A. - Hasnaoui, A. - Maurin, G. - Badawi, M. **Adsorption of NO, NO2 and H2O in divalent cation faujasite type zeolites: a density functional theory screening approach** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 15565 - 15578

2022 [01/20] / **CHE** - Mazurek, A.H. - Szeleszczuk, L. **Current Status of Quantum Chemical Studies of Cyclodextrin Host-Guest Complexes** [elektronický dokument] In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 27, č. 12, [online]. ISSN (online) 1420-3049. - SCO, s. Art. No. 3874

2022 [01/20] / **NLD** - Mei, Z.-G. - Ponciroli, R. - Petersen, A. **Wigner energy in irradiated graphite: A first-principles study** [elektronický dokument] In: **Journal of Nuclear Materials**. Amsterdam: Elsevier, 2022, Roč. 563, [tlačená forma] [online]. ISSN 0022-3115. ISSN (online) 1873-4820. - SCO, s. Art. No. 153663

2022 [01/20] / **USA** - Shepelenko, M. - Hirsch, A. - Varsano, N. - Beghi, F. - Addadi, L. - Kronik, L. - Leiserowitz, L. **Polymorphism, Structure, and Nucleation of Cholesterol.H2O at Aqueous Interfaces and in Pathological Media: Revisited from a Computational Perspective** [elektronický dokument] In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2022, Roč. 144, č. 12, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 5304 - 5314

2022 [01/20] / **GBR** - Mukherjee, S. - Aiswarya, T. - Mondal, S. - Vaitheeswaran, G. **Electronic structure, phonons and optical properties of baryte type scintillators TlXO4(X = Cl, Br)** In: **Journal of Physics Condensed Matter**, 2022, Roč. 34, č. 11. - SCO, s. Art. No. 115502

2022 [01/20] / **USA** - Pathak, S. - Rakib, T. - Hou, R. - Nevidomskyy, A. - Ertekin, E. - Johnson, H.T. - Wagner, L.K. **Accurate tight-binding model for twisted bilayer graphene describes topological flat bands without geometric relaxation** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 105, č. 11, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 115141

2022 [01/20] / **GBR** - Reza Rezapour, M. - Biel, B. **DNA/RNA sequencing using germanene nanoribbons via two dimensional molecular electronic spectroscopy: an ab initio study** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 14, č. 13, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 5147 - 5153

2022 [01/20] / **GBR** - Nguyen, B.D. - Hernandez, D.J. - Flores, E.V. - Furche, F. **Dispersion size-consistency** [elektronický dokument] In: **Electronic Structure**. Bristol: Institute of Physics. IOP Publishing, 2022, Roč. 4, č. 1. ISSN (online) 2516-1075. - SCO, s. Art. No. 014003

2022 [01/20] / **NLD** - Ryu, J.H. - Park, J. - Park, J. - Mun, J. - Im, E. - Lee, H. - Hong, S.Y. - An, K. - Lee, G. - Kim, Y. - Jo, P.S. - Kang, S.J. **Carbothermal shock-induced bifunctional Pt-Co alloy electrocatalysts for high-performance seawater batteries** [elektronický dokument] In: **Energy storage materials**. [Amsterdam] : Elsevier, 2022, Roč. 45, [tlačená forma] [online]. ISSN 2405-8297. ISSN (online) 2405-8289. - SCO, s. 281 - 290

2022 [01/20] / **USA** - Piotrowski, M.J. - Orenha, R.P. - Parreira, R.L.T. - Guedes-Sobrinho, D. **Assessment of the van der Waals, Hubbard U parameter and spin-orbit coupling corrections on the 2D/3D structures from metal gold congeners clusters** [elektronický dokument] In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2022, Roč. 43, č. 4, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO, s. 230 - 243

2022 [01/20] / **GBR** - Hassani, N. - Neek-Amal, M. **The interaction between atomic-scale pores and particles** In: **Journal of Physics Condensed Matter**, 2022, Roč. 34, č. 3. - SCO, s. Art. No. 035001

2021 [01/20] / **GBR** - Zhang, H.-P. - Zhang, R. - Sun, C. - Jiao, Y. - Zhang, Y. **CO2reduction to CH4on Cu-doped phosphorene: A first-principles study** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 13, č. 48, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 20541 - 20549

2021 [01/20] / **CHE** - Ponciroli, R. - Stauff, N. - Mei, Z.-G. - Shriwise, P. - Brockmeyer, L. - Cao, Y. - Feng, B. - Romano, P. **Integration of a Wigner effect-based energy storage system with an advanced nuclear reactor** [elektronický dokument] In: **Nuclear Engineering and Design**: an International Journal devoted to all aspects of Nuclear Fission Energy. Lausanne: Elsevier, 2021, Roč. 385, [tlačená forma] [online]. ISSN 0029-5493. ISSN (online) 1872-759X. - SCO, s. Art. No. 111521

2021 [01/20] / **GBR** - Wei, F. - Smeets, E.W.F. - Voss, J. - Kroes, G.-J. - Lin, S. - Guo, H. **Assessing density functionals for describing methane dissociative chemisorption on Pt(110)-(2x1) surface** [elektronický dokument] In: **Chinese Journal of Chemical Physics**. New York: American Institute of Physics. AIP Publishing, 2021, Roč. 34, č. 6, [tlačená forma] [online]. ISSN 1674-0068. ISSN (online) 2327-2244. - SCO, s. 883 - 895

2021 [01/20] / **CHE** - Wang, J. - Zhao, X. - Hu, G. - Ren, J. - Yuan, X. **Manipulable electronic and optical properties of two-dimensional MoSTe/MoGe2N4 van der Waals heterostructures** [elektronický dokument] In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 11, č. 12, [online]. ISSN (online) 2079-4991. - SCO, s. Art. No. 3338

2021 [01/20] / **CHE** - Shakil, M. - Naz, A. - Zeba, I. - Gillani, S.S.A. - Rafique, M. - Ahmed, S. - Zafar, M. **Structural and Magnetic Behavior of MoS2 on Doping of Transition Metals: a DFT Study** [elektronický dokument] In: **Journal of Superconductivity and Novel Magnetism**. Cham: Springer Nature, 2021, Roč. 34, č. 12, [tlačená forma] [online]. ISSN 1557-1939. ISSN (online) 1557-1947. - SCO, s. 3441 - 3453

2021 [01/20] / **CHN** - Chen, J. - Ling, Y. - Sun, Y. - Liu, L. - Min, F. **Molecular simulation study of quaternary ammonium salts adsorption on kaolinite surfaces** In: **Zhongguo Kuangye Daxue Xuebao/Journal of China University of Mining and Technology**. Jiangsu: China University of Mining and Technology, 2021, Roč. 50, č. 6. ISSN 1000-1964. - SCO, s. 1204 - 1211

2021 [01/20] / **NLD** - Rakib, T. - Ertekin, E. - Pochet, P. - Johnson, H.T. **An efficient computational framework for charge density estimation in twisted bilayer graphene** [elektronický dokument] In: **Computational Materials Science**. Amsterdam: Elsevier, 2021, Roč. 199, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO, s. Art. No. 110746

2021 [01/20] / **USA** - Villarreal, R. - Lin, P.-C. - Faraji, F. - Hassani, N. - Bana, H. - Zarkua, Z. - Nair, M.N. - Tsai, H.-C. - Auge, M. - Junge, F. - Hofsaess, H.C. - De Gendt, S. - De Feyter, S. - Brems, S. - Ahlgren, E.H. - Neyts, E.C. - Covaci, L. - Peeters, F.M. - Neek-Amal, M. - Pereira, L.M.C. **Breakdown of Universal Scaling for Nanometer-Sized Bubbles in Graphene** [elektronický dokument] In: **Nano letters**. Washington: American Chemical Society, 2021, Roč. 21, č. 19, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCO, s. 8103 - 8110

2021 [01/20] / **GBR** - Pastukh, S. - Laskowska, M. - Dulski, M. - Krzykawski, T. - Parlinski, K. - Piekarz, P. **Ab initio studies for characterization and identification of nanocrystalline copper pyrophosphate confined in mesoporous silica** [elektronický dokument] In: **Nanotechnology**. Bristol : Institute of Physics. IOP Publishing, 2021, Roč. 32, č. 41, [tlačená forma] [online]. ISSN 0957-4484. ISSN (online) 1361-6528. - SCO, s. Art. No. 415701

2021 [01/20] / **GBR** - Hassani, N. - Rashidi, R. - Milosevic, M.V. - Neek-Amal, M. **Evaluating gas permeance through**

graphene nanopores and porous 2D-membranes: A generalized approach [elektronický dokument] In: **Carbon trends**. [Oxford]: Elsevier, 2021, Roč. 5, [online]. ISSN (online) 2667-0569. - SCO, s. Art. No. 100086

2021 [01/20] / **GBR** - Cuautli, C. - Romero-Ibarra, I. - Vazquez-Arenas, J. - Galvan, M. **Determination of active sites on Na2SiO3 and Li2SiO3 catalysts for methanol dissociation and methoxide stabilization concerning biodiesel production** [elektronický dokument] In: **Fuel**: the science and technology of fuel and energy. Oxford: Elsevier, 2021, Roč. 298, [tlačená forma] [online]. ISSN 0016-2361. ISSN (online) 1873-7153. - SCO, s. Art. No. 120840

2021 [01/20] / **CHE** - Du, L. - Jin, S. - Nie, P. - She, C. - Wang, J. **Initial decomposition mechanism of 3-nitro-1,2,4-triazol-5-one (Nto) under shock loading: Reaxff parameterization and molecular dynamic study** [elektronický dokument] In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 26, č. 16, [online]. ISSN (online) 1420-3049. - SCO, s. Art. No. 4808

2021 [01/20] / **USA** - Muhli, H. - Chen, X. - Bartok, A.P. - Hernandez-Leon, P. - Csanyi, G. - Ala-Nissila, T. - Caro, M.A. **Machine learning force fields based on local parametrization of dispersion interactions: Application to the phase diagram of C60** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 104, č. 5, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 054106

2021 [01/20] / **USA** - Shan, W. - Wang, G. **Enhancing Catalytic Properties of Iron- And Nitrogen-Doped Carbon for Nitrogen Reduction through Structural Distortion: A Density Functional Theory Study** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 29. - SCO, s. 16004 - 16012

2021 [01/20] / **USA** - Yonezawa, A.F. - Nagurniak, G.R. - Orenha, R.P. - Silva, E.H.D. - Parreira, R.L.T. - Piotrowski, M.J. **Stability Changes in Iridium Nanoclusters via Monoxide Adsorption: A DFT Study within the van der Waals Corrections** In: **Journal of Physical Chemistry A**, 2021, Roč. 125, č. 22. - SCO, s. 4805 - 4818

2021 [01/20] / **GBR** - Zhao, D. - Wang, Y. - Dong, C.-L. - Huang, Y.-C. - Chen, J. - Xue, F. - Shen, S. - Guo, L. **Boron-doped nitrogen-deficient carbon nitride-based Z-scheme heterostructures for photocatalytic overall water splitting** [elektronický dokument] In: **Nature energy**. Londýn: Springer Nature. Macmillan Education, 2021, Roč. 6, č. 4, [online]. ISSN (online) 2058-7546. - SCO, s. 388 - 397

2021 [01/20] / **NLD** - Tunega, D. - Zaoui, A. **Adsorption of polycyclic aromatic hydrocarbons on FeOOH polymorphs: A theoretical study** [elektronický dokument] In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2021, Roč. 706, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO, s. Art. No. 121795

2021 [01/20] / **NLD** - Shukla, N. - Ahmed, G.A. **Sb2Te3 an optically potent topological insulator: A density functional study** In: **Materials Today: Proceedings**, 2021, Roč. 45. - SCO, s. 4819 - 4823

2020 [01/12] / **NLD** - Ji, W. - Tang, Q. - Shen, Z. - Fan, M. - Li, F. **The adsorption of phosphate on hydroxylated alpha-SiO2 (0 0 1) surface and influence of typical anions: A theoretical study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 501, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 144233

2020 [01/12] / **NLD** - Berro, Y. - Badawi, M. - El Haj Hassan, F. - Kassir, M. - Tielens, F. **Water-silanol interactions on the amorphous silica surface: A dispersion-corrected DFT investigation** [elektronický dokument] In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2020, Roč. 320, [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. Art. No. 114496

2020 [01/12] / **USA** - Duan, X. - Liu, Z. - Hanrahan, B.M. - Zhu, W. - Liu, S. **Designing xenes with two-dimensional triangular lattice** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics.

American Physical Society, 2020, Roč. 4, č. 12, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 124003

2020 [01/12] / **USA** - Kumar, J. - Ansh - Shrivastava, M. **Stone-Wales Defect and Vacancy-Assisted Enhanced Atomic Orbital Interactions between Graphene and Ambient Gases: A First-Principles Insight** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 48, [online]. ISSN (online) 2470-1343. - SCO, s. 31281 - 31288

2020 [01/12] / **CHE** - Naicker, S.-A. - Moodley, M. **The Reactivity of the Corrosion Mechanism in Transformers: A Computational Study** [elektronický dokument] In: **Journal of Bio- and Tribo-Corrosion**. Cham: Springer Nature, 2020, Roč. 6, č. 4. ISSN 2198-4220. ISSN (online) 2198-4239. - SCO, s. Art. No. 125

2020 [01/12] / **GBR** - Abdulsalam, M. - Rugut, E. - Joubert, D.P. **Mechanical, thermal and thermoelectric properties of MX2 (M = Zr, Hf; X = S, Se)** In: **Materials Today Communications**, 2020, Roč. 25. - SCO, s. Art. No. 101434

2020 [01/12] / **DEU** - Wang, H. - Narasaki, M. - Zhang, Z. - Takahashi, K. - Chen, J. - Zhang, X. **Ultra-strong stability of double-sided fluorinated monolayer graphene and its electrical property characterization** In: **Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2020, Roč. 10, č. 1, [tlačená forma]. ISSN 1437-7624. - SCO, s. Art. No. 17562

2020 [01/12] / **GBR** - Jagielski, J. - Solari, S.F. - Jordan, L. - Scullion, D. - Blulle, B. - Li, Y.-T. - Krumeich, F. - Chiu, Y.-C. - Ruhstaller, B. - Santos, E.J.G. - Shih, C.-J. **Scalable photonic sources using two-dimensional lead halide perovskite superlattices** [elektronický dokument] In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2020, Roč. 11, č. 1, [online]. ISSN (online) 2041-1723. - SCO, s. Art. No. 387

2020 [01/12] / **USA** - Xu, P. - Alkan, M. - Gordon, M.S. **Many-Body Dispersion** [elektronický dokument] In: **Chemical Reviews**. Washington: American Chemical Society, 2020, Roč. 120, č. 22, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO, s. 12343 - 12356

2020 [01/12] / **GBR** - Valchev, G. - Djondjorov, P. - Vassilev, V. - Dantchev, D. **Behavior of the van der Waals force between a plate and a single-walled carbon nanotube under uniform hydrostatic pressure: A theoretical study** In: **Journal of Physics Condensed Matter**, 2020, Roč. 32, č. 40. - SCO, s. Art. No. 405001

2020 [01/12] / **USA** - Hernangomez-Perez, D. - Schlor, J. - Egger, D.A. - Patera, L.L. - Repp, J. - Evers, F. **Reorganization energy and polaronic effects of pentacene on NaCl films** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 11, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 115419

2020 [01/12] / **USA** - Zhang, X. - Shen, T. - Kan, D. - Zhang, D. - Dong, R. - An, Z. - Song, Y. - Zheng, K. - Sheng, Y. - Shi, Z. - Zou, H. **Study on the Local Structure and Luminescence Properties of a Y2Mg2Al2Si2O12:Eu3+Red Phosphor for White-Light-Emitting Diodes** [elektronický dokument] In: **Inorganic Chemistry**. Washington: American Chemical Society, 2020, Roč. 59, č. 14, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO, s. 9927 - 9937

2020 [01/12] / **USA** - Syam Kumar, R. - Akande, A. - El-Mellouhi, F. - Park, H. - Sanvito, S. **Theoretical investigation of the structural, elastic, electronic, and dielectric properties of alkali-metal-based bismuth ternary chalcogenides** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 7, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 075401

2020 [01/12] / Zhang, X. - Fan, X. - Zhu, G. - Wang, Y. - Ding, H. - Lin, H. - Li, Y. - Li, Q. - Gao, J. - Pan, M. - Guo, Q. **Two-Dimensional van der Waals Supramolecular Frameworks from Co-Hosted Molecular Assembly and C60Dimerization** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 23. - SCO, s. 12589 - 12595

2020 [01/12] / Wei, J. - Shaw, L. - Chen, W. **First-Principles Prediction of Na Diffusivity in Doped NaCrO2Layered Cathode Materials with van der Waals Interactions** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 23. - SCO, s. 12239 - 12248

2020 [01/12] / **USA** - Xi, Y. - Heyden, A. **Selective activation of methane C[sbnd]H bond in the presence of methanol** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2020, Roč. 386, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 12 - 18

2020 [01/12] / **GBR** - de Amorim, R.V. - Batista, K.E.A. - Nagurniak, G.R. - Orenha, R.P. - Parreira, R.L.T. - Piotrowski, M.J. **CO, NO, and SO adsorption on Ni nanoclusters: A DFT investigation** [elektronický dokument] In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2020, Roč. 49, č. 19, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO, s. 6407 - 6417

2020 [01/12] / **CHE** - Varadwaj, P.R. **Combined molecular dynamics and DFT simulation study of the molecular and polymer properties of a catechol-based cyclic oligomer of polyether Ether Ketone** [elektronický dokument] In: **Polymers**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 12, č. 5, [online]. ISSN (online) 2073-4360. - SCO, s. Art. No. 1054

2020 [01/12] / **USA** - Zhang, Z. - Guo, Y. - Robertson, J. **Phase dependence of Schottky barrier heights for Ge-Sb-Te and related phase-change materials** [elektronický dokument] In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2020, Roč. 127, č. 15, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO, s. Art. No. 155301

2020 [01/12] / **GBR** - Rehak, F.R. - Piccini, G. - Alessio, M. - Sauer, J. **Including dispersion in density functional theory for adsorption on flat oxide surfaces, in metal-organic frameworks and in acidic zeolites** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 7577 - 7585

2020 [01/12] / **GBR** - Cai, X. - Jia, X. - Liu, Y. - Zhang, L. - Yu, W. - Wang, B. - Yang, X. - Wang, Q. - Jia, Y. **Enhanced carrier mobility and tunable electronic properties in alfa-tellurene monolayer: Via an alfa-tellurene and h-BN heterostructure** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 11, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 6434 - 6440

2020 [01/12] / **NLD** - Fang, F. - Min, F. - Liu, L. - Chen, J. - Ren, B. - Liu, C. **Adsorption of Al(OH)n(3-n)+ (n = 2-4) on Kaolinite (001) Surfaces: A DFT study** [elektronický dokument] In: **Applied Clay Science**: An International Journal on Physics, Chemistry, Geology and Technology of Clays and Clay Minerals. Amsterdam: Elsevier, 2020, Roč. 187, [tlačená forma] [online]. ISSN 0169-1317. ISSN (online) 1872-9053. - SCO, s. Art. No. 105455

2020 [01/12] / **DEU** - Asher, M. - Angerer, D. - Korobko, R. - Diskin-Posner, Y. - Egger, D.A. - Yaffe, O. **Anharmonic Lattice Vibrations in Small-Molecule Organic Semiconductors** [elektronický dokument] In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2020, Roč. 32, č. 10, [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO, s. Art. No. 1908028

2020 [01/12] / **GBR** - Liu, N. - Luo, X. - Yuan, X. - Luo, K. - He, J. - Yu, D. - Zhao, Y. **Effect of the bond polarity on interlayer interactions in B-C-N layered materials: A dispersion-corrected density functional study** In: **Materials Today Communications**, 2020, Roč. 22. - SCO, s. Art. No. 100781

2020 [01/12] / **NLD** - Santos, S.S.M. - Marcondes, M.L. - Justo, J.F. - Assali, L.V.C. **Calcium carbonate at high pressures and high temperatures: A first-principles investigation** [elektronický dokument] In: **Physics of the Earth and Planetary Interiors**: a journal devoted to observational and experimental studies of the earth and planetary interiors and their theoretical interpretation by the physical sciences. Amsterdam: Elsevier, 2020, Roč. 299, [tlačená forma] [online]. ISSN 0031-9201. ISSN (online) 1872-7395. - SCO, s. Art. No. 106327

2020 [01/12] / **USA** - Jana, S. - Patra, A. - Constantin, L.A. - Samal, P. **Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 152, č. 4, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 044111

2020 [01/12] / **USA** - Ouyang, W. - Azuri, I. - Mandelli, D. - Tkatchenko, A. - Kronik, L. - Urbakh, M. - Hod, O. **Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 1, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 666 - 676

2020 [01/12] / **CHN** - Min, F. - Ren, B. - Chen, J. - Liu, C. - Peng, C. **Mechanism and experimental study on promoting coal slime dewatering based on weakening of hydration layer** In: **Meitan Xuebao/Journal of the China Coal Society**. Peking: China Coal Society, 2020, Roč. 45, č. 1, [tlačená forma]. ISSN 0253-9993. - SCO, s. 368 - 376

2020 [01/12] / **GBR** - Kim, E.M. - Javaid, S. - Park, J.H. - Lee, G. **Edge functionalized graphene nanoribbons with tunable band edges for carrier transport interlayers in organic-inorganic perovskite solar cells** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 5, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 2955 - 2962

2020 [01/12] / **GBR** - Peraca, C.S.T. - Nagurniak, G.R. - Orenha, R.P. - Parreira, R.L.T. - Piotrowski, M.J. **A theoretical indicator of transition-metal nanoclusters applied in the carbon nanotube nucleation process: A DFT study** [elektronický dokument] In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2020, Roč. 49, č. 2, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO, s. 492 - 503

2020 [01/12] / Angyan, J. - Dobson, J. - Jansen, G. - Gould, T. **London Dispersion Forces in Molecules, Solids and Nano-structures: An Introduction to Physical Models and Computational Methods** In: **RSC Theoretical and Computational Chemistry Series**. London: Royal Society of Chemistry, 2020. - SCO, s. 1 - 434

2019 [01/12] / Zhao, X.M. - Wang, P. - Ma, Z.Y. - Pei, Y. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 3. - SCIE ; WOS CC, s. 1710 - 1719

2019 [01/12] / **DEU** - Shahbaz, M. - Szalewicz, K. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2019, Roč. 138, č. 2, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 25

2019 [01/12] / **GBR** - Zheng, S. - Lu, H.C. - Liu, H. - Liu, D.M. - Robertson, J. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 11, č. 11, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 4811 - 4821

2019 [01/12] / **CHE** - Kouarta, H. - Zanat, K. - Belkhir, H. **In: Journal of Superconductivity and Novel Magnetism**. Cham: Springer Nature, 2019, Roč. 32, č. 4, [tlačená forma] [online]. ISSN 1557-1939. ISSN (online) 1557-1947. - SCIE ; WOS CC, s. 805 - 819

2019 [01/12] / **USA** - Zhang, F. - Wang, Y.X. - Erb, C. - Wang, K. - Moradifar, P. - Crespi, V.H. - Alem, N. **In: Physical**

Review B. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 99, č. 15, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 155430

2019 [01/12] / **NLD** - Chen, J. - Min, F.F. - Liu, L.Y. - Liu, C.F. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 476, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 6 - 15

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. - Cole, D.J. - Limas, N.G. - Fiszbein, B. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 34, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 19297 - 19324

2019 [01/12] / **USA** - Hirsch, A. - Palmer, B.A. - Ramasubramaniam, A. - Williams, P.A. - Harris, K.D.M. - Pokroy, B. - Weiner, S. - Addadi, L. - Leiserowitz, L. - Kronik, L. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2019, Roč. 31, č. 12, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 4479 - 4489

2019 [01/12] / **NLD** - Yong, Y.L. - Cui, H.L. - Zhou, Q.X. - Su, X.Y. - Kuang, Y.M. - Li, X.H. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 487, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 488 - 495

2019 [01/12] / Salazar, J.M. - Badawi, M. - Radola, B. - Macaud, M. - Simon, J.M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 38. - SCIE ; WOS CC, s. 23455 - 23463

2019 [01/12] / **USA** - Liu, C.F. - Min, F.F. - Liu, L.Y. - Chen, J. **In: ACS Omega**. Washington: American Chemical Society, 2019, Roč. 4, č. 7, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 12711 - 12718

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 57, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 33310 - 33336

2019 [01/12] / **GBR** - Yuan, D.W. - Liao, H.T. - Hu, W.Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 21049 - 21056

2019 [01/12] / **NLD** - Silva, N.J. - Borges, I. - Tone, P.A. - Green, M.J. - Lischka, H. - Aquino, A.J.A. **In: Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2019, Roč. 527, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / Rezapour, M.R. - Lee, G. - Kim, K.S. **In: Carbon**, 2019, Roč. 153. - SCIE ; WOS CC, s. 525 - 530

2019 [01/12] / **NLD** - Freire, R.L.H. - Masteghin, M.G. - Da Silva, J.L.F. - Orlandi, M.O. **In: Computational Materials Science**. Amsterdam: Elsevier, 2019, Roč. 170, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/12] / **GBR** - Mroz, D. - George, J. - Kremer, M. - Wang, R. - Englert, U. - Dronskowski, R. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 42, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 6396 - 6404

2019 [01/12] / Patra, A. - Jana, S. - Samal, P. **In: Journal of Physical Chemistry A**, 2019, Roč. 123, č. 49. - SCIE ; WOS CC, s. 10582 - 10593

2019 [01/12] / **USA** - Smolyanyuk, A. - Aichhorn, M. - Mazin, I.I. - Boeri, L. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 23, [tlačená forma] [online]. ISSN 2469-9950.

ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235114

2019 [01/12] / **USA** - Terentjev, A.V. - Constantin, L.A. - Artacho, E. - Pitarke, J.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235439

2019 [01/12] / **USA** - Zhang, G. - Hirsch, A. - Shmul, G. - Avram, L. - Elad, N. - Brumfeld, V. - Pinkas, I. - Feldman, Y. - Ben Asher, R. - Palmer, B.A. - Kronik, L. - Leiserowitz, L. - Weiner, S. - Addadi, L. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2019, Roč. 141, č. 50, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 19736 - 19745

2019 [01/12] / **USA** - Tran, F. - Kalantari, L. - Traore, B. - Rocquefelte, X. - Blaha, P. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 6, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 63602

2019 [01/12] / Khalil, R.M.A. - Hussain, F. - Rana, A.M. - Imran, M. - Murtaza, G. **In: Physica E-Low-Dimensional Systems & Nanostructures**, 2019, Roč. 106. - SCIE ; WOS CC, s. 338 - 345

2019 [01/12] / **NLD** - Jun, C. - Fan-fei, M. - Ling-yun, L. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 467, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 12 - 21

2018 [01/12] / Freire, R.L.H. - Guedes-Sobrinho, D. - Kiejna, A. - Da Silva, J.L.F. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 3. - SCIE ; WOS CC, s. 1577 - 1588

2018 [01/12] / **GBR** - Bijoy, T.K. - Murugan, P. - Kumar, V. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 15, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 10060 - 10068

2018 [01/12] / **GBR** - Khabibullin, A.R. - Karolak, A. - Budzevich, M.M. - McLaughlin, M.L. - Morse, D.L. - Woods, L.M. **In: MedChemComm**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 9, č. 7, [tlačená forma] [online]. ISSN 2040-2503. ISSN (online) 2040-2511. - SCIE ; WOS CC, s. 1155 - 1163

2018 [01/12] / **USA** - Yaghoubi, A. - Masenelli-Varlot, K. - Boisron, O. - Ramesh, S. - Melinon, P. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2018, Roč. 30, č. 20, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 7234 - 7244

2018 [01/12] / **USA** - de Oliveira, J.B. - de Oliveira, I.S.S. - Padilha, J.E. - Miwa, R.H. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 97, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045107

2018 [01/12] / **NLD** - Huang, Y. - Hu, Z.Y. - Gong, X. - Shao, X.H. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2018, Roč. 691, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 341 - 346

2018 [01/12] / **GBR** - Zhao, Q.Y. - Guo, Y.H. - Zhou, Y.X. - Yao, Z.H. - Ren, Z.Y. - Bai, J.T. - Xu, X.L. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 10, č. 7, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 3547 - 3555

2018 [01/12] / **USA** - Tao, J.M. - Perdew, J.P. - Tang, H. - Shahi, C. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 148, č. 7, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-

7690. - SCIE ; WOS CC, s. Art. No. 074110

2018 [01/12] / **CHN** - Zhang, Y.Y. - Chen, S.Y. - Xu, P. - Xiang, H. - Gong, X.G. - Walsh, A. - Wei, S.H. **In: Chinese Physics Letters**. Peking: Chinese Physical Society, 2018, Roč. 35, č. 3, [tlačená forma] [online]. ISSN 0256-307X. ISSN (online) 1741-3540. - SCIE ; WOS CC, s. Art. No. 036104

2018 [01/12] / **USA** - Curutchet, C. - Cupellini, L. - Kongsted, J. - Corni, S. - Frediani, L. - Steindal, A.H. - Guido, C.A. - Scalmani, G. - Mennucci, B. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 3, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 1671 - 1681

2018 [01/12] / **USA** - Li, J.Y. - Fleurat-Lessard, P. - Zaera, F. - Delbecq, F. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 3067 - 3075

2018 [01/12] / **CHN** - Hu, C.Z. - Ni, P. - Zhan, L. - Zhao, H.J. - He, J. - Tritt, T.M. - Huang, J.S. - Sumpter, B.G. **In: Rare Metals**. Beijing: Metallurgical Industry Press, 2018, Roč. 37, č. 4, [tlačená forma] [online]. ISSN 1001-0521. ISSN (online) 1867-7185. - SCIE ; WOS CC, s. 316 - 325

2018 [01/12] / **USA** - Ko, H.Y. - DiStasio, R.A. - Santra, B. - Car, R. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 2, č. 5, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 055603

2018 [01/12] / **GBR** - Marcondes, M.L. - Wentzcovitch, R.M. - Assali, L.V.C. **In: Solid State Communications**: an International Journal. Oxford: Elsevier, 2018, Roč. 273, [tlačená forma] [online]. ISSN 0038-1098. ISSN (online) 1879-2766. - SCIE ; WOS CC, s. 11 - 16

2018 [01/12] / **DEU** - Cha, J. - Sung, D. - Min, K.A. - Hong, S. **In: Journal of the Korean Physical Society**. Berlín: Springer Nature, 2018, Roč. 73, č. 1, [tlačená forma] [online]. ISSN 0374-4884. ISSN (online) 1976-8524. - SCIE ; WOS CC, s. 100 - 104

2018 [01/12] / Wang, N. - Zhang, W.B. - Tang, B.Y. - Gao, H.T. - He, E.J. - Wang, L. **In: Physica B-Condensed Matter**, 2018, Roč. 540. - SCIE ; WOS CC, s. 38 - 42

2018 [01/12] / **GBR** - Elias, B.H. - Ilyas, B.M. - Saadi, N.S. **In: Materials Research Express**. Bristol: Institute of Physics. IOP Publishing, 2018, Roč. 5, č. 8, [online]. ISSN (online) 2053-1591. - SCIE ; WOS CC, s. Art. No. 086302

2018 [01/12] / **GBR** - Kabakova, I.V. - Azuri, I. - Chen, Z.Y. - Nayak, P.K. - Snaith, H.J. - Kronik, L. - Paterson, C. - Bakulin, A.A. - Egger, D.A. **In: Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2018, Roč. 6, č. 15, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCIE ; WOS CC, s. 3861 - 3868

2018 [01/12] / **NLD** - Jaimes, R. - Cervantes-Alcala, R. - Garcia-Garcia, W. - Miranda-Hernandez, M. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2018, Roč. 284, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 108 - 118

2018 [01/12] / **DEU** - Rerat, M. - Pascale, F. - Noel, Y. - Carbonniere, P. - Dovesi, R. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2018, Roč. 137, č. 11, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 150

2018 [01/12] / **USA** - Mosyagin, I. - Gambino, D. - Sangiovanni, D.G. - Abrikosov, I.A. - Caffrey, N.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 17, [tlačená forma]

[online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 174103

2018 [01/12] / **USA** - Zupanic, E. - van Midden, H.J.P. - van Midden, M.A. - Sturm, S. - Tchernychova, E. - Pokrovskii, V.Y. - Zybtsev, S.G. - Nasretdinova, V.F. - Zaitsev-Zotov, S.V. - Chen, W.T. - Pai, W.W. - Bennett, J.C. - Prodan, A. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 17, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 174113

2018 [01/12] / **USA** - Sivadas, N. - Okamoto, S. - Xu, X.D. - Fennie, C.J. - Xiao, D. **In: Nano letters**. Washington: American Chemical Society, 2018, Roč. 18, č. 12, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 7658 - 7664

2018 [01/12] / **GBR** - Piotrowski, M.J. - Nagurniak, G.R. - da Silva, E.H. - Parreira, R.L.T. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 46, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 29480 - 29492

2018 [01/12] / **USA** - Terentjev, A.V. - Constantin, L.A. - Pitarke, J.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 214108

2017 [01/12] / **USA** - Wang, F. - Cao, Y.H. - Wei, S.Q. - Zhou, Y. **In: Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2017, Roč. 23, č. 1, [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCIE ; WOS CC, s. Art. No. 23

2017 [01/12] / de Oliveira, I.S.S. - Scopel, W.L. - Miwa, R.H. **In: Journal of Physics-Condensed Matter**, 2017, Roč. 29, č. 4. - SCIE ; WOS CC, s. Art. No. 045302

2017 [01/12] / **USA** - Kebede, G.G. - Spangberg, D. - Mitev, P.D. - Broqvist, P. - Hermansson, K. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 6, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 064703

2017 [01/12] / **NLD** - Jaimes, R. - Vazquez-Arenas, J. - Gonzalez, I. - Galvan, M. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2017, Roč. 229, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 345 - 351

2017 [01/12] / **NLD** - Takaba, H. - Kimura, S. - Alam, M.K. **In: Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2017, Roč. 485, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCIE ; WOS CC, s. 22 - 28

2017 [01/12] / **USA** - Al-Hamdani, Y.S. - Alfe, D. - Michaelides, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094701

2017 [01/12] / **USA** - Hermann, J. - DiStasio, R.A. - Tkatchenko, A. **In: Chemical Reviews**. Washington: American Chemical Society, 2017, Roč. 117, č. 6, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 4714 - 4758

2017 [01/12] / **USA** - Singh, S. - Romero, A.H. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 16, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 165444

2017 [01/12] / **USA** - Hu, C.Z. - Zeng, X.Y. - Liu, Y.F. - Zhou, M.H. - Zhao, H.J. - Tritt, T.M. - He, J. - Jakowski, J. - Kent,

P.R.C. - Huang, J.S. - Sumpter, B.G. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 16, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 165204

2017 [01/12] / **USA** - Rego, C.R.C. - Tereshchuk, P. - Oliveira, L.N. - Da Silva, J.L.F. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235422

2017 [01/12] / **USA** - Wang, Y.H. - Yang, S. - Fuentes-Cabrera, M. - Li, S. - Liu, W. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2017, Roč. 139, č. 24, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 8167 - 8173

2017 [01/12] / **GBR** - Falin, A. - Cai, Q.R. - Santos, E.J.G. - Scullion, D. - Qian, D. - Zhang, R. - Yang, Z. - Huang, S.M. - Watanabe, K. - Taniguchi, T. - Barnett, M.R. - Chen, Y. - Ruoff, R.S. - Li, L.H. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2017, Roč. 8, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 15815

2017 [01/12] / **USA** - Aykol, M. - Doak, J.W. - Wolverton, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 214115

2017 [01/12] / **NLD** - Perea-Ramirez, L.I. - Vargas, R. - Dominguez, Z. - Salas-Reyes, M. - Matus, M.H. - Galvan, M. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2017, Roč. 242, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 66 - 72

2017 [01/12] / **GBR** - Singh, B. - Gupta, M.K. - Mishra, S.K. - Mittal, R. - Sastry, P.U. - Rols, S. - Chaplot, S.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 27, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 17967 - 17984

2017 [01/12] / **NLD** - Chen, J. - Min, F.F. - Liu, L.Y. - Liu, C.F. - Lu, F.Q. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2017, Roč. 419, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 241 - 251

2017 [01/12] / Huang, L.F. - Rondinelli, J.M. **In: Journal of Physics-Condensed Matter**, 2017, Roč. 29, č. 47. - SCIE ; WOS CC, s. Art. No. 475501

2017 [01/12] / Lu, J.Y. - Ge, Q.Y. - Li, H.X. - Raza, A. - Zhang, T.J. **In: Journal of Physical Chemistry Letters**, 2017, Roč. 8, č. 21. - SCIE ; WOS CC, s. 5309 - 5316

2017 [01/12] / Shinde, P.P. - Groning, O. - Wang, S.Y. - Ruffieux, P. - Pignedoli, C.A. - Fasel, R. - Passerone, D. **In: Carbon**, 2017, Roč. 124. - SCIE ; WOS CC, s. 123 - 132

2017 [01/12] / **USA** - Gong, W.B. - Zhang, W. - Wang, C.B. - Yao, Y.G. - Lu, W.B. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 96, č. 17, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 174101

2017 [01/12] / Shi, X.F. - Wang, H.C. - Tang, P.Y. - Tang, B.Y. **In: Physica B-Condensed Matter**, 2017, Roč. 521. - SCIE ; WOS CC, s. 339 - 346

2017 [01/12] / **NLD** - Shi, X.F. - Yao, X.J. - Yang, Y. - Tang, B.Y. **In: Journal of Solid State Chemistry**. Amsterdam: Elsevier, 2017, Roč. 254, [tlačená forma] [online]. ISSN 0022-4596. ISSN (online) 1095-726X. - SCIE ; WOS CC, s. 75 -

81

2016 [01/12] / **GBR** - Cheung, P.M. - Berger, R.F. - Zakharov, L.N. - Gilbertson, J.D. **In: Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 52, č. 22, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCIE ; WOS CC, s. 4156 - 4159

2016 [01/12] / **USA** - Tao, J.M. - Rappe, A.M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 144, č. 3, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 031102

2016 [01/12] / **GBR** - de Oliveira, I.S.S. - Miwa, R.H. **In: Nanotechnology**. Bristol : Institute of Physics. IOP Publishing, 2016, Roč. 27, č. 3, [tlačená forma] [online]. ISSN 0957-4484. ISSN (online) 1361-6528. - SCIE ; WOS CC, s. Art. No. 035704

2016 [01/12] / Lechner, C. - Pannier, B. - Baranek, P. - Forero-Martinez, N.C. - Vach, H. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 9. - SCIE ; WOS CC, s. 5083 - 5100

2016 [01/12] / **USA** - Rangel, T. - Berland, K. - Sharifzadeh, S. - Brown-Altvater, F. - Lee, K. - Hyldgaard, P. - Kronik, L. - Neaton, J.B. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 11, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 115206

2016 [01/12] / **DEU** - Tonkikh, A.A. - Voloshina, E.N. - Werner, P. - Blumtritt, H. - Senkovskiy, B. - Guntherodt, G. - Parkin, S.S.P. - Dedkov, Y.S. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2016, Roč. 6, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 23547

2016 [01/12] / **USA** - Caskey, C.M. - Holder, A. - Shulda, S. - Christensen, S.T. - Diercks, D. - Schwartz, C.P. - Biagioni, D. - Nordlund, D. - Kukliansky, A. - Natan, A. - Prendergast, D. - Orvananos, B. - Sun, W. - Zhang, X. - Ceder, G. - Ginley, D.S. - Tumas, W. - Perkins, J.D. - Stevanovic, V. - Pylypenko, S. - Lany, S. - Richards, R.M. - Zakutayev, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 144, č. 14, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 144201

2016 [01/12] / **USA** - Mayo, M. - Griffith, K.J. - Pickard, C.J. - Morris, A.J. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2016, Roč. 28, č. 7, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 2011 - 2021

2016 [01/12] / **USA** - Yang, B. - Keum, J. - Ovchinnikova, O.S. - Belianinov, A. - Chen, S.Y. - Du, M.H. - Ivanov, I.N. - Rouleau, C.M. - Geohegan, D.B. - Xiao, K. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 15, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 5028 - 5035

2016 [01/12] / **GBR** - Potticary, J. - Terry, L.R. - Bell, C. - Papanikolopoulos, A.N. - Christianen, P.C.M. - Engelkamp, H. - Collins, A.M. - Fontanesi, C. - Kociok-Kohn, G. - Crampin, S. - Da Como, E. - Hall, S.R. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2016, Roč. 7, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 11555

2016 [01/12] / **DEU** - Abdulsalam, M. - Joubert, D.P. **In: Physica Status Solidi B-Basic Solid State Physics**. Weinheim: John Wiley & Sons. Wiley-VCH, 2016, Roč. 253, č. 5, [tlačená forma] [online]. ISSN 0370-1972. ISSN (online) 1521-3951. - SCIE ; WOS CC, s. 868 - 874

2016 [01/12] / **GBR** - Zhang, R.W. - Ji, W.X. - Zhang, C.W. - Li, S.S. - Li, P. - Wang, P.J. - Li, F. - Ren, M.J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 17, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 12169 - 12174

2016 [01/12] / **USA** - Grimme, S. - Hansen, A. - Brandenburg, J.G. - Bannwarth, C. **In: Chemical Reviews**. Washington: American Chemical Society, 2016, Roč. 116, č. 9, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 5105 - 5154

2016 [01/12] / **USA** - Tran, F. - Stelzl, J. - Blaha, P. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 144, č. 20, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 204120

2016 [01/12] / **GBR** - Klett, B. - Cocchi, C. - Pithan, L. - Kowarik, S. - Draxl, C. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 21, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 14603 - 14609

2016 [01/12] / **NLD** - Ranea, V.A. - de Andres, P.L. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2016, Roč. 648, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 256 - 261

2016 [01/12] / Yuan, D.W. - Han, Z.M. - Czap, G. - Chiang, C.L. - Xu, C. - Ho, W. - Wu, R.Q. **In: Journal of Physical Chemistry Letters**, 2016, Roč. 7, č. 12. - SCIE ; WOS CC, s. 2228 - 2233

2016 [01/12] / **DEU** - Munoz-Galan, H. - Vines, F. - Gebhardt, J. - Gorling, A. - Illas, F. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2016, Roč. 135, č. 7, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 165

2016 [01/12] / **GBR** - Fischer, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 23, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 15738 - 15750

2016 [01/12] / Flores-Huerta, A.G. - Tkatchenko, A. - Galvan, M. **In: Journal of Physical Chemistry A**, 2016, Roč. 120, č. 24. - SCIE ; WOS CC, s. 4223 - 4230

2016 [01/12] / **USA** - Lee, J.H. - Park, J.H. - Soon, A. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 2, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 024108

2016 [01/12] / **USA** - Ambrosetti, A. - Silvestrelli, P.L. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045124

2016 [01/12] / Endres, J. - Egger, D.A. - Kulbak, M. - Kerner, R.A. - Zhao, L.F. - Silver, S.H. - Hodes, G. - Rand, B.P. - Cahen, D. - Kronik, L. - Kahn, A. **In: Journal of Physical Chemistry Letters**, 2016, Roč. 7, č. 14. - SCIE ; WOS CC, s. 2722 - 2729

2016 [01/12] / **GBR** - Silva, N.J. - Machado, F.B.C. - Lischka, H. - Aquino, A.J.A. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 32, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 22300 - 22310

2016 [01/12] / **USA** - Sadhukhan, M. - Manby, F.R. **In: Physical Review B**. College Park: American Institute of Physics.

American Physical Society, 2016, Roč. 94, č. 11, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 115106

2016 [01/12] / **USA** - Klimes, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094506

2016 [01/12] / Le, N.B. - Woods, L.M. **In: Journal of Physics-Condensed Matter**, 2016, Roč. 28, č. 36. - SCIE ; WOS CC, s. Art. No. 364001

2016 [01/12] / Deringer, V.L. - Csanyi, G. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 38. - SCIE ; WOS CC, s. 21552 - 21560

2016 [01/12] / **NLD** - Lee, J. - Sorescu, D.C. - Lee, J.G. - Dougherty, D. **In: Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2016, Roč. 652, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCIE ; WOS CC, s. 82 - 90

2016 [01/12] / **USA** - Silvestrelli, P.L. - Ambrosetti, A. **In: Journal of Low Temperature Physics**. New York: Springer Nature, 2016, Roč. 185, č. 1-2, [tlačená forma] [online]. ISSN 0022-2291. ISSN (online) 1573-7357. - SCIE ; WOS CC, s. 183 - 197

2016 [01/12] / **USA** - Boese, A.D. - Sauer, J. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2016, Roč. 37, č. 26, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 2374 - 2385

2016 [01/12] / **USA** - Woods, L.M. - Dalvit, D.A.R. - Tkatchenko, A. - Rodriguez-Lopez, P. - Rodriguez, A.W. - Podgornik, R. **In: Reviews of modern physics**. Melville: American Institute of Physics. American Physical Society, 2016, Roč. 88, č. 4, [tlačená forma] [online]. ISSN 0034-6861. ISSN (online) 1539-0756. - SCIE ; WOS CC, s. Art. No. 045003

2016 [01/12] / **GBR** - De Jesus, L.R. - Horrocks, G.A. - Liang, Y.F. - Parija, A. - Jaye, C. - Wangoh, L. - Wang, J. - Fischer, D.A. - Piper, L.F.J. - Prendergast, D. - Banerjee, S. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2016, Roč. 7, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 12022

2016 [01/12] / **USA** - Besse, R. - Sabino, F.P. - Da Silva, J.L.F. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 16, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. nestr.

2016 [01/12] / **DEU** - Yu, X.M. - Robertson, J. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2016, Roč. 6, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 37325

2016 [01/12] / **NLD** - Khalil, R.M.A. **In: Chinese Journal of Physics**. Amsterdam: Elsevier, 2016, Roč. 54, č. 6, [tlačená forma] [online]. ISSN 0577-9073. ISSN (online) 2309-9097. - SCIE ; WOS CC, s. 890 - 894

2016 [01/12] / **USA** - George, J. - Deringer, V.L. - Wang, A. - Muller, P. - Englert, U. - Dronskowski, R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 23, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 234512

2016 [01/12] / **USA** - Huang, D. - Kaxiras, E. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 24, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online)

2469-9969. - SCIE ; WOS CC, s. Art. No. 241303

2016 [01/12] / Piotrowski, M.J. - Ungureanu, C.G. - Tereshchuk, P. - Batista, K.E.A. - Chaves, A.S. - Guedes-Sobrinho, D. - Da Silva, J.L.F. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 50. - SCIE ; WOS CC, s. 28844 - 28856

2016 [01/12] / **GBR** - Chiter, F. - Nguyen, V.B. - Tarrat, N. - Benoit, M. - Tang, H. - Lacaze-Dufaure, C. **In: Materials Research Express**. Bristol: Institute of Physics. IOP Publishing, 2016, Roč. 3, č. 4, [online]. ISSN (online) 2053-1591. - SCIE ; WOS CC, s. Art. No. 046501

2015 [01/12] / **GBR** - Hu, M. - Dong, X. - Yang, B.C. - Xu, B. - Yu, D.L. - He, J.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 19, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 13028 - 13033

2015 [01/12] / **GBR** - Reilly, A.M. - Tkatchenko, A. **In: Chemical Science**. Cambridge: The Royal Society of Chemistry, 2015, Roč. 6, č. 6, [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCIE ; WOS CC, s. 3289 - 3301

2015 [01/12] / **GBR** - Gautier, S. - Steinmann, S.N. - Michel, C. - Fleurat-Lessard, P. - Sautet, P. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 43, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 28921 - 28930

2015 [01/12] / **GBR** - Tristant, D. - Puech, P. - Gerber, L.C. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2015, Roč. 17, č. 44, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 30045 - 30051

2015 [01/12] / **GBR** - Junkaew, A. - Rungnim, C. - Kunaseth, M. - Arroyave, R. - Promarak, V. - Kungwan, N. - Namuangruk, S. **In: New Journal of Chemistry**: a journal for new directions in chemistry. Cambridge: The Royal Society of Chemistry, 2015, Roč. 39, č. 12, [tlačená forma] [online]. ISSN 1144-0546. ISSN (online) 1369-9261. - SCIE ; WOS CC, s. 9650 - 9658

2015 [01/12] / **USA** - Guevara-Garcia, A. - Ireta, J. - Galvan, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 142, č. 1, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 014504

2015 [01/12] / **USA** - de Oliveira, I.S.S. - Miwa, R.H. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 142, č. 4, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 044301

2015 [01/12] / **USA** - Lopez-Estrada, O. - Orgaz, E. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075428

2015 [01/12] / **USA** - Boese, A.D. - Boese, R. **In: Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2015, Roč. 15, č. 3, [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCIE ; WOS CC, s. 1073 - 1081

2015 [01/12] / **DEU** - Zhang, R.W. - Zhang, C.W. - Ji, W.X. - Ren, M.J. - Li, F. - Yuan, M. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2015, Roč. 156, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 89 - 94

2015 [01/12] / **USA** - Tao, J.M. - Yang, J. - Rappe, A.M. **In: Journal of Chemical Physics**. Melville: American Institute of

Physics. AIP Publishing, 2015, Roč. 142, č. 16, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 164302

2015 [01/12] / **NLD** - Knuth, F. - Carbogno, C. - Atalla, V. - Blum, V. - Scheffler, M. **In: Computer Physics Communications**: An International Journal and Program Library for Computational Physics and Physical Chemistry. Amsterdam: Elsevier, 2015, Roč. 190, [tlačená forma] [online]. ISSN 0010-4655. ISSN (online) 1879-2944. - SCIE ; WOS CC, s. 33 - 50

2015 [01/12] / **USA** - Dong, L. - Wang, J. - Namburu, R. - O'Regan, T.P. - Dubey, M. - Dongare, A.M. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2015, Roč. 117, č. 24, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 244303

2015 [01/12] / Abdulsalam, M. - Joubert, D.P. **In: European Physical Journal B**, 2015, Roč. 88, č. 7. - SCIE ; WOS CC, s. Art. No. 177

2015 [01/12] / Xu, C.Y. - Brown, P.A. - Lu, J. - Shuford, K.L. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 30. - SCIE ; WOS CC, s. 17271 - 17277

2015 [01/12] / **NLD** - Park, J. - Yu, B.D. - Hong, S. **In: Current Applied Physics**. Amsterdam: Elsevier. Elsevier Science, 2015, Roč. 15, č. 8, [tlačená forma] [online]. ISSN 1567-1739. ISSN (online) 1878-1675. - SCIE ; WOS CC, s. 885 - 891

2015 [01/12] / **USA** - Tian, Y.H. - Huang, J.S. - Sheng, X.L. - Sumpter, B.G. - Yoon, M. - Kertesz, M. **In: Nano letters**. Washington: American Chemical Society, 2015, Roč. 15, č. 8, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCIE ; WOS CC, s. 5482 - 5491

2015 [01/12] / Aykol, M. - Kim, S. - Wolverton, C. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 33. - SCIE ; WOS CC, s. 19053 - 19058

2015 [01/12] / **NLD** - Sun, T. - Wang, Y. - Zhang, H.M. - Liu, P.R. - Zhao, H.J. **In: Journal of colloid and interface science**. Amsterdam: Elsevier, 2015, Roč. 454, [tlačená forma] [online]. ISSN 0021-9797. ISSN (online) 1095-7103. - SCIE ; WOS CC, s. 180 - 186

2015 [01/12] / **DEU** - Shen, Y.Q. - Oganov, A.R. - Qian, G.R. - Zhang, J. - Dong, H.F. - Zhu, Q. - Zhou, Z.X. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2015, Roč. 5, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 14204

2015 [01/12] / Yanagisawa, S. - Okuma, K. - Inaoka, T. - Hamada, I. **In: Journal of Electron Spectroscopy and Related Phenomena**, 2015, Roč. 204. ISSN 03682048. - SCIE ; WOS CC, s. 159 - 167

2015 [01/12] / Rego, C.R.C. - Oliveira, L.N. - Tereshchuk, P. - Da Silva, J.L.F. **In: Journal of Physics-Condensed Matter**, 2015, Roč. 27, č. 41. - SCIE ; WOS CC, s. Art. No. 415502

2015 [01/12] / **NLD** - Razumovskiy, V.I. - Ghosh, G. **In: Computational Materials Science**. Amsterdam: Elsevier, 2015, Roč. 110, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 169 - 181

2015 [01/12] / Robledo, M. - Pacchioni, G. - Martin, F. - Alcami, M. - Diaz-Tendero, S. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 8. - SCIE ; WOS CC, s. 4062 - 4071

2015 [01/12] / **USA** - Greathouse, J.A. - Geatches, D.L. - Pike, D.Q. - Greenwell, H.C. - Johnston, C.T. - Wilcox, J. - Cygan, R.T. **In: Clays and Clay Minerals**. Bloomington: Clay Minerals Society, 2015, Roč. 63, č. 3-4, [tlačená forma] [online].

ISSN 0009-8604. ISSN (online) 1552-8367. - SCIE ; WOS CC, s. 185 - 198

2015 [01/12] / **USA** - Li, H.S. - Chen, W.G. - Han, X.Y. - Li, L.B. - Sun, Q. - Guo, Z.X. - Jia, Y. **In: Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2015, Roč. 36, č. 25, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCIE ; WOS CC, s. 1919 - 1927

2015 [01/12] / **USA** - Hirsch, A. - Gur, D. - Polishchuk, I. - Levy, D. - Pokroy, B. - Cruz-Cabeza, A.J. - Addadi, L. - Kronik, L. - Leiserowitz, L. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2015, Roč. 27, č. 24, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 8289 - 8297

2014 [01/12] / **GBR** - Peng, Q. - R.a.h.u.l. - Wang, G.Y. - Liu, G.R. - De, S. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 19972 - 19983

2014 [01/12] / **USA** - He, J.G. - Hummer, K. - Franchini, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075409

2014 [01/12] / **USA** - Luder, J. - Sanyal, B. - Eriksson, O. - Puglia, C. - Brena, B. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045416

2014 [01/12] / **GBR** - Wang, X. - Cheng, X.Y. - Zhang, Y.T. - Li, R.H. - Xing, W.W. - Zhang, P.C. - Chen, X.Q. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2014, Roč. 16, č. 48, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 26974 - 26982

2014 [01/12] / **USA** - Silvestrelli, P.L. - Ambrosetti, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124107

2014 [01/12] / **USA** - Luder, J. - Eriksson, O. - Sanyal, B. - Brena, B. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124711

2014 [01/12] / **USA** - Oh, M.W. - Son, J.H. - Kim, B.S. - Park, S.D. - Min, B.K. - Lee, H.W. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2014, Roč. 115, č. 13, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 133706

2014 [01/12] / **USA** - Tran, H.D. - Amsler, M. - Botti, S. - Marques, M.A.L. - Goedecker, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124708

2014 [01/12] / Moellmann, J. - Grimme, S. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 14. - SCIE ; WOS CC, s. 7615 - 7621

2014 [01/12] / **USA** - Bremond, E. - Golubev, N. - Steinmann, S.N. - Corminboeuf, C. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 18, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 18516

2014 [01/12] / **USA** - Hirsch, A. - Azuri, I. - Addadi, L. - Weiner, S. - Yang, K.S. - Curtarolo, S. - Kronik, L. **In: Chemistry**

of Materials: a Publication of the American Chemical Society. Washington: American Chemical Society, 2014, Roč. 26, č. 9, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 2934 - 2942

2014 [01/12] / **NLD** - Bokareva, O.S. - Kuhn, O. **In: Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2014, Roč. 435, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCIE ; WOS CC, s. 40 - 48

2014 [01/12] / **USA** - Ambrosetti, A. - Reilly, A.M. - DiStasio, R.A. - Tkatchenko, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 18, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 18508

2014 [01/12] / Gao, W. - Xiao, P.H. - Henkelman, G. - Liechti, K.M. - Huang, R. **In: Journal of Physics D-Applied Physics**, 2014, Roč. 47, č. 25. - SCIE ; WOS CC, s. Art. No. 255301

2014 [01/12] / **USA** - Dobson, J.F. - Gould, T. - Vignale, G. **In: Physical Review X**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 4, č. 2, [online]. ISSN (online) 2160-3308. - SCIE ; WOS CC, s. Art. No. 021040

2014 [01/12] / Egger, D.A. - Kronik, L. **In: Journal of Physical Chemistry Letters**, 2014, Roč. 5, č. 15. - SCIE ; WOS CC, s. 2728 - 2733

2014 [01/12] / **USA** - Bereau, T. - von Lilienfeld, O.A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 141, č. 3, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 034101

2014 [01/12] / Tetlow, H. - de Boer, J.P. - Ford, I.J. - Vvedensky, D.D. - Coraux, J. - Kantorovich, L. **In: Physics Reports-Review Section of Physics Letters**, 2014, Roč. 542, č. 3. - SCIE ; WOS CC, s. 195 - 295

2014 [01/12] / **USA** - Yu, F. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 10, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4400 - 4407

2014 [01/12] / **USA** - Zhu, Q. - Sharma, V. - Oganov, A.R. - Ramprasad, R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 141, č. 15, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 154102

2014 [01/12] / **USA** - Sorescu, D.C. - Byrd, E.F.C. - Rice, B.M. - Jordan, K.D. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4982 - 4994

2014 [01/12] / Zhang, R.W. - Zhang, C.W. - Ji, W.X. - Hu, S.J. - Yan, S.S. - Li, S.S. - Li, P. - Wang, P.J. - Liu, Y.S. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 43. - SCIE ; WOS CC, s. 25278 - 25283

2014 [01/12] / **USA** - Ganesh, P. - Kim, J. - Park, C. - Yoon, M. - Reboredo, F.A. - Kent, P.R.C. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2014, Roč. 10, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 5318 - 5323

2014 [01/12] / **USA** - Samanta, A. - Pandey, T. - Singh, A.K. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 90, č. 17, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 174301

2014 [01/12] / **USA** - Kronik, L. - Tkatchenko, A. **In: Accounts of Chemical Research**. Washington: American Chemical Society, 2014, Roč. 47, č. 11, [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCIE ; WOS CC, s. 3208 - 3216

2013 [01/12] / Zhou, J. - Huang, J.S. - Sumpter, B.G. - Kent, P.R.C. - Terrones, H. - Smith, S.C. **In: Journal of Physical Chemistry C**, 2013, Roč. 117, č. 48. - SCIE ; WOS CC, s. 25817 - 25825

2013 [01/12] / **USA** - Bamidele, J. - Brndiar, J. - Gulans, A. - Kantorovich, L. - Stich, I. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2013, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 5578 - 5584

2013 [01/12] / **USA** - Cerny, R. - Schouwink, P. - Sadikin, Y. - Stare, K. - Smrcok, L. - Richter, B. - Jensen, T.R. **In: Inorganic Chemistry**. Washington: American Chemical Society, 2013, Roč. 52, č. 17, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCIE ; WOS CC, s. 9941 - 9947

2013 [01/12] / **USA** - Silvestrelli, P.L. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 139, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 054106

2013 [01/12] / **USA** - Agrawal, P. - Tkatchenko, A. - Kronik, L. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2013, Roč. 9, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 3473 - 3478

2013 [01/12] / **USA** - Gao, W. - Tkatchenko, A. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2013, Roč. 111, č. 4, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s. Art. No. 045501

2013 [01/12] / **USA** - Reilly, A.M. - Tkatchenko, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2013, Roč. 139, č. 2, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 024705

2013 [01/12] / **GBR** - Ling, S.L. - Watkins, M.B. - Shluger, A.L. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 45, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 19615 - 19624

2013 [01/12] / **GBR** - Dudenko, D.V. - Yates, J.R. - Harris, K.D.M. - Brown, S.P. **In: CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2013, Roč. 15, č. 43, [tlačená forma] [online]. ISSN 1466-8033. - SCIE ; WOS CC, s. 8797 - 8807

2013 [01/12] / **GBR** - Gobre, V.V. - Tkatchenko, A. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2013, Roč. 4, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 2341

ADC_040: / Egger, David A. (Autor) (18%) - Ruiz, Viktor G. (Autor) (18%) - Saidi, Wissam A. (Autor) (18%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (10%) - Tkatchenko, Alexandre (Autor) (18%) - Zojer, Egbert (Autor) (18%): **Understanding Structure and Bonding of Multilayered Metal-Organic Nanostructures**. – [recenzované]. – CCC ; SCO ; WOS CC ; SCIE ; OA.
In: *The Journal of Physical Chemistry C* [textový dokument (print)] [elektronický dokument] : Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. – Washington (USA) : American Chemical

Society. – ISSN 1932-7447. – ISSN (online) 1932-7455. – Roč. 117, č. 6 (2013), s. 3055-3061 [tlačená forma] [online]
Počet všetkých autorov: 6
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,434 - 2013
SJR: 2,143 - 2013
CiteScore: 8,3 - 2013

Ohlasy (22):

2025 [01/20] / **DEU** - Li, Jingtai - Schröder, Carsten - Schmidt, Marvin - Smyczek, Jan - Schauermann, Swetlana - Liu, Wei. **Understanding Heterogeneously Catalyzed Hydrogenation of Carbonyl Compounds Through Keto-Enol Tautomerization** [elektronický dokument]. DOI 10.1002/smll.202504104 In: **Small**. Weinheim: John Wiley & Sons, 2025, Roč. 21, č. 23, art. no. 2504104 [tlačená forma] [online]. ISSN 1613-6810. ISSN (online) 1613-6829. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2021 [01/20] / **DEU** - Forker, R. - Gruenewald, M. - Kirchhuebel, T. - Fritz, T. **Recent Progress in the Consistent Interpretation of Complementary Spectroscopic Results Obtained on Molecular Systems** In: **Advanced Optical Materials**. Weinheim: John Wiley & Sons, 2021, Roč. 9, č. 14, [online]. ISSN 2195-1071. - SCO, s. Art. No. 2100200

2021 [01/20] / **GBR** - Yang, J. - Wang, Q. - Wan, S. - Wu, D. - Chen, M. - Kashtanov, S. - Duhm, S. **Photoelectron spectroscopy reveals molecular diffusion through physisorbed template layers on Au(111)** [elektronický dokument] In: **Electronic Structure**. Bristol: Institute of Physics. IOP Publishing, 2021, Roč. 3, č. 2. ISSN (online) 2516-1075. - SCO, s. Art. No. 024002

2020 [01/12] / **GBR** - Franco-Canellas, A. - Duhm, S. - Gerlach, A. - Schreiber, F-. **Binding and electronic level alignment of pí-conjugated systems on metals** [elektronický dokument] In: **Reports on Progress in Physics**: a journal recognized by the European Physical Society. Bristol: Institute of Physics. IOP Publishing, 2020, Roč. 83, č. 6, [tlačená forma]. ISSN 0034-4885. ISSN (online) 1361-6633. - SCO, s. Art. No. 066501

2019 [01/12] / Niu, T.C. - Si, N. - Zhou, D.C. - Zhou, M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 12. - SCIE ; WOS CC, s. 7178 - 7184

2019 [01/12] / Thussing, S. - Fernandez, L. - Jakob, P. **In: Journal of Physics-Condensed Matter**, 2019, Roč. 31, č. 13. - SCIE ; WOS CC, s. Art. No. 134002

2019 [01/12] / **USA** - Eschmann, L. - Sabitova, A. - Temirov, R. - Tautz, F.S. - Kruger, P. - Rohlfing, M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 12, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 125155

2018 [01/12] / Wang, Q. - Franco-Canellas, A. - Ji, P.H. - Burker, C. - Wang, R.B. - Broch, K. - Thakur, P.K. - Lee, T.L. - Zhang, H.M. - Gerlach, A. - Chi, L.F. - Duhm, S. - Schreiber, F. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 17. - SCIE ; WOS CC, s. 9480 - 9490

2018 [01/12] / van Straaten, G. - Franke, M. - Soubatch, S. - Stadtmuller, B. - Duncan, D.A. - Lee, T.L. - Tautz, F.S. - Kumpf, C. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 15. - SCIE ; WOS CC, s. 8491 - 8504

2017 [01/12] / Thussing, S. - Jakob, P. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 25. - SCIE ; WOS CC, s. 13680 - 13691

2015 [01/12] / Stadtmuller, B. - Schroder, S. - Kumpf, C. **In: Journal of Electron Spectroscopy and Related Phenomena**,

2015, Roč. 204. ISSN 03682048. - SCIE ; WOS CC, s. 80 - 91

2015 [01/12] / **USA** - Gruenewald, M. - Sauer, C. - Peuker, J. - Meissner, M. - Sojka, F. - Scholl, A. - Reinert, F. - Forker, R. - Fritz, T. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 15, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 155432

2015 [01/12] / **USA** - Stadtmuller, B. - Willenbockel, M. - Schroder, S. - Kleimann, C. - Reinisch, E.M. - Ules, T. - Soubatch, S. - Ramsey, M.G. - Tautz, F.S. - Kumpf, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 91, č. 15, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 155433

2015 [01/12] / **USA** - Wagner, M. - Berkebile, S. - Netzer, F.P. - Ramsey, M.G. **In: ACS Nano**. Washington: American Chemical Society, 2015, Roč. 9, č. 12, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 12070 - 12078

2014 [01/12] / Stadtmuller, B. - Gruenewald, M. - Peuker, J. - Forker, R. - Fritz, T. - Kumpf, C. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 49. - SCIE ; WOS CC, s. 28592 - 28602

2014 [01/12] / **USA** - Stadtmuller, B. - Schroder, S. - Bocquet, F.C. - Henneke, C. - Kleimann, C. - Soubatch, S. - Willenbockel, M. - Detlefs, B. - Zegenhagen, J. - Lee, T.L. - Tautz, F.S. - Kumpf, C. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 16, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 161407

2014 [01/12] / **NLD** - Sarasola, A. - Barja, S. - de Parga, A.L.V. - Arnau, A. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2014, Roč. 612, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 45 - 50

2014 [01/12] / **GBR** - Stadtmuller, B. - Luftner, D. - Willenbockel, M. - Reinisch, E.M. - Sueyoshi, T. - Koller, G. - Soubatch, S. - Ramsey, M.G. - Puschnig, P. - Tautz, F.S. - Kumpf, C. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2014, Roč. 5, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 3685

2014 [01/12] / **USA** - Niederhausen, J. - Duhm, S. - Heimel, G. - Burker, C. - Xin, Q. - Wilke, A. - Vollmer, A. - Schreiber, F. - Kera, S. - Rabe, J.P. - Ueno, N. - Koch, N. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2014, Roč. 140, č. 1, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 014705

2014 [01/12] / **USA** - Luder, J. - Sanyal, B. - Eriksson, O. - Puglia, C. - Brena, B. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045416

2014 [01/12] / **USA** - Droghetti, A. - Steil, S. - Grossmann, N. - Haag, N. - Zhang, H.T. - Willis, M. - Gillin, W.P. - Drew, A.J. - Aeschlimann, M. - Sanvito, S. - Cinchetti, M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2014, Roč. 89, č. 9, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 94412

2014 [01/12] / Kleimann, C. - Stadtmuller, B. - Schroder, S. - Kumpf, C. **In: Journal of Physical Chemistry C**, 2014, Roč. 118, č. 3. - SCIE ; WOS CC, s. 1652 - 1660

2014 - spolu : **2**

ADC_041: / Bučko, Tomáš (Autor) [UKOPRCFZ] (80%) - Lebegue, Sebastien (Autor) (5%) - Ángyán, János G. (Autor) (5%) - Hafner, Jürgen (Autor) (10%): **Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning**. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 141, č. 3 (2014), Art. No. 34114, s. [1-1] [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,026 - 2014
SJR: 1,446 - 2014
CiteScore: 5,1 - 2014
Nordic List: 1 - 2014

Ohlasy (167):
2025 [01/20] / **CHE** - Herbert, John M. - Gray, Montgomery - Liu, Kuan Yu - Carter-Fenk, Kevin. **Extended Symmetry-Adapted Perturbation Theory (XSAPT): A Cubic-Scaling Platform for Computing Accurate Intermolecular Interaction Energies and ab Initio Energy Decomposition Analysis** [elektronický dokument]. DOI 10.1007/430_2025_98 In: **Structure and Bonding Computational Methods for the Analysis of Non-Covalent Interactions**. Cham: Springer Nature, 2025, s. 137-222 [tlačená forma] [online]. ISBN 978-3-032-01542-6. ISBN (online) 978-3-032-01543-3. ISSN 00815993. ISSN (online) 16168550. - SCO, s. 137 - 222

2025 [01/20] / **USA** - Gao, Xiang - Ouyang, Wengen - Kronik, Leeor - Urbakh, Michael - Hod, Oded. **Anisotropic interlayer force fields for van der Waals interfaces: Development and applications** [elektronický dokument]. DOI 10.1063/5.0273079 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 4, art. no. 041001 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **GBR** - Garrido Aldea, Jaime - Esteras, Dorye L. - Roche, Stephan - Garcia, Jose H. **Challenges and strategies for first-principles simulations of two-dimensional magnetic phenomena** [elektronický dokument]. DOI 10.1039/d4nr05503a In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 43, s. 24955-24989 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 24955 - 24989

2025 [01/20] / **USA** - Pfeiffer, Florian - Krenz, Marvin - Sanna, Simone. **Theoretical Investigation and Simulated Imaging of Halogenated Tetracenes on Coinage Metal (111) Surfaces** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c06015 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 49, s. 21686-21695 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 21686 - 21695

2025 [01/20] / **DEU** - Chen, Xiaokai - Xuan, Xiaoyu - Guo, Wanlin - Zhang, Zhuhua. **Ferroelectricity in van der Waals multilayers via interfacial polarization engineering** [elektronický dokument]. DOI 10.1038/s41699-025-00531-x In: **NPJ 2D Materials and Applications**. Berlín: Nature Research, 2025, Roč. 9, č. 1, art. no. 10. ISSN (online) 2397-7132. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 10

2025 [01/20] / **GBR** - Núñez-Murillo, F. A. - López, L. A. - Mejía-Burgos, D. - Mazo-Zuluaga, J. - Mejía-López, J. **Single-layer CrI2as a magnetic semiconductor: a detailed first-principles study** [elektronický dokument]. DOI 10.1039/d5nr01077b In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 44, s. 25833-25845 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; WOS CC ; SCIE ; OA, s. 25833 - 25845

2025 [01/20] / **USA** - Lopes, Daniel S. - da Costa, Diego R. - Dias, Alexandre C. - Barcelos, Ingrid D. - Cadore, Alisson R. - Teldo, A. S.Pereira - de Sousa, Jeanlex S. **Tunable Electronic Properties of Multilayer Talc: Combined First-Principles and Experimental Insights** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c05824 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 45, s. 20404-20417 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 20404 - 20417

2025 [01/20] / **GBR** - Dickbreder, Tobias - Schneider, Florian - Klausfering, Lea - Dreier, Kim Noelle - Sabath, Franziska - Foster, Adam S. - Bechstein, Ralf - Kühnle, Angelika. **Water desorption from microcline (001): insights into the first water layer** [elektronický dokument]. DOI 10.1039/d5cp01796c In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 35, s. 18317-18325 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 18317 - 18325

2025 [01/20] / **USA** - Heggemann, Jonas - Huang, Jie - Aeschlimann, Simon - Spiller, Simon - Foster, Adam S. - Rahe, Philipp. **Sidestepping Intermolecular Hydrogen Bonds: How Single Water Molecules Adsorb and Assemble on the Calcite(104)–(2 × 1) Surface** [elektronický dokument]. DOI 10.1021/acsnano.5c05845 In: **ACS Nano**. Washington: American Chemical Society, 2025, Roč. 19, č. 29, s. 26650-26658 [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO ; WOS CC ; SCIE ; OA, s. 26650 - 26658

2025 [01/20] / **USA** - Ikwa, Emmanuel - Rivallan, Mickael - Nardin, Thibaud - Hugon, Antoine - Loffreda, David. **How Morphological Descriptors Capture the Stability Order in Palladium Nanoparticles** [elektronický dokument]. DOI 10.1021/acs.jpclett.5c01188 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2025, Roč. 16, č. 25, s. 6513-6522 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC ; SCIE, s. 6513 - 6522

2025 [01/20] / **CHE** - Dubok, Aleksandr S. - Rychkov, Denis A. **What Is More Important When Calculating the Thermodynamic Properties of Organic Crystals, Density Functional, Supercell, or Energy Second-Order Derivative Method Choice?** [elektronický dokument]. DOI 10.3390/cryst15030274 In: **Crystals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 3, art. no. 274 [online]. ISSN (online) 2073-4352. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 274

2025 [01/20] / **USA** - Yadav, Shivam - Sekh, Sajid - Ptok, Andrzej. **Low temperature phase of AuSn4 induced by the van der Waals interactions** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.9.034202 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 9, č. 3, art. no. 034202 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. art. no. 034202

2025 [01/20] / **USA** - Li, Zhe - Xue, Feng - Tang, Xin Yi - Hong, Xiyu - Chen, Yang - Feng, Xiao - He, Ke. **Universally optimizable strategy for magnetic gaps towards high-temperature quantum anomalous Hall states via magnetic-insulator/topological-insulator building blocks** [elektronický dokument]. DOI 10.1103/PhysRevB.111.075106 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 111, č. 7, art. no. 075106 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 075106

2025 [01/20] / **USA** - Jin, Jiaxi - Shang, Yanbo - Lai, Hao - Ling, Shisheng - Cai, Jinpeng - Shen, Peilun - Wei, Xiao - Liu, Dianwen. **Selective Separation of Galena from Sphalerite with a Novel Depressant Sodium Thiophosphate: Flotation and Adsorption Mechanism** [elektronický dokument]. DOI 10.1021/acs.langmuir.5c03873 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2025, Roč. 41, č. 41, s. 28038-28051 [tlačená forma]

[online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC ; SCIE, s. 28038 - 28051

2025 [01/20] / **USA** - Saniz, Rolando - Li, Shangkun - Lamoen, Dirk - Bogaerts, Annemie - Partoens, Bart. **CO2Adsorption on Stoichiometric Ceria (110) Revisited** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c01747 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 28, s. 12814-12826 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; WOS CC ; SCIE, s. 12814 - 12826

2025 [01/20] / **USA** - Hassett, Michael P. - Binns, Jack - Brown, Stuart J. - Karim, Akib - Brand, Helen E.A. - Bryant, Gary - Martin, Andrew V. - Greaves, Tamar L. **Crystal structures of protic ionic liquids** [elektronický dokument]. DOI 10.1063/5.0279110 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 1, art. no. 014503 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 014503

2025 [01/20] / **USA** - Banaev, Maksim V. - Sagatova, Dinara N. - Sagatov, Nursultan E. - Gavryushkin, Pavel N. **K2C2O5─The First Finding of Pyrocarbonate Stable at Ambient Pressure** [elektronický dokument]. DOI 10.1021/acs.cgd.5c00200 In: **Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2025, Roč. 25, č. 11, s. 3786-3792 [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCO ; CCC ; WOS CC ; SCIE, s. 3786 - 3792

2025 [01/20] / **USA** - Hessou, Etienne P. - Virot, François - Calatayud, Monica - Souvi, Sidi M.O. **Ab Initio Investigation of the Competitive Adsorption of RuO4 and NOX on a RuO2 Surface: Assessment of RuO4 Release in a Severe Nuclear Accident** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c00359 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 23, s. 10463-10472 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 10463 - 10472

2025 [01/20] / **CHE** - Yan, Jingyi - Dai, Weiju - Zou, Dexu - Sun, Haoruo - Tang, Chao - Gui, Yingang. **A TMO-ZnO Heterojunction-Based Sensor for Transformer Defect Detection: A DFT Study** [elektronický dokument]. DOI 10.3390/nano15110856 In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 15, č. 11, art. no. 856 [online]. ISSN (online) 2079-4991. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 856

2025 [01/20] / **USA** - Keller, Elisabeth - Blum, Volker - Reuter, Karsten - Margraf, Johannes T. **Exploring atom-pairwise and many-body dispersion corrections for the BEEF-vdW functional** [elektronický dokument]. DOI 10.1063/5.0248728 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 162, č. 7, art. no. 074111 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 074111

2025 [01/20] / **GBR** - Shawon, Md Jahirul Islam - Dash, Bivas Kumar - Rafat, Al - Piya, Afiya Akter - Shamim, Siraj Ud Daula. **Exploring the sensing properties of Janus ScSTe, TiSTe, and ZrSTe nanosheets for nitrogen based toxic gases via DFT** [elektronický dokument]. DOI 10.1038/s41598-025-21091-6 In: **Scientific reports**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 15, č. 1, art. no. 37200 [online]. ISSN (online) 2045-2322. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 37200

2025 [01/20] / **DEU** - Shi, Benjamin X. - Rosen, Andrew S. - Schäfer, Tobias - Grüneis, Andreas - Kapil, Venkat - Zen, Andrea - Michaelides, Angelos. **An accurate and efficient framework for modelling the surface chemistry of ionic materials** [elektronický dokument]. DOI 10.1038/s41557-025-01884-y In: **Nature Chemistry**. Berlín: Springer Nature. Springer. Nature Portfolio, 2025, Roč. 17, č. 11, s. 1688-1695. ISSN 17554330. ISSN (online) 17554349. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 1688 - 1695

2025 [01/20] / **USA** - Carneiro Queiroz da Silva, G. - Salazar, J. Marcos. **Emergence of an Icosahedral (H2)13 Cluster**

inside a Pure Silica Faujasite [elektronický dokument]. DOI 10.1021/acs.jpcc.4c08679 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 14, s. 7031-7039 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 7031 - 7039

2024 [01/20] / **USA** - González, José E. - Besse, Rafael - Lima, Matheus P. - Da Silva, Juarez L.F. **Decoding Van der Waals Impact on Chirality Transfer in Perovskite Structures: Density Functional Theory Insights** [elektronický dokument]. DOI 10.1021/acs.jcim.3c01895 In: **Journal of Chemical Information and Modeling**. Washington, D.C.: American Chemical Society, 2024, Roč. 64, č. 4, s. 1306-1318 [tlačená forma] [online]. ISSN 1549-9596. ISSN (online) 1549-960X. - SCO ; CCC ; WOS CC, s. 1306 - 1318

2024 [01/20] / **USA** - Guedes-Sobrinho, Diego - Caldeira Rêgo, Celso R. - Da Silva, Gabriel Reynald - Da Silva, Henrique R. - Wenzel, W. - Piotrowski, Maurício J. - Cavalheiro Dias, Alexandre. **Theoretical Exploration of Structural and Excitonic Properties in Black Phosphorus: From First-Principles to a Semi-Empirical Approach** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c08414 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 17, s. 7242-7251 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 7242 - 7251

2024 [01/20] / **DEU** - Liu, Modan - Elsing, David - Esmaeilpour, Meysam - Kozlowska, Mariana - Wenzel, Wolfgang - Wöll, Christof. **Layer-By-Layer Assembly of Asymmetric Linkers into Non-Centrosymmetric Metal Organic Frameworks: A Thorough Theoretical Treatment** [elektronický dokument]. DOI 10.1002/adfm.202302516 In: **Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 34, č. 20, art. no. 2302516 [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Malik, Asif A. - Saeed, Zeinab M. - Ahmad, Ishtiyaq - Alkhidir, Tamador - Managutti, Praveen B. - Mohamed, Sharmarke - Dar, Aijaz A. **Polymorphism Steered Thermochromism in a Sulfonamide** [elektronický dokument]. DOI 10.1021/acsaom.4c00260 In: **ACS Applied Optical Materials**. Washington: American Chemical Society, 2024, Roč. 2, č. 8, s. 1709-1720 [online]. ISSN (online) 27719855. - SCO ; WOS CC, s. 1709 - 1720

2024 [01/20] / **GBR** - Caicedo-Dávila, Sebastián - Cohen, Adi - Motti, Silvia G. - Isobe, Masahiko - McCall, Kyle M. - Grumet, Manuel - Kovalenko, Maksym V. - Yaffe, Omer - Herz, Laura M. - Fabini, Douglas H. - Egger, David A. **Disentangling the effects of structure and lone-pair electrons in the lattice dynamics of halide perovskites** [elektronický dokument]. DOI 10.1038/s41467-024-48581-x In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2024, Roč. 15, č. 1, art. no. 4184 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Deng, Linjie - Ran, Jingyi - Wang, Bipeng - Boziki, Ariadni - Tkatchenko, Alexandre - Jiang, Jun - Prezhdo, Oleg V. **Strong Dependence of Point Defect Properties in Metal Halide Perovskites on Description of van der Waals Interaction** [elektronický dokument]. DOI 10.1021/acs.jpclett.4c02390 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2024, Roč. 15, č. 42, s. 10465-10472 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 10465 - 10472

2024 [01/20] / **USA** - O'Neill, Niamh - Shi, Benjamin X. - Fong, Kara - Michaelides, Angelos - Schran, Christoph. **To Pair or not to Pair? Machine-Learned Explicitly-Correlated Electronic Structure for NaCl in Water** [elektronický dokument]. DOI 10.1021/acs.jpclett.4c01030 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2024, Roč. 15, č. 23, s. 6081-6091 [online]. ISSN (online) 1948-7185. - SCO, s. 6081 - 6091

2024 [01/20] / **USA** - Drużbicki, Kacper - Gila-Herranz, Pablo - Marin-Villa, Pelayo - Gaboardi, Mattia - Armstrong, Jeff - Fernandez-Alonso, Felix. **Cation Dynamics as Structure Explorer in Hybrid Perovskites─The Case of MAPbI3** [elektronický dokument]. DOI 10.1021/acs.cgd.3c01112 In: **Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2024, Roč. 24, č. 1, s. 391-404 [tlačená forma] [online]. ISSN 1528-7483. ISSN

(online) 1528-7505. - SCO ; CCC ; WOS CC, s. 391 - 404

2024 [01/20] / **USA** - Novotný, Michal - Dubecký, Matúš - Karlický, František. **Toward accurate modeling of structure and energetics of bulk hexagonal boron nitride** [elektronický dokument]. DOI 10.1002/jcc.27222 In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2024, Roč. 45, č. 2, s. 115-121 [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO ; CCC ; WOS CC, s. 115 - 121

2023 [01/20] / **NLD** - Srikaew, Manmanut - Wongnongwa, Yutthana - Jungsuitiwong, Siriporn - Kaiyasuan, Chokchai - Promarak, Vinich - Saengsuwan, Sayant. **Improvement of adsorption performance and selectivity of GO-COOH towards MB dye through effective carboxylation approach: Combined experimental and DFT studies** [elektronický dokument]. DOI 10.1016/j.colsurfa.2023.131920 In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2023, Roč. 673, art. no. 131920 [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO ; CCC ; WOS CC, s. art. no. 131920

2023 [01/20] / **USA** - Askenazi, Evan M. - Lazar, Emanuel A. - Grinberg, Ilya. **Identification of High-Reliability Regions of Machine Learning Predictions Based on Materials Chemistry** [elektronický dokument]. DOI 10.1021/acs.jcim.3c01684 In: **Journal of Chemical Information and Modeling**. Washington, D.C.: American Chemical Society, 2023, Roč. 63, č. 23, s. 7350-7362 [tlačená forma] [online]. ISSN 1549-9596. ISSN (online) 1549-960X. - SCO ; CCC ; WOS CC, s. 7350 - 7362

2023 [01/20] / **USA** - Seidl, Stefan A. - Zhu, Xiangzhou - Reuveni, Guy - Aharon, Sigalit - Gehrmann, Christian - Caicedo-Dávila, Sebastián - Yaffe, Omer - Egger, David A. **Anharmonic fluctuations govern the band gap of halide perovskites** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.7.L092401 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 7, č. 9, art. no. L092401 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC, s. art. no. L092401

2023 [01/20] / **GBR** - Chu, Jifeng - Pan, Jianbin - Wang, Qiongyuan - Yang, Aijun - Song, Shizhen - Yuan, Huan - Rong, Mingzhe - Wang, Xiaohua. **Research progress and prospects on gas-sensitive mechanisms of semiconductor sensors** [elektronický dokument]. DOI 10.1039/d3cp00030c In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 18, s. 12668-12683 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 12668 - 12683

2023 [01/20] / **GBR** - Dickbreder, Tobias - Sabath, Franziska - Reischl, Bernhard - Nilsson, Rasmus V.E. - Foster, Adam S. - Bechstein, Ralf - Kühnle, Angelika. **Atomic structure and water arrangement on K-feldspar microcline (001)** [elektronický dokument]. DOI 10.1039/d3nr05585j In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 16, č. 7, s. 3462-3473 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC, s. 3462 - 3473

2023 [01/20] / **USA** - Menachekanian, Sevan - Mora Perez, Carlos - Pennathur, Anuj K. - Voegtle, Mattew J. - Blauth, Drew - Prezhdo, Oleg V. - Dawlaty, Jahan M. **Phenol as a Tethering Group to Gold Surfaces: Stark Response and Comparison to Benzenethiol** [elektronický dokument]. DOI 10.1021/acs.jpclett.3c02058 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 37, s. 8353-8359 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 8353 - 8359

2023 [01/20] / **USA** - Zhao, Qiyi - Ren, Yani - Li, Lu - He, Chuan - Che, Junling - Jia, Rongkai - Xu, Yonggang - Zhu, Lipeng - Xu, Xinlong. **Flexibility and anisotropy of MX3 (M = Zr, Hf; X = S, Se): New semiconductors with high photovoltaic performance** [elektronický dokument]. DOI 10.1063/5.0164156 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2023, Roč. 134, č. 12, art. no. 124302 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC, s. art. no. 124302

2023 [01/20] / **USA** - Al-Hamdani, Yasmine S. - Zen, Andrea - Alfè, Dario. **Unraveling H2 chemisorption and physisorption on metal decorated graphene using quantum Monte Carlo** [elektronický dokument]. DOI 10.1063/5.0174232 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 20, art. no. 204708 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 204708

2023 [01/20] / **GBR** - Ghojavand, Sajjad - Dib, Eddy - Rey, Jérôme - Daouli, Ayoub - Clatworthy, Edwin B. - Bazin, Philippe - Ruaux, Valérie - Badawi, Michael - Mintova, Svetlana. **Interplay between alkali-metal cations and silanol sites in nanosized CHA zeolite and implications for CO2 adsorption** [elektronický dokument]. DOI 10.1038/s42004-023-00918-1 In: **Communications chemistry**. [London]: Springer Nature, 2023, Roč. 6, č. 1, art. no. 134 [online]. ISSN (online) 2399-3669. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **DEU** - Cohen, Bat El - Alafi, Ron - Beinglass, Jonathan - Shpatz Dayan, Adva - Goldberg, Oren - Gold, Shachar - Balberg, Isaac - Kronik, Leeor - Etgar, Lioz - Millo, Oded - Azulay, Doron. **In-gap States and Carrier Recombination in Quasi-2D Perovskite Films** [elektronický dokument]. DOI 10.1002/solr.202300813 In: **Solar RRL**. Weinheim : John Wiley & Sons. Wiley-VCH, 2023, Roč. 7, č. 24, art. no. 2300813 [online]. ISSN (online) 2367-198X. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Mostaghimi, Mersad - Pacheco Hernandez, Helmy - Jiang, Yunzhe - Wenzel, Wolfgang - Heinke, Lars - Kozlowska, Mariana. **On–off conduction photoswitching in modelled spiropyran-based metal-organic frameworks** [elektronický dokument]. DOI 10.1038/s42004-023-01072-4 In: **Communications chemistry**. [London]: Springer Nature, 2023, Roč. 6, č. 1, art. no. 275 [online]. ISSN (online) 2399-3669. - SCO ; CCC ; WOS CC, s. art. no. 275

2023 [01/20] / **GBR** - Delachaux, F. - Hessou, E. P. - Vallières, C. - Monnier, H. - Badawi, M. **A dispersion-corrected DFT method for zeolite-based CO2/N2separation: Assessment and application** [elektronický dokument]. DOI 10.1016/j.jece.2022.109052 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2023, Roč. 11, č. 1, art. no. 109052 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s.

2023 [01/20] / **USA** - Hermann, Jan - Stöhr, Martin - Góger, Szabolcs - Chaudhuri, Shayantan - Aradi, Bálint - Maurer, Reinhard J. - Tkatchenko, Alexandre. **libMBD: A general-purpose package for scalable quantum many-body dispersion calculations** [elektronický dokument]. DOI 10.1063/5.0170972 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 17, art. no. 174802 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Manz, Thomas A. **Density-Derived Electrostatic and Chemical Methods** [elektronický dokument]. DOI 10.1016/B978-0-12-821978-2.00072-6 In: **Comprehensive Computational Chemistry**. Oxford: Elsevier, 2023, s. 362-405 [tlačená forma] [online]. ISBN 978-0-12-821978-2. ISBN (online) 978-0-12-823256-9. ISBN (chybné) 978-0-12-823256-9. - SCO, s. 362 - 405

2023 [01/20] / **USA** - Bryenton, Kyle R. - Johnson, Erin R. **Many-body dispersion in model systems and the sensitivity of self-consistent screening** [elektronický dokument]. DOI 10.1063/5.0142465 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 20, art. no. 204110 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Zhour, Kazem - Daouli, Ayoub - Postnikov, Andrei - Hasnaoui, Abdellatif - Badawi, Michael. **Potential of nanostructured carbon materials for iodine detection in realistic environments revealed by first-principles calculations** [elektronický dokument]. DOI 10.1039/d3cp02205f In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 39, s. 26461-26474 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 26461 - 26474

2023 [01/20] / **DEU** - Zhang, Chaoyang - Huang, Jing - Bu, Rupeng. **Intrinsic Structures and Properties of Energetic**

Materials [textový dokument (print)] . Berlín: Springer Nature, 2023. 1. vyd. ISBN 9789819926992. - SCO, s.

2022 [01/20] / **GBR** - Guha, S. - Kabiraj, A. - Mahapatra, S. **High-throughput design of functional-engineered MXene transistors with low-resistive contacts** [elektronický dokument] In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2022, Roč. 8, č. 1, [online]. ISSN (online) 2057-3960. - SCO, s. Art. No. 202

2022 [01/20] / **USA** - Ma, C. - Li, Q.M. - Gao, W. **Regulating Rolling and Sliding of Carbon Nanotubes on Graphite Through Doping and Charging** In: **Tribology Letters**, 2022, Roč. 70, č. 4. - SCO, s. Art. No. 112

2022 [01/20] / **USA** - Hurdax, P. - Kern, C.S. - Bone, T.G. - Haags, A. - Hollerer, M. - Egger, L. - Yang, X. - Kirschner, H. - Gottwald, A. - Richter, M. - Bocquet, F.C. - Soubatch, S. - Koller, G. - Tautz, F.S. - Sterrer, M. - Puschnig, P. - Ramsey, M.G. **Large Distortion of Fused Aromatics on Dielectric Interlayers Quantified by Photoemission Orbital Tomography** [elektronický dokument] In: **ACS Nano**. Washington: American Chemical Society, 2022, Roč. 16, č. 10, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO, s. 17435 - 17443

2022 [01/20] / **USA** - Liu, G. - Wei, S.-H. - Zhang, C. **Verification of the Accuracy and Efficiency of Dispersion-Corrected Density Functional Theory Methods to Describe the Lattice Structure and Energy of Energetic Cocrystals** In: **Crystal Growth and Design**, 2022, Roč. 22, č. 9. - SCO, s. 5307 - 5321

2022 [01/20] / **USA** - Abella, L. - Autschbach, J. **Density Functional Response Calculations of Dispersion Coefficients C6and C9of Closed- and Open-Shell Systems** In: **Journal of Physical Chemistry A**, 2022, Roč. 126, č. 34. - SCO, s. 5821 - 5831

2022 [01/20] / **NLD** - Malcioglu, O.B. - Bockstedte, M. **Self-metalation of a free-base porphyrin on a metal oxide surface mediated by extended defects: Insight from ab initio molecular dynamics simulations** [elektronický dokument] In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2022, Roč. 723, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO, s. Art. No. 122101

2022 [01/20] / **USA** - Fabila, J. - Romero, D. - Paz-Borbon, O. - Buendia, F. **Role of bimetallic Au-Ir subnanometer clusters mediating O2adsorption and dissociation on anatase TiO2(101)** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2022, Roč. 157, č. 8, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 084309

2022 [01/20] / **USA** - Ramakers, S. - Marusczyk, A. - Amsler, M. - Eckl, T. - Mrovec, M. - Hammerschmidt, T. - Drautz, R. **Effects of thermal, elastic, and surface properties on the stability of SiC polytypes** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 106, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 075201

2022 [01/20] / **GBR** - Bartaquim, E.O. - Bezerra, R.C. - Bittencourt, A.F.B. - Da, Silva J.L.F. **Computational investigation of van der Waals corrections in the adsorption properties of molecules on the Cu(111) surface** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 34, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 20294 - 20302

2022 [01/20] / **USA** - De Rezende, A. - Malmali, M. - Dral, P.O. - Lischka, H. - Tunega, D. - Aquino, A.J.A. **Machine Learning for Designing Mixed Metal Halides for Efficient Ammonia Separation and Storage** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 29. - SCO, s. 12184 - 12196

2022 [01/20] / **GBR** - Daouli, A. - Hessou, E.P. - Monnier, H. - Dziurla, M.-A. - Hasnaoui, A. - Maurin, G. - Badawi, M. **Adsorption of NO, NO2 and H2O in divalent cation faujasite type zeolites: a density functional theory screening approach** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 25, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 15565 - 15578

2022 [01/20] / **USA** - Gray, M. - Herbert, J.M. **Comprehensive Basis-Set Testing of Extended Symmetry-Adapted Perturbation Theory and Assessment of Mixed-Basis Combinations to Reduce Cost** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 4, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 2308 - 2330

2022 [01/20] / **GBR** - Vogt, J. **Strain modulation in small molecule physisorption in two dimensions: LEED structure analysis and DFT modeling of the system NaCl(100)/(3root2xroot2)R45degrees C2H2** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 16, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 9168 - 9175

2021 [01/20] / **GBR** - Zhang, H.-P. - Zhang, R. - Sun, C. - Jiao, Y. - Zhang, Y. **CO2reduction to CH4on Cu-doped phosphorene: A first-principles study** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 13, č. 48, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 20541 - 20549

2021 [01/20] / **USA** - Ouyang, W. - Sofer, R. - Gao, X. - Hermann, J. - Tkatchenko, A. - Kronik, L. - Urbakh, M. - Hod, O. **Anisotropic interlayer force field for transition metal dichalcogenides: The case of molybdenum disulfide** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 7237 - 7245

2021 [01/20] / **GBR** - Pastukh, S. - Laskowska, M. - Dulski, M. - Krzykawski, T. - Parlinski, K. - Piekarz, P. **Ab initio studies for characterization and identification of nanocrystalline copper pyrophosphate confined in mesoporous silica** [elektronický dokument] In: **Nanotechnology**. Bristol : Institute of Physics. IOP Publishing, 2021, Roč. 32, č. 41, [tlačená forma] [online]. ISSN 0957-4484. ISSN (online) 1361-6528. - SCO, s. Art. No. 415701

2021 [01/20] / **GBR** - Williams, L. - Mukherjee, A. - Dasgupta, A. - Rajan, K. **Monitoring the role of site chemistry on the formation energy of perovskitesviadeep learning analysis of Hirshfeld surfaces** [elektronický dokument] In: **Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2021, Roč. 9, č. 34, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO, s. 11153 - 11162

2021 [01/20] / **GBR** - Oliveira, M. - Hunenberger, P.H. **Systematic optimization of a fragment-based force field against experimental pure-liquid properties considering large compound families: Application to oxygen and nitrogen compounds** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 33, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 17774 - 17793

2021 [01/20] / **CHE** - Hessou, E.P. - Bede, L.A. - Jabraoui, H. - Semmeq, A. - Badawi, M. - Valtchev, V. **Adsorption of toluene and water over cationic-exchanged y zeolites: A dft exploration** [elektronický dokument] In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 26, č. 18, [online]. ISSN (online) 1420-3049. - SCO, s. Art. No. 5486

2021 [01/20] / **USA** - Li, Y. - Liu, C. - Zhao, G.-D. - Hu, T. - Ren, W. **Two-dimensional multiferroics in a breathing kagome lattice** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 104, č. 6, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. L060405

2021 [01/20] / **USA** - Cockayne, E. - Wong-Ng, W. - Chen, Y.-S. - Culp, J.T. - Allen, A.J. **Density Functional Theory Study of the Structure of the Pillared Hofmann Compound Ni(3-Methyl-4,4¸-bipyridine)[Ni(CN)4] (Ni-BpyMe or PICNIC-21)** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 29. - SCO, s. 15882 - 15889

2021 [01/20] / **USA** - Henkel, P. - Mollenhauer, D. **Uncertainty of exchange-correlation functionals in density functional theory calculations for lithium-based solid electrolytes on the case study of lithium phosphorus oxynitride** [elektronický dokument] In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2021, Roč. 42, č. 18, [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO, s. 1283 - 1295

2021 [01/20] / **USA** - Srikulwong, U. - Phanchai, W. - Srepusharawoot, P. - Sakonsinsiri, C. - Puangmali, T. **Computational Insights into Molecular Adsorption Characteristics of Methylated DNA on Graphene Oxide for Multicancer Early Detection** [elektronický dokument] In: **Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2021, Roč. 125, č. 24, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCO, s. 6697 - 6708

2021 [01/20] / **USA** - Bowskill, D.H. - Sugden, I.J. - Konstantinopoulos, S. - Adjiman, C.S. - Pantelides, C.C. **Crystal Structure Prediction Methods for Organic Molecules: State of the Art** [elektronický dokument] In: **Annual Review of Chemical and Biomolecular Engineering**. San Mateo (Kalifornia): Annual Reviews, 2021, Roč. 12. ISSN 1947-5438. ISSN (online) 1947-5446. - SCO, s. 593 - 623

2021 [01/20] / **USA** - Pisarra, M. - Diaz, C. - Martin, F. **Theoretical study of structural and electronic properties of 2H-phase transition metal dichalcogenides** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 103, č. 19, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 195416

2021 [01/20] / **GBR** - Hofmann, O.T. - Zojer, E. - Hormann, L. - Jeindl, A. - Maurer, R.J. **First-principles calculations of hybrid inorganic-organic interfaces: From state-of-the-art to best practice** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 8132 - 8180

2021 [01/20] / **USA** - Welsh, I.D. - Crittenden, D.L. **New atoms-in-molecules dispersion models for use in ab initio derived force fields** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 0037157

2021 [01/20] / **NLD** - Hessou, E.P. - Jabraoui, H. - Khalil, I. - Dziurla, M.-A. - Badawi, M. **Ab initio screening of zeolite Y formulations for efficient adsorption of thiophene in presence of benzene** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2021, Roč. 541, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 148515

2020 [01/12] / **GBR** - Santos, I.C. - Gama, V. - Rabaca, S. - Veiros, L.F. - Nogueira, F. - Paixao, J.A. - Almeida, M. **Structural diversity in conducting bilayer salts (CNB-EDT-TTF)4A** In: **CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 48, [tlačená forma] [online]. ISSN 1466-8033. - SCO, s. 8313 - 8321

2020 [01/12] / **USA** - Li, Z. - Huang, J. - Ye, L. - Lv, Y. - Zhou, Z. - Shen, Y. - He, Y. - Jiang, L. **Encapsulation of Highly Volatile Fragrances in y Zeolites for Sustained Release: Experimental and Theoretical Studies** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 49, [online]. ISSN (online) 2470-1343. - SCO, s. 31925 - 31935

2020 [01/12] / **NLD** - Berro, Y. - Badawi, M. - El Haj Hassan, F. - Kassir, M. - Tielens, F. **Water-silanol interactions on the amorphous silica surface: A dispersion-corrected DFT investigation** [elektronický dokument] In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2020, Roč. 320, [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. Art. No. 114496

2020 [01/12] / **USA** - Duan, X. - Liu, Z. - Hanrahan, B.M. - Zhu, W. - Liu, S. **Designing xenes with two-dimensional triangular lattice** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 12, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 124003

2020 [01/12] / **USA** - Kashefolgheta, S. - Oliveira, M.P. - Rieder, S.R. - Horta, B.A.C. - Acree, W.E. - Hunenberger, P.H. **Evaluating Classical Force Fields against Experimental Cross-Solvation Free Energies** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 7556 - 7580

2020 [01/12] / **USA** - Oliveira, M.P. - Andrey, M. - Rieder, S.R. - Kern, L. - Hahn, D.F. - Riniker, S. - Horta, B.A.C. - Hunenberger, P.H. **Systematic Optimization of a Fragment-Based Force Field against Experimental Pure-Liquid Properties Considering Large Compound Families: Application to Saturated Haloalkanes** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 7525 - 7555

2020 [01/12] / **NLD** - Guo, H. - Zheng, K. - Cui, H. - Yu, J. - Tao, L.-Q. - Li, X. - Liao, C. - Xie, L. - Chen, X. **Tellurene based biosensor for detecting DNA/RNA nucleobases and amino acids: A theoretical insight** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 532, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. Art. No. 147451

2020 [01/12] / **USA** - Yang, H. - Savory, C.N. - Morgan, B.J. - Scanlon, D.O. - Skelton, J.M. - Walsh, A. **Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O2(NMC) Battery Cathodes** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2020, Roč. 32, č. 17, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 7542 - 7550

2020 [01/12] / Williams, L. - Mukherjee, A. - Rajan, K. **Deep Learning Based Prediction of Perovskite Lattice Parameters from Hirshfeld Surface Fingerprints** In: **Journal of Physical Chemistry Letters**, 2020, Roč. 11, č. 17. - SCO, s. 7462 - 7468

2020 [01/12] / **USA** - Li, H. - Shi, W. - Guo, Y. - Guo, W. **Nonmonotonic interfacial friction with normal force in two-dimensional crystals** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 085427

2020 [01/12] / **USA** - Paleico, M.L. - Behler, J. **Global optimization of copper clusters at the ZnO(10 1 ¯ 0) surface using a DFT-based neural network potential and genetic algorithms** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 054704

2020 [01/12] / Yuan, D. - Zhang, Y. - Ho, W. - Wu, R. **Effects of van der Waals Dispersion Interactions in Density Functional Studies of Adsorption, Catalysis, and Tribology on Metals** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 31. - SCO, s. 16926 - 16942

2020 [01/12] / **USA** - Blowey, P.J. - Blowey, P.J. - Sohail, B. - Rochford, L.A. - Lafosse, T. - Duncan, D.A. - Ryan, P.T.P. - Ryan, P.T.P. - Warr, D.A. - Lee, T.-L. - Costantini, G. - Maurer, R.J. - Woodruff, D.P. **Alkali Doping Leads to Charge-Transfer Salt Formation in a Two-Dimensional Metal-Organic Framework** [elektronický dokument] In: **ACS Nano**. Washington: American Chemical Society, 2020, Roč. 14, č. 6, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO, s. 7475 - 7483

2020 [01/12] / **USA** - Oliva, R. - Wozniak, T. - Dybala, F. - Tolloczko, A. - Kopaczek, J. - Scharoch, P. - Kudrawiec, R.

Valley polarization investigation of GeS under high pressure [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 101, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 235205

2020 [01/12] / **GBR** - Caldeweyher, E. - Mewes, J.-M. - Ehlert, S. - Grimme, S. **Extension and evaluation of the D4 London-dispersion model for periodic systems** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 16, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 8499 - 8512

2020 [01/12] / **GBR** - Rehak, F.R. - Piccini, G. - Alessio, M. - Sauer, J. **Including dispersion in density functional theory for adsorption on flat oxide surfaces, in metal-organic frameworks and in acidic zeolites** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 7577 - 7585

2020 [01/12] / **USA** - Silva, A.F. - Duarte, L.J. - Popelier, P.L.A. **Contributions of IQA electron correlation in understanding the chemical bond and non-covalent interactions** [elektronický dokument] In: **Structural Chemistry**: an international journal concerned with energy, structure, and their relationships to chemical, physical, and biological properties: Computational and Experimental Studies of Chemical and Biological Systems. New York: Springer Nature, 2020, Roč. 31, č. 2, [tlačená forma]. ISSN 1040-0400. ISSN (online) 1572-9001. - SCO, s. 507 - 519

2020 [01/12] / **USA** - Kim, J. - Kim, K.-W. - Kim, B. - Kang, C.-J. - Shin, D. - Lee, S.-H. - Min, B.-C. - Park, N. **Exploitable Magnetic Anisotropy of the Two-Dimensional Magnet CrI3** [elektronický dokument] In: **Nano letters**. Washington: American Chemical Society, 2020, Roč. 20, č. 2, [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCO, s. 929 - 935

2020 [01/12] / **GBR** - Demirci, S. - Gurel, H.H. - Jahangirov, S. - Ciraci, S. **Temperature, strain and charge mediated multiple and dynamical phase changes of selenium and tellurium** [elektronický dokument] In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 12, č. 5, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO, s. 3249 - 3258

2020 [01/12] / Shepelenko, M. - Feldman, Y. - Leiserowitz, L. - Kronik, L. **Order and Disorder in Calcium Oxalate Monohydrate: Insights from First-Principles Calculations** In: **Crystal Growth and Design**, 2020, Roč. 20, č. 2. - SCO, s. 858 - 865

2020 [01/12] / **NLD** - Sheng, C. - Fan, D. - Liu, H. **High thermoelectric performance can be achieved in two-dimensional (PbTe)2 layer** In: **Physics Letters, Section A: General, Atomic and Solid State Physics**, 2020, Roč. 384, č. 2. - SCO, s. Art. No. 126044

2020 [01/12] / **USA** - Ouyang, W. - Azuri, I. - Mandelli, D. - Tkatchenko, A. - Kronik, L. - Urbakh, M. - Hod, O. **Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 1, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 666 - 676

2020 [01/12] / Angyan, J. - Dobson, J. - Jansen, G. - Gould, T. **London Dispersion Forces in Molecules, Solids and Nano-structures: An Introduction to Physical Models and Computational Methods** In: **RSC Theoretical and Computational Chemistry Series**. London: Royal Society of Chemistry, 2020. - SCO, s. 1 - 434

2019 [01/12] / **USA** - Kebede, G. - Mitev, P.D. - Broqvist, P. - Eriksson, A. - Hermansson, K. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2019, Roč. 15, č. 1, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 584 - 594

2019 [01/12] / **USA** - Garcia-Muelas, R. - Rellan-Pineiro, M. - Li, Q. - Lopez, N. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 1, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 357 - 367

2019 [01/12] / **DEU** - Shahbaz, M. - Szalewicz, K. **In: Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2019, Roč. 138, č. 2, [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCIE ; WOS CC, s. Art. No. 25

2019 [01/12] / **USA** - Beck, H. - Gehrmann, C. - Egger, D.A. **In: APL materials**. Melville: ACA and AIP Publishing, 2019, Roč. 7, č. 2, [online]. ISSN (online) 2166-532X. - SCIE ; WOS CC, s. Art. No. 021108

2019 [01/12] / **USA** - Dues, C. - Schmidt, W.G. - Sanna, S. **In: ACS Omega**. Washington: American Chemical Society, 2019, Roč. 4, č. 2, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 3850 - 3859

2019 [01/12] / **CHE** - Allen, A.J. - Wong-Ng, W. - Cockayne, E. - Culp, J.T. - Matranga, C. **In: Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 3, [online]. ISSN (online) 2079-4991. - SCIE ; WOS CC, s. Art. No. 354

2019 [01/12] / **GBR** - Kiruthika, S. - Fjellvag, H. - Ravindran, P. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2019, Roč. 7, č. 11, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 6228 - 6240

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. - Cole, D.J. - Limas, N.G. - Fiszbein, B. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 34, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 19297 - 19324

2019 [01/12] / **CHE** - Hessou, E.P. - Ponce-Vargas, M. - Mensah, J.B. - Tielens, F. - Santos, J.C. - Badawi, M. **In: Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 5, [online]. ISSN (online) 2079-4991. - SCIE ; WOS CC, s. Art. No. 715

2019 [01/12] / Hessou, E.R. - Jabraoui, H. - Houngue, M.T.A.K. - Mensah, J.B. - Pastore, M. - Badawi, M. **In: Zeitschrift fur Kristallographie-Crystalline Materials**, 2019, Roč. 234, č. 7-8. - SCIE ; WOS CC, s. 469 - 482

2019 [01/12] / **GBR** - Stohr, M. - Van Voorhis, T. - Tkatchenko, A. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 48, č. 15, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 4118 - 4154

2019 [01/12] / Caicedo-Davila, S. - Funk, H. - Lovrincic, R. - Muller, C. - Sendner, M. - Cojocaru-Miredin, O. - Lehmann, F. - Gunder, R. - Franz, A. - Levcenco, S. - Cohen, A.V. - Kronik, L. - Haas, B. - Koch, C.T. - Abou-Ras, D. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 29. - SCIE ; WOS CC, s. 17666 - 17677

2019 [01/12] / Cohen, A.V. - Egger, D.A. - Rappe, A.M. - Kronik, L. **In: Journal of Physical Chemistry Letters**, 2019, Roč. 10, č. 16. - SCIE ; WOS CC, s. 4490 - 4498

2019 [01/12] / **DEU** - Zheng, J.Y. - Manning, H.G. - Zhang, Y.H. - Wang, J.J. - Purcell-Milton, F. - Pokle, A. - Porter, S.B. - Zhong, C. - Li, J. - Meehan, R.O. - Enright, R. - Gun'ko, Y.K. - Nicolosi, V. - Boland, J.J. - Sanvito, S. - Donegan, J.F. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2019, Roč. 9, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 11738

2019 [01/12] / **USA** - Mozara, R. - Kamlapure, A. - Valentyuk, I.M. - Cornils, L. - Lichtenstein, A.I. - Wiebe, J. -

Wiesendanger, R. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 9, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 094801

2019 [01/12] / Yang, H. - Yang, J.Y. - Savory, C.N. - Skelton, J.M. - Morgan, B.J. - Scanlon, D.O. - Walsh, A. **In: Journal of Physical Chemistry Letters**, 2019, Roč. 10, č. 18. - SCIE ; WOS CC, s. 5552 - 5556

2019 [01/12] / **GBR** - Yuan, D.W. - Liao, H.T. - Hu, W.Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 21049 - 21056

2019 [01/12] / Salazar, J.M. - Badawi, M. - Radola, B. - Macaud, M. - Simon, J.M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 38. - SCIE ; WOS CC, s. 23455 - 23463

2019 [01/12] / **GBR** - Liu, J. - Lu, H.G. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 59, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 34481 - 34485

2019 [01/12] / **USA** - Klimes, J. - Tew, D.P. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 151, č. 23, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 234108

2019 [01/12] / Shukri, N.S. - Johari, Z. - Alias, N.E. - Zakaria, N.A. - Yusoff, M.F.M. **Improved Sensing Properties of Amino Acid on Black Phosphorene: A Computational Study** In: **20189 Ieee International Conference on Sensors and Nanotechnology (sn), 2019**. NewYork: Institute of Electrical and Electronics Engineers, 2019. - CPCI-S ; WOS CC, s. 205 - 208

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 57, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 33310 - 33336

2018 [01/12] / **NLD** - Hesselmann, A. - Meitei, O.R. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2018, Roč. 1129, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 57 - 69

2018 [01/12] / **GBR** - Wang, X.H. - Wang, D.W. - Yang, A.J. - Koratkar, N. - Chu, J.F. - Lv, P.L. - Rong, M.Z. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 6, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 4058 - 4066

2018 [01/12] / **USA** - Wang, D.W. - Wang, X.H. - Yang, A.J. - Chu, J.F. - Lv, P.L. - Liu, Y. - Rong, M.Z. **In: IEEE Electron Device Letters**. Piscataway: Institute of Electrical and Electronics Engineers, 2018, Roč. 39, č. 2, [tlačená forma] [online]. ISSN 0741-3106. ISSN (online) 1558-0563. - SCIE ; WOS CC, s. 292 - 295

2018 [01/12] / **GBR** - Liang, T. - Chen, W.Q. - Hu, C.E. - Chen, X.R. - Chen, Q.F. **In: Solid State Communications**: an International Journal. Oxford: Elsevier, 2018, Roč. 272, [tlačená forma] [online]. ISSN 0038-1098. ISSN (online) 1879-2766. - SCIE ; WOS CC, s. 28 - 32

2018 [01/12] / **GBR** - Zhao, Q.Y. - Guo, Y.H. - Zhou, Y.X. - Yao, Z.H. - Ren, Z.Y. - Bai, J.T. - Xu, X.L. **In: Nanoscale**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 10, č. 7, [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCIE ; WOS CC, s. 3547 - 3555

2018 [01/12] / **USA** - Lao, K.U. - Herbert, J.M. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. -

SCIE ; WOS CC, s. 2955 - 2978

2018 [01/12] / Meitei, O.R. - Hesselmann, A. **In: Journal of Theoretical & Computational Chemistry**, 2018, Roč. 17, č. 5. - SCIE ; WOS CC, s. 57 - 69

2018 [01/12] / **DEU** - Wang, D.W. - Wang, X.H. - Yang, A.J. - Lv, P.L. - Chu, J.F. - Liu, Y. - Rong, M.Z. - Wang, C.Q. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2018, Roč. 212, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 453 - 460

2018 [01/12] / **USA** - Sun, M.L. - Chou, J.P. - Shi, L.H. - Gao, J.F. - Hu, A. - Tang, W.C. - Zhang, G. **In: ACS Omega**. Washington: American Chemical Society, 2018, Roč. 3, č. 6, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 5971 - 5979

2018 [01/12] / **USA** - Bereau, T. - DiStasio, R.A. - Tkatchenko, A. - von Lilienfeld, O.A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 148, č. 24, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 241706

2018 [01/12] / Fang, H.J. - Awati, R. - Boulfelfel, S.E. - Ravikovitch, P.I. - Sholl, D.S. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 24. - SCIE ; WOS CC, s. 12880 - 12891

2018 [01/12] / Zhang, Y.H. - Sanvito, S. **In: Journal of the American Ceramic Society**, 2018, Roč. 101, č. 9. ISSN 0002-7220. - SCIE ; WOS CC, s. 4118 - 4127

2018 [01/12] / **USA** - Bedoya-Martinez, N. - Giunchi, A. - Salzillo, T. - Venuti, E. - Della Valle, R.G. - Zojer, E. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4380 - 4390

2018 [01/12] / **USA** - Srour, J. - Badawi, M. - Hassan, F.E. - Postnikov, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 054106

2018 [01/12] / **USA** - Mosyagin, I. - Gambino, D. - Sangiovanni, D.G. - Abrikosov, I.A. - Caffrey, N.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 17, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 174103

2018 [01/12] / **USA** - Islas-Vargas, C. - Guevara-Garcia, A. - Oliver-Tolentino, M. - Ramos-Sanchez, G. - Gonzalez, I. - Galvan, M. **In: Journal of the Electrochemical Society**. Pennington: The Electrochemical Society, 2018, Roč. 166, č. 3, 5139- [tlačená forma] [online]. ISSN 0013-4651. ISSN (online) 1945-7111. - SCIE ; WOS CC, s.

2018 [01/12] / Hijazi, H. - Cantrel, L. - Paul, J.F. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 46. - SCIE ; WOS CC, s. 26401 - 26408

2018 [01/12] / **USA** - Liu, P.F. - Bo, T. - Xu, J.P. - Yin, W. - Zhang, J.R. - Wang, F.W. - Eriksson, O. - Wang, B.T. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. UNSP

2017 [01/12] / **USA** - Wang, J.Z. - Dong, B.J. - Guo, H.H. - Yang, T. - Zhu, Z. - Hu, G. - Saito, R. - Zhang, Z.D. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045404

2017 [01/12] / **NLD** - Chebbi, M. - Chibani, S. - Paul, J.F. - Cantrel, L. - Badawi, M. **In: Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2017, Roč. 239, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCIE ; WOS CC, s. 111 - 122

2017 [01/12] / **NLD** - Lebedeva, I.V. - Lebedev, A.V. - Popov, A.M. - Knizhnik, A.A. **In: Computational Materials Science**. Amsterdam: Elsevier, 2017, Roč. 128, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 45 - 58

2017 [01/12] / **USA** - Hermann, J. - DiStasio, R.A. - Tkatchenko, A. **In: Chemical Reviews**. Washington: American Chemical Society, 2017, Roč. 117, č. 6, [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCIE ; WOS CC, s. 4714 - 4758

2017 [01/12] / **USA** - Boese, A.D. - Sauer, J. **In: Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2017, Roč. 17, č. 4, [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCIE ; WOS CC, s. 1636 - 1646

2017 [01/12] / **GBR** - Lozano, A. - Escribano, B. - Akhmatskaya, E. - Carrasco, J. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 15, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 10133 - 10139

2017 [01/12] / **USA** - Yang, A.J. - Wang, D.W. - Wang, X.H. - Chu, J.F. - Lv, P.L. - Liu, Y. - Rong, M.Z. **In: IEEE Electron Device Letters**. Piscataway: Institute of Electrical and Electronics Engineers, 2017, Roč. 38, č. 7, [tlačená forma] [online]. ISSN 0741-3106. ISSN (online) 1558-0563. - SCIE ; WOS CC, s. 963 - 966

2017 [01/12] / Bedoya-Martinez, N. - Schrode, B. - Jones, A.O.F. - Salzillo, T. - Ruzie, C. - Demitri, N. - Geerts, Y.H. - Venuti, E. - Della Valle, R.G. - Zojer, E. - Resel, R. **In: Journal of Physical Chemistry Letters**, 2017, Roč. 8, č. 15. - SCIE ; WOS CC, s. 3690 - 3695

2017 [01/12] / Makoudi, Y. - Jeannoutot, J. - Palmino, F. - Cherioux, F. - Copie, G. - Krzeminski, C. - Cleri, F. - Grandidier, B. **In: Surface Science Reports**: a Review Journal, 2017, Roč. 72, č. 4, [tlačená forma]. ISSN 0167-5729. ISSN (online) 1879-274X. - SCIE ; WOS CC, s. 316 - 349

2017 [01/12] / **USA** - Amsler, M. - Yao, Z.P. - Wolverton, C. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2017, Roč. 29, č. 22, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 9819 - 9828

2017 [01/12] / **DEU** - Zhao, Q.Y. - Guo, Y.H. - Si, K.Y. - Ren, Z.Y. - Bai, J.T. - Xu, X.L. **In: Physica Status Solidi B-Basic Solid State Physics**. Weinheim: John Wiley & Sons. Wiley-VCH, 2017, Roč. 254, č. 9, [tlačená forma] [online]. ISSN 0370-1972. ISSN (online) 1521-3951. - SCIE ; WOS CC, s. Art. No. 1700033

2017 [01/12] / **USA** - Tsatsoulis, T. - Hummel, F. - Usvyat, D. - Schutz, M. - Booth, G.H. - Binnie, S.S. - Gillan, M.J. - Alfe, D. - Michaelides, A. - Gruneis, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 20, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 204108

2017 [01/12] / Zhao, Q.Y. - Guo, Y.H. - Zhou, Y.X. - Xu, X. - Ren, Z.Y. - Bai, J.T. - Xu, X.L. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 42. - SCIE ; WOS CC, s. 23744 - 23751

2017 [01/12] / Wang, D.W. - Yang, A.J. - Chu, J.F. - Lv, P.L. - L. - Wang, X.H. - Rong, M.Z. **In: 2017 Ieee Sensors**, 2017. - SCIE ; WOS CC, s. 169 - 171

2016 [01/12] / Kolobov, A.V. - Tominaga, J. **In: Two-Dimensional Transition-Metal Dichalcogenides**, 2016, Roč. 239. - SCIE ; WOS CC, s. 29 - 77

2016 [01/12] / **GBR** - Limas, N.G. - Manz, T.A. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2016, Roč. 6, č. 51, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 45727 - 45747

2016 [01/12] / **USA** - Cole, D.J. - Vilseck, J.Z. - Tirado-Rives, J. - Payne, M.C. - Jorgensen, W.L. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 5, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2312 - 2323

2016 [01/12] / **USA** - Li, J.R. - Rinke, P. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045201

2016 [01/12] / **USA** - Verstraelen, T. - Vandenbrande, S. - Heidar-Zadeh, F. - Vanduyfhuys, L. - Van Speybroeck, V. - Waroquier, M. - Ayers, P.W. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 3894 - 3912

2016 [01/12] / Deringer, V.L. - Csanyi, G. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 38. - SCIE ; WOS CC, s. 21552 - 21560

2016 [01/12] / **USA** - Woods, L.M. - Dalvit, D.A.R. - Tkatchenko, A. - Rodriguez-Lopez, P. - Rodriguez, A.W. - Podgornik, R. **In: Reviews of modern physics**. Melville: American Institute of Physics. American Physical Society, 2016, Roč. 88, č. 4, [tlačená forma] [online]. ISSN 0034-6861. ISSN (online) 1539-0756. - SCIE ; WOS CC, s. Art. No. 045003

2016 [01/12] / **USA** - Liu, X.F. - Hermann, J. - Tkatchenko, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 24, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 241101

2015 [01/12] / **USA** - Gao, W. - Tkatchenko, A. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 114, č. 9, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s. Art. No. 096101

2015 [01/12] / **USA** - Ferri, N. - DiStasio, R.A. - Ambrosetti, A. - Car, R. - Tkatchenko, A. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 114, č. 17, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s. Art. No. 176802

2015 [01/12] / **NLD** - Sun, T. - Wang, Y. - Zhang, H.M. - Liu, P.R. - Zhao, H.J. **In: Journal of colloid and interface science**. Amsterdam: Elsevier, 2015, Roč. 454, [tlačená forma] [online]. ISSN 0021-9797. ISSN (online) 1095-7103. - SCIE ; WOS CC, s. 180 - 186

2015 [01/12] / Yanagisawa, S. - Okuma, K. - Inaoka, T. - Hamada, I. **In: Journal of Electron Spectroscopy and Related Phenomena**, 2015, Roč. 204. ISSN 03682048. - SCIE ; WOS CC, s. 159 - 167

2015 [01/12] / Zhou, P.S. - Xu, Q. - Li, H.X. - Wang, Y. - Yan, B. - Zhou, Y.C. - Chen, J.F. - Zhang, J.N. - Wang, K.X. **In: Angewandte Chemie-International Edition**, 2015, Roč. 54, č. 50. - SCIE ; WOS CC, s. 15226 - 15230

ADC_042: / Huang, Yu Li (Autor) (10%) - Wruss, Elisabeth (Autor) (20%) - Egger, David A. (Autor) (10%) - Kera, Satoshi (Autor) (10%) - Ueno, Nobuo (Autor) (10%) - Saidi, Wissam A. (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (10%) - Wee, Andrew T. S. (Autor) (10%) - Zojer, Egbert (Autor) (10%): **Understanding the Adsorption of CuPc and ZnPc on Noble Metal Surfaces by Combining Quantum-Mechanical Modelling and Photoelectron Spectroscopy**. – CCC ; SCO ; WOS CC.
In: *Molecules* [elektronický dokument] . – Bazilej (Švajčiarsko) : Multidisciplinary Digital Publishing Institute. – ISSN (online) 1420-3049. – Roč. 19, č. 3 (2014), s. 2969-2992 [online]
Počet všetkých autorov: 9
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,312 - 2014
SJR: 0,738 - 2014
CiteScore: 3,7 - 2014
Kvartil Q:
2013, JIF - Chemistry, organic - Q3; **2013, Scimago** - Analytical chemistry - Q2; **2013, Scimago** - Chemistry (miscellaneous) - Q2; **2013, Scimago** - Drug discovery - Q2; **2013, Scimago** - Medicine (miscellaneous) - Q2; **2013, Scimago** - Molecular medicine - Q3; **2013, Scimago** - Organic chemistry - Q2; **2013, Scimago** - Pharmaceutical science - Q1; **2013, Scimago** - Physical and theoretical chemistry - Q2

Ohlasy (59):
2025 [01/20] / **USA** - Wang, Zihao - Li, Wan-Lu - Li, Shaowei. **Computational analysis of interface-driven spin-orbit coupling in molecular adsorbates on transition metal dichalcogenides** [elektronický dokument]. DOI 10.1103/zsmc-pd17 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 112, č. 16, s. [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - WOS CC ; SCO, s.

2025 [01/20] / **GBR** - Oh, Soyoung - Cho, Franklin H. - Soe, We Hyo - Yu, Jisoo - Bui, Hong Thi - Spree, Lukas - Hommel, Caroline - Jang, Won Jun - Phark, Soo Hyon - Colazzo, Luciano - Wolf, Christoph - Donati, Fabio. **Tailoring the electronic configurations of YPc2 on Cu(111): decoupling strategies for molecular spin qubit platforms** [elektronický dokument]. DOI 10.1039/d5nr02516h In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 38, s. 22163-22173 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC ; SCIE, s. 22163 - 22173

2025 [01/20] / **USA** - Sharma, Mayank - Jo, Junhyeon - Avedissian, Garen - Bayindir, Bertuğ - Kang, Jun - Sahin, Hasan - Casanova, Fèlix - Gobbi, Marco - Hueso, Luis E. **Molecular Engineering of Exchange Bias in Fe3GeTe2/Molecule Heterostructures** [elektronický dokument]. DOI 10.1021/acsaelm.5c01598 In: **ACS Applied Electronic Materials**. Washington: American Chemical Society, 2025, Roč. 7, č. 19, s. 9204-9211 [online]. ISSN (online) 2637-6113. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 9204 - 9211

2025 [01/20] / **CHE** - Morari, Vadim - Lungu, Ion - Suman, Victor - Ghimpu, Lidia - Potlog, Tamara - Tigoianu, Radu - Stoica, Iuliana - Gherasim, Carmen - Airinei, Anton. **Spectral Relationships of ZnPc and CuPc: UV-VIS and Fluorescence Behavior in Liquids and Thin Films** [elektronický dokument]. DOI 10.3390/molecules30214262 In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 30, č. 21, art. no. 4262 [online]. ISSN (online) 1420-3049. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 4262

2025 [01/20] / **NLD** - Drivas, Charalampos - Kennou, Stella - Kyriakou, Georgios. **Phthalocyanine interfaces with MoS2(0001): The effect of the metal centre on the charge transfer** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.161672 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 682, art. no. 161672 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 161672

2024 [01/20] / **USA** - Antczak, Grażyna - Kamiński, Wojciech - Morgenstern, Karina. **Apparent Height of the Metal Atom**

in Phthalocyanine: Co vs Cu [elektronický dokument]. DOI 10.1021/acs.jpcc.4c03449 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 33, s. 14056-14064 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 14056 - 14064

2023 [01/20] / **GBR** - Castrillo-Bodero, R. - Blanco-Rey, M. - Ali, K. - Ortega, J. E. - Schiller, F. - Fernández, L. **Tuning the carrier injection barrier of hybrid metal-organic interfaces on rare earth-gold surface compounds** [elektronický dokument]. DOI 10.1039/d2nr06440e In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 15, č. 8, s. 4090-4100 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC, s. 4090 - 4100

2023 [01/20] / **USA** - Baklanov, Aleksandr - Küchle, Johannes T. - Duncan, David A. - Ryan, Paul T.P. - Maurer, Reinhard J. - Schwarz, Martin - Rascon, Eduardo Corral - Piquero-Zulaica, Ignacio - Ngo, Huynh Thien - Riss, Alexander - Allegretti, Francesco - Auwärter, Willi. **Zinc-Porphine on Coinage Metal Surfaces: Adsorption Configuration and Ligand-Induced Central Atom Displacement** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c00232 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 15, s. 7501-7512 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 7501 - 7512

2022 [01/20] / **USA** - Belser, A. - Greulich, K. - Nagel, P. - Merz, M. - Schuppler, S. - Chasse, T. - Peisert, H. **Interface Properties of Perfluorinated Iron Phthalocyanine on Au(111) and Ag(111): The Influence of Iron and the Macrocycle** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 33. - SCO, s. 14245 - 14254

2022 [01/20] / **GBR** - Odintsova, E.G. - Petrenko, V.E. - Kolker, A.M. - Borovkov, N.Y. **Molecular origin of structural defects in the zinc phthalocyanine film** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 33, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 19956 - 19964

2022 [01/20] / **USA** - Greulich, K. - Belser, A. - Basova, T. - Chasse, T. - Peisert, H. **Interfaces between Different Iron Phthalocyanines and Au(111): Influence of the Fluorination on Structure and Interfacial Interactions** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 1. - SCO, s. 716 - 727

2022 [01/20] / **JPN** - Koshida, H. - Takahashi, Y. - Okuyama, H. - Hatta, S. - Aruga, T. **CuPc Adsorption on Au(110)-(1 x 2): From a Monomer to a Periodic Chain** [elektronický dokument] In: **e-Journal of Surface Science and Nanotechnology**. Tokio: The Japan Society of Vacuum and Surface Science, 2022, Roč. 20, č. 1. ISSN (online) 13480391. - SCO, s. 25 - 30

2021 [01/20] / **NLD** - Mabrouk, M. - Majewski, J.A. **Stability, electronic structure, and magnetic moment of vanadium phthalocyanine grafted to the Au(1 1 1) surface** [elektronický dokument] In: **Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2021, Roč. 1202, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCO, s. Art. No. 113319

2021 [01/20] / **USA** - Fernandez, L. - Thussing, S. - Brion-Rios, A.X. - Sanchez-Portal, D. - Jakob, P. **Lateral Interactions and Order-Disorder Phase Transitions of Metal Phthalocyanines on Ag(111)** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 28. - SCO, s. 15623 - 15635

2021 [01/20] / **USA** - Belser, A. - Greulich, K. - Gruninger, P. - Karstens, R. - Ovsyannikov, R. - Giangrisostomi, E. - Nagel, P. - Merz, M. - Schuppler, S. - Chasse, T. - Peisert, H. **Perfluorinated Phthalocyanines on Cu(110) and Cu(110)-(2 x 1)O: The Special Role of the Central Cobalt Atom** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 16. - SCO, s. 8803 - 8814

2020 [01/12] / Koshida, H. - Okuyama, H. - Hatta, S. - Aruga, T. - Hamamoto, Y. - Hamada, I. - Morikawa, Y. **Identifying**

Atomic-Level Correlation between Geometric and Electronic Structure at a Metal-Organic Interface In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 32. - SCO, s. 17696 - 17701

2020 [01/12] / Greulich, K. - Belser, A. - Bolke, S. - Gruninger, P. - Karstens, R. - Sattele, M.S. - Ovsyannikov, R. - Giangrisostomi, E. - Basova, T.V. - Klyamer, D. - Chasse, T. - Peisert, H. **Charge Transfer from Organic Molecules to Molybdenum Disulfide: Influence of the Fluorination of Iron Phthalocyanine** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 31. - SCO, s. 16990 - 16999

2020 [01/12] / Azuri, I. - Ali, M.E. - Tarafder, K. - Oppeneer, P.M. - Kronik, L. **Fe-porphyrin on Co(001) and Cu(001): A Comparative Dispersion-augmented Density Functional Theory Study** In: **Israel Journal of Chemistry**, 2020, Roč. 60, č. 8-9. - SCO, s. 870 - 875

2020 [01/12] / Granet, J. - Sicot, M. - Gerber, I.C. - Kremer, G. - Pierron, T. - Kierren, B. - Moreau, L. - Fagot-Revurat, Y. - Lamare, S. - Cherioux, F. - Malterre, D. **Adsorption-Induced Kondo Effect in Metal-Free Phthalocyanine on Ag(111)** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 19. - SCO, s. 10441 - 10452

2020 [01/12] / Qin, H. - Xu, L. - Zhong, D. **First-Principles Study of Zinc Phthalocyanine Molecules Adsorbed on Methylammonium Lead Iodide Surfaces** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 9. - SCO, s. 5167 - 5173

2020 [01/12] / Herper, H.C. - Brena, B. - Puglia, C. - Bhandary, S. - Wende, H. - Eriksson, O. - Sanyal, B. **Interaction with substrates** In: **SpringerBriefs in Applied Sciences and Technology**. Cham: Springer, 2020. - SCO, s. 45 - 64

2019 [01/12] / **USA** - Rumetshofer, M. - Bauernfeind, D. - Arrigoni, E. - von der Linden, W. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 99, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 045148

2019 [01/12] / **DEU** - Belser, A. - Karstens, R. - Nagel, P. - Merz, M. - Schuppler, S. - Chasse, T. - Peisert, H. **In: Physica Status Solidi B-Basic Solid State Physics**. Weinheim: John Wiley & Sons. Wiley-VCH, 2019, Roč. 256, č. 2, [tlačená forma] [online]. ISSN 0370-1972. ISSN (online) 1521-3951. - SCIE ; WOS CC, s. Art. No. 1800292

2019 [01/12] / **DEU** - Buimaga-Iarinca, L. - Morari, C. **In: Beilstein Journal of Nanotechnology**. Frankfurt nad Mohanom: Beilstein-Institut zur Förderung der Chemischen Wissenschaften, 2019, Roč. 10, [online]. ISSN (online) 2190-4286. - SCIE ; WOS CC, s. 706 - 717

2019 [01/12] / **DEU** - Widdascheck, F. - Hauke, A.A. - Witte, G. **In: Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2019, Roč. 29, č. 17, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCIE ; WOS CC, s. Art. No. 1808385

2019 [01/12] / Balle, D. - Schedel, C. - Chasse, T. - Peisert, H. **In: Journal of Physics-Condensed Matter**, 2019, Roč. 31, č. 17. - SCIE ; WOS CC, s. Art. No. 174004

2019 [01/12] / Montenegro-Pohlhammer, N. - Sanchez-de-Armas, R. - Cardenas-Jiron, G. - Calzado, C.J. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 46. - SCIE ; WOS CC, s. 28359 - 28369

2019 [01/12] / **DEU** - Gajda, L. - Kupka, T. - Malolepszy, A. - Stobinski, L. - Buczek, A. - Broda, M.A. - Wrzalik, R. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2019, Roč. 231, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 301 - 310

2019 [01/12] / **CHE** - Karstens, R. - Glaser, M. - Belser, A. - Balle, D. - Polek, M. - Ovsyannikov, R. - Giangrisostomi, E. - Chasse, T. - Peisert, H. **In: Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 24, č. 24, [online]. ISSN (online) 1420-3049. - SCIE ; WOS CC, s. Art. No. 4579

2019 [01/12] / **GBR** - Zhu, H. - Song, H.J. - Zhao, W.H. - Peng, Z.T. - Liu, D. - Xing, L.B. - Dai, J.X. - Huang, Z.C. - Liao, P.L. - Wang, Y. - Wu, K. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 29, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 16323 - 16328

2018 [01/12] / van Straaten, G. - Franke, M. - Soubatch, S. - Stadtmuller, B. - Duncan, D.A. - Lee, T.L. - Tautz, F.S. - Kumpf, C. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 15. - SCIE ; WOS CC, s. 8491 - 8504

2018 [01/12] / Birmingham, B. - Liege, Z. - Larson, N. - Lu, W.G. - Park, K.T. - Lee, H.W.H. - Voronine, D.V. - Scully, M.O. - Zhang, Z.R. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 5. - SCIE ; WOS CC, s. 2753 - 2760

2018 [01/12] / **DEU** - Buimaga-larinca, L. - Morari, C. **In: Scientific reports. Journal of the University of Applied Sciences Mittweida**: Journal of the University of Applied Sciences Mittweida: Wissenschaftliche Zeitschrift der Hochschule Mittweida . Mittweida: University of Applied Sciences Mittweida, 2018, Roč. 8, [tlačená forma]. ISSN 1437-7624. - SCIE ; WOS CC, s. Art. No. 12728

2018 [01/12] / **DEU** - Dreher, M. - Bischof, D. - Widdascheck, F. - Huttner, A. - Breuer, T. - Witte, G. **In: Advanced Materials Interfaces**. Weinheim: John Wiley & Sons. Wiley-VCH, 2018, Roč. 5, č. 21, [online]. ISSN 2196-7350. - SCIE ; WOS CC, s. Art. No. 1800920

2017 [01/12] / Borghetti, P. - Sarasola, A. - Merino-Diez, N. - Vasseur, G. - Floreano, L. - Lobo-Checa, J. - Arnau, A. - de Oteyza, D.G. - Ortega, J.E. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 51. - SCIE ; WOS CC, s. 28412 - 28419

2017 [01/12] / Fernandez, L. - Thussing, S. - Manz, A. - Witte, G. - Brion-Rios, A.X. - Cabrera-Sanfelix, P. - Sanchez-Portal, D. - Jakob, P. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 3. - SCIE ; WOS CC, s. 1608 - 1617

2017 [01/12] / **USA** - Lin, M.K. - Nakayama, Y. - Zhuang, Y.J. - Su, K.J. - Wang, C.Y. - Pi, T.W. - Metz, S. - Papadopoulos, T.A. - Chiang, T.C. - Ishii, H. - Tang, S.J. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 085425

2017 [01/12] / Thussing, S. - Jakob, P. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 25. - SCIE ; WOS CC, s. 13680 - 13691

2017 [01/12] / **DEU** - Tang, H. - Tarrat, N. - Langlais, V. - Wang, Y.F. **In: Beilstein Journal of Nanotechnology**. Frankfurt nad Mohanom: Beilstein-Institut zur Förderung der Chemischen Wissenschaften, 2017, Roč. 8, [online]. ISSN (online) 2190-4286. - SCIE ; WOS CC, s. 2484 - 2491

2017 [01/12] / Lerch, A. - Fernandez, L. - Ilyn, M. - Gastaldo, M. - Paradinas, M. - Valbuena, M.A. - Mugarza, A. - Ibrahim, A.B.M. - Sundermeyer, J. - Hofer, U. - Schiller, F. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 45. - SCIE ; WOS CC, s. 25353 - 25363

2017 [01/12] / **USA** - Baby, A. - Gruenewald, M. - Zwick, C. - Otto, F. - Forker, R. - van Straaten, G. - Franke, M. - Stadtmuller, B. - Kumpf, C. - Brivio, G.P. - Fratesi, G. - Fritz, T. - Zojer, E. **In: ACS Nano**. Washington: American Chemical Society, 2017, Roč. 11, č. 10, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 10495 - 10508

2017 [01/12] / Balle, D. - Adler, H. - Gruninger, P. - Karstens, R. - Ovsyannikov, R. - Giangrisostomi, E. - Chasse, T. - Peisert, H. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 34. - SCIE ; WOS CC, s. 18564 - 18574

2017 [01/12] / **USA** - Wang, C. - Niu, D.M. - Xie, H.P. - Liu, B.X. - Wang, S.T. - Zhu, M.L. - Gao, Y.L. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 147, č. 6, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 064702

2017 [01/12] / **USA** - Ferri, N. - Ambrosetti, A. - Tkatchenko, A. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 1, č. 2, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 026003

2017 [01/12] / **GBR** - Liang, Z.F. - Sun, H.L. - Shen, K.C. - Hu, J.B. - Song, B. - Lu, Y.H. - Jiang, Z. - Song, F. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2017, Roč. 7, č. 82, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 52143 - 52150

2016 [01/12] / **DEU** - Goiri, E. - Borghetti, P. - El-Sayed, A. - Ortega, J.E. - de Oteyza, D.G. **In: Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2016, Roč. 28, č. 7, [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCIE ; WOS CC, s. 1340 - 1368

2016 [01/12] / **DEU** - Balliou, A. - Kazim, S. - Pfleger, J. - Rakusan, J. - Skoulatakis, G. - Kennou, S. - Glezos, N. **In: Physica Status Solidi B-Basic Solid State Physics**. Weinheim: John Wiley & Sons. Wiley-VCH, 2016, Roč. 253, č. 5, [tlačená forma] [online]. ISSN 0370-1972. ISSN (online) 1521-3951. - SCIE ; WOS CC, s. 1009 - 1019

2016 [01/12] / Thussing, S. - Jakob, P. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 18. - SCIE ; WOS CC, s. 9904 - 9913

2016 [01/12] / **DEU** - Perfetti, M. - Serri, M. - Poggini, L. - Mannini, M. - Rovai, D. - Sainctavit, P. - Heutz, S. - Sessoli, R. **In: Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2016, Roč. 28, č. 32, 6946- [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCIE ; WOS CC, s.

2016 [01/12] / **USA** - Stadtmuller, B. - Seidel, J. - Haag, N. - Grad, L. - Tusche, C. - van Straaten, G. - Franke, M. - Kirschner, J. - Kumpf, C. - Cinchetti, M. - Aeschlimann, M. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 117, č. 9, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s. Art. No. 096805

2016 [01/12] / Yamane, H. - Kosugi, N. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 42. - SCIE ; WOS CC, s. 24307 - 24313

2016 [01/12] / Polek, M. - Latteyer, F. - Basova, T.V. - Petraki, F. - Aygul, U. - Uihlein, J. - Nagel, P. - Merz, M. - Schuppler, S. - Chasse, T. - Peisert, H. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 43. - SCIE ; WOS CC, s. 24715 - 24723

2016 [01/12] / **USA** - Novko, D. - Tremblay, J.C. - Blanco-Rey, M. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 24, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 244701

2015 [01/12] / **USA** - Kostyrko, T. - Slusarski, T. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2015, Roč. 117, č. 3, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. Art. No. 034302

2015 [01/12] / **USA** - Glaser, M. - Peisert, H. - Adler, H. - Aygul, U. - Ivanovic, M. - Nagel, P. - Merz, M. - Schuppler, S. -

Chasse, T. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2015, Roč. 142, č. 10, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 101918

2015 [01/12] / Adler, H. - Paszkiewicz, M. - Uihlein, J. - Polek, M. - Ovsyannikov, R. - Basova, T.V. - Chasse, T. - Peisert, H. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 16. - SCIE ; WOS CC, s. 8755 - 8762

2015 [01/12] / **USA** - Snezhkova, O. - Luder, J. - Wiengarten, A. - Burema, S.R. - Bischoff, F. - He, Y.Q. - Rusz, J. - Knudsen, J. - Bocquet, M.L. - Seufert, K. - Barth, J.V. - Auwarter, W. - Brena, B. - Schnadt, J. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2015, Roč. 92, č. 7, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 075428

2015 [01/12] / Peisert, H. - Uihlein, J. - Petraki, F. - Chasse, T. **In: Journal of Electron Spectroscopy and Related Phenomena**, 2015, Roč. 204. ISSN 03682048. - SCIE ; WOS CC, s. 49 - 60

2015 [01/12] / Gottfried, J.M. **In: Surface Science Reports**: a Review Journal, 2015, Roč. 70, č. 3, [tlačená forma]. ISSN 0167-5729. ISSN (online) 1879-274X. - SCIE ; WOS CC, s. 259 - 379

2015 - spolu : **2**

ADC_043: / Lazar, Petr (Autor) (20%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (60%) - Hafner, Jürgen (Autor) (20%): **Negative thermal expansion of ScF3: Insights from density-functional molecular dynamics in the isothermal-isobaric ensemble**. – [recenzované]. – CCC ; SCO ; WOS CC ; SCIE.
In: *Physical Review B, Condensed matter and materials physics* [textový dokument (print)] [elektronický dokument] . – College Park (USA) : American Institute of Physics. American Physical Society. – ISSN 1098-0121. – ISSN (online) 1550-235X. – Roč. 92, č. 22 (2015), s. 4302-4302 [tlačená forma] [online] [CD-ROM]
Počet všetkých autorov: 3
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 3,718 - 2015
SJR: 2,377 - 2015
CiteScore: 6,8 - 2015
Kvartil Q:
2014, AIS - Physics, condensed matter - Q1; **2015, JIF** - Physics, condensed matter - Q1

Ohlasy (62):
2025 [01/20] / **NLD** - El Hyani, Houda - Habib, Haris - Tian, Dongsheng - Li, Gong. **Unveiling structural phase transitions and Negative Linear Compressibility of ScF3 under high pressure** [elektronický dokument]. DOI 10.1016/j.physb.2025.416976 In: **Physica B**: Condensed Matter. Amsterdam: Elsevier, 2025, Roč. 701, art. no. 416976 [tlačená forma] [online]. ISSN 0921-4526. ISSN (online) 1873-2135. - SCO ; CCC ; WOS CC, s. art. no. 416976

2025 [01/20] / **GBR** - Yan, Haiyan - Chen, Lei - Zhang, Yun - Cao, Xuanyu - Zhang, Meiguang - Wei, Qun. **Temperature-dependent structural stability, mechanical strength, and thermodynamics of pyrite-type silicon pernitride** [elektronický dokument]. DOI 10.1039/d5cp03090k In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 45, s. 24558-24568 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 24558 - 24568

2025 [01/20] / **USA** - Hyani, Houda El - Habib, Haris - Gong, Li. **Exploring negative linear compressibility in the**

orthorhombic polymorph of ScF3 space group C222 under high pressure [elektronický dokument]. DOI 10.1007/s00894-025-06468-8 In: **Journal of Molecular Modeling**: Computational Chemistry: Life Science: Advanced Materials: New Methods. New York: Springer Nature. Springer-VDI-Verlag, 2025, Roč. 31, č. 9, art. no. 242 [tlačená forma] [online]. ISSN 1610-2940. ISSN (online) 0948-5023. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 242

2024 [01/20] / **NLD** - Wang, Lei - Sun, Ya Ning - Yao, Zhi Hao - Chen, Ying - Wang, Cong. **Anharmonicity in negative thermal expansion materials ZrW2O8 and ZrV2O7: Three-phonon interactions** [elektronický dokument]. DOI 10.1016/j.physleta.2024.129667 In: **Physics Letters A**: General Physics, Nonlinear Science, Statistical Physics, Atomic, Molecular and Cluster Physics, Plasma and Fluid Physics, Condensed Matter, Cross-disciplinary Physics, Biological Physics, Nanosciences, Quantum Physics, Optical physics. Amsterdam: Elsevier, 2024, Roč. 517, art. no. 129667 [tlačená forma] [online]. ISSN 0375-9601. ISSN (online) 1873-2429. - SCO ; CCC ; WOS CC, s. art. no. 129667

2024 [01/20] / **USA** - Zhao, Kaiyue - Jiao, Yixin - Sun, Qiang - He, Ri - Sanson, Andrea - Zhong, Zhicheng - Liang, Erjun - Gao, Qilong. **Octahedral tilt distortion in negative thermal expansion in the fluorides CaZr F6 and Sc F3** [elektronický dokument]. DOI 10.1103/PhysRevB.110.064322 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2024, Roč. 110, č. 6, art. no. 064322 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 064322

2024 [01/20] / **USA** - Saßnick, Holger Dietrich - Machado Ferreira De Araujo, Fabiana - Edzards, Joshua - Cocchi, Caterina. **Impact of Ligand Substitution and Metal Node Exchange in the Electronic Properties of Scandium Terephthalate Frameworks** [elektronický dokument]. DOI 10.1021/acs.inorgchem.3c03945 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2024, Roč. 63, č. 4, s. 2098-2108 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 2098 - 2108

2023 [01/20] / **USA** - Machado Ferreira de Araujo, Fabiana - Duarte-Ruiz, Daniel - Saßnick, Holger Dietrich - Gentzmann, Marie C. - Huthwelker, Thomas - Cocchi, Caterina. **Electronic Structure and Core Spectroscopy of Scandium Fluoride Polymorphs** [elektronický dokument]. DOI 10.1021/acs.inorgchem.2c04357 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2023, Roč. 62, č. 10, s. 4238-4247 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 4238 - 4247

2023 [01/20] / **CHE** - Sulyanova, Elena A. - Sobolev, Boris P. **Thermodynamic Origin of Negative Thermal Expansion Based on a Phase Transition-Type Mechanism in the GdF3-TbF3 System** [elektronický dokument]. DOI 10.3390/ijms241914944 In: **International journal of molecular sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 24, č. 19, art. no. 14944 [online] [tlačená forma]. ISSN 1661-6596. ISSN (online) 1422-0067. - SCO ; CCC ; WOS CC, s. art. no. 14944

2023 [01/20] / **CHE** - Sobolev, Boris P. - Sulyanova, Elena A. **Two-Component Rare-Earth Fluoride Materials with Negative Thermal Expansion Based on a Phase Transition-Type Mechanism in 50 RF3-R'F3 (R = La-Lu) Systems** [elektronický dokument]. DOI 10.3390/ijms241814000 In: **International journal of molecular sciences**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 24, č. 18, art. no. 14000 [online] [tlačená forma]. ISSN 1661-6596. ISSN (online) 1422-0067. - SCO ; CCC ; WOS CC, s. art. no. 14000

2023 [01/20] / **USA** - Stoppelman, John P. - Wilkinson, Angus P. - McDaniel, Jesse G. **Equation of state predictions for ScF3 and CaZrF6 with neural network-driven molecular dynamics** [elektronický dokument]. DOI 10.1063/5.0157615 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 8, art. no. 084707 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 084707

2023 [01/20] / **USA** - Denisenko, Yuriy G. - Molokeev, Maxim S. - Jiang, Xingxing - Sedykh, Alexander E. - Aleksandrovsky, Aleksandr S. - Oreshonkov, Aleksandr S. - Roginskii, Evgenii M. - Zhernakov, Maksim A. - Heuler, Dominik - Seuffert, Marcel - Lin, Zheshuai - Andreev, Oleg V. - Müller-Buschbaum, Klaus. **Negative Thermal Expansion in the Polymorphic Modification of Double Sulfate β-AEu(SO4)2 (A-Rb+, Cs+)** [elektronický dokument]. DOI

10.1021/acs.inorgchem.3c01624 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2023, Roč. 62, č. 31, s. 12423-12433 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 12423 - 12433

2023 [01/20] / **USA** - Dove, Martin T. - Wei, Zhongsheng - Phillips, Anthony E. - Keen, David A. - Refson, Keith. **Which phonons contribute most to negative thermal expansion in ScF3?** [elektronický dokument]. DOI 10.1063/5.0147610 In: **APL materials**. Melville: ACA and AIP Publishing, 2023, Roč. 11, č. 4, art. no. 041130 [online]. ISSN (online) 2166-532X. - SCO, s. art. no. 041130

2022 [01/20] / **USA** - Wang, Lei - Chen, Ying - Ni, Jun - Ye, Feng - Wang, Cong. **Anharmonic Interaction in Negative Thermal Expansion Material CaTiF6** [elektronický dokument]. DOI 10.1021/acs.inorgchem.2c03263 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2022, Roč. 61, č. 43, s. 17378-17386 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 17378 - 17386

2022 [01/20] / **USA** - Wang, L. - Chen, Y. - Ni, J. - Ye, F. - Wang, C. **Anharmonic Interaction in Negative Thermal Expansion Material CaTiF6** [elektronický dokument] In: **Inorganic Chemistry**. Washington: American Chemical Society, 2022, Roč. 61, č. 43, [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO, s. 17378 - 17386

2021 [01/20] / **USA** - Tkachenko, A.V. - Zaliznyak, I.A. **Empty perovskites as Coulomb floppy networks: Entropic elasticity and negative thermal expansion** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 103, č. 13, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 134106

2021 [01/20] / **USA** - Ren, B. - Chen, B. - Zhao, J. - Guo, Y. - Zhang, X. - Chen, X. - Du, Y. - Deng, Z. - Zhu, G. - Wang, F. **Synthesis of Core-Shell ScF3Nanoparticles for Thermal Enhancement of Upconversion** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2021, Roč. 33, č. 1, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 158 - 163

2021 [01/20] / **USA** - Tkachenko, Alexei V. - Zaliznyak, Igor A. **Empty perovskites as Coulomb floppy networks: Entropic elasticity and negative thermal expansion** [elektronický dokument]. DOI 10.1103/PhysRevB.103.134106 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 103, č. 13, art. no. 134106 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 134106

2021 [01/20] / **USA** - Ren, Biyun - Chen, Bing - Zhao, Jianxiong - Guo, Yang - Zhang, Xin - Chen, Xian - Du, Yangyang - Deng, Zhiqin - Zhu, Guangyu - Wang, Feng. **Synthesis of Core-Shell ScF3 Nanoparticles for Thermal Enhancement of Upconversion** [elektronický dokument]. DOI 10.1021/acs.chemmater.0c03124 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2021, Roč. 33, č. 1, s. 158-163 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC, s. 158 - 163

2020 [01/20] / **USA** - Dove, Martin T. - Du, Juan - Wei, Zhongsheng - Keen, David A. - Tucker, Matthew G. - Phillips, Anthony E. **Quantitative understanding of negative thermal expansion in scandium trifluoride from neutron total scattering measurements** [elektronický dokument]. DOI 10.1103/PhysRevB.102.094105 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 9, art. no. 094105 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 094105

2020 [01/20] / **GBR** - Handunkanda, Sahan U. - Curry, Erin B. - Voronov, Vladimir - Hancock, Jason N. **Infrared lattice dynamics in negative thermal expansion material in single-crystal ScF3** [elektronický dokument]. DOI 10.1088/1361-648X/ab4955 In: **Journal of Physics**: Condensed Matter. Bristol: Institute of Physics. IOP Publishing, 2020, Roč. 32, č. 3, art. no. 035403 [tlačená forma] [online]. ISSN 0953-8984. ISSN (online) 1361-648X. - SCO ; CCC ; WOS CC, s. art. no. 035403

2020 [01/20] / **NLD** - Bocharov, D. - Krack, M. - Rafalskij, Yu - Kuzmin, A. - Purans, J. **Ab initio molecular dynamics simulations of negative thermal expansion in ScF<inf>3</inf>: The effect of the supercell size** [elektronický dokument]. DOI 10.1016/j.commatsci.2019.109198 In: **Computational Materials Science**. Amsterdam: Elsevier, 2020, Roč. 171, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO, s.

2020 [01/12] / **NLD** - Bocharov, D. - Krack, M. - Rafalskij, Y. - Kuzmin, A. - Purans, J. **In: Computational Materials Science**. Amsterdam: Elsevier, 2020, Roč. 171, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. Art. No. UNSP

2020 [01/12] / **GBR** - Handunkanda, S.U. - Curry, E.B. - Voronov, V. - Hancock, J.N. **Infrared lattice dynamics in negative thermal expansion material in single-crystal ScF3** In: **Journal of Physics Condensed Matter**, 2020, Roč. 32, č. 3. - SCO, s. Art. No. 035403

2020 [01/12] / **USA** - Dove, M.T. - Du, J. - Wei, Z. - Keen, D.A. - Tucker, M.G. - Phillips, A.E. **Quantitative understanding of negative thermal expansion in scandium trifluoride from neutron total scattering measurements** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 9, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 094105

2019 [01/12] / **USA** - Oba, Y. - Tadano, T. - Akashi, R. - Tsuneyuki, S. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 3, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 033601

2019 [01/12] / Bocharov, D. - Rafalskij, Y. - Krack, M. - Putnina, M. - Kuzmin, A. **In: Functional Materials and Nanotechnologies (fm&nt 2018)**, 2019, Roč. 503. - SCIE ; WOS CC, s. Art. No. UNSP

2019 [01/20] / **GBR** - Bocharov, Dmitry - Rafalskij, Yuri - Krack, Matthias - Putnina, Mara - Kuzmin, Alexei. **Negative thermal expansion of ScF3: First principles vs empirical molecular dynamics**. DOI 10.1088/1757-899X/503/1/012001 In: **Functional Materials and Nanotechnologies (FM&NT 2018)**: 2–5 October 2018, Riga, Latvia. Bristol: Institute of Physics. IOP Publishing, 2019, [online]. - SCO, s.

2019 [01/20] / **USA** - Oba, Yusuke - Tadano, Terumasa - Akashi, Ryosuke - Tsuneyuki, Shinji. **First-principles study of phonon anharmonicity and negative thermal expansion in ScF3** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.3.033601 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 3, art. no. 033601 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC, s. art. no. 033601

2018 [01/20] / **CHE** - Singh, Baltej - Gupta, Mayanak K. - Mittal, Ranjan - Zbiri, Mohamed - Hodgson, Sarah A. - Goodwin, Andrew L. - Schober, Helmut - Chaplot, Samrath L. **Anomalous lattice dynamics in AgC4N3: Insights from inelastic neutron scattering and density functional calculations** [elektronický dokument]. DOI 10.3389/fchem.2018.00544 In: **Frontiers in Chemistry**. Lausanne: Frontiers Media, 2018, Roč. 6, č. NOV, art. no. 544 [online]. ISSN (online) 2296-2646. - SCO ; CCC ; WOS CC, s. art. no. 544

2018 [01/20] / **USA** - Singh, Baltej - Gupta, Mayanak K. - Mittal, Ranjan - Chaplot, Samrath L. **Density Functional Studies Revealing Anomalous Lattice Behavior in Metal Cyanide, AgC8N5** [elektronický dokument]. DOI 10.1021/acs.jpcc.8b04398 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2018, Roč. 122, č. 27, s. 15575-15581 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 15575 - 15581

2018 [01/20] / **USA** - Gupta, M. K. - Singh, Baltej - Mittal, R. - Chaplot, S. L. **Negative thermal expansion behavior in MZr F6 (M=Ca,Mg,Sr): Ab initio lattice dynamical studies** [elektronický dokument]. DOI 10.1103/PhysRevB.98.014301 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 1, art. no. 014301 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 014301

2018 [01/20] / **USA** - Winter, I. S. - Montoya, J. - Persson, K. A. - Chrzan, D. C. **Ab initio calculation of thermal expansion with application to understanding Invar behavior in gum metal** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.2.073601 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 2, č. 7, art. no. 073601 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC, s. art. no. 073601

2018 [01/20] / **GBR** - Mittal, R. - Gupta, M. K. - Chaplot, S. L. **Phonons and anomalous thermal expansion behaviour in crystalline solids** [elektronický dokument]. DOI 10.1016/j.pmatsci.2017.10.002 In: **Progress in Materials Science**: An International Review Journal. Oxford : Elsevier. Pergamon Press, 2018, Roč. 92, s. 360-445 [online] [tlačená forma]. ISSN 0079-6425. ISSN (online) 1873-2208. - SCO, s. 360 - 445

2018 [01/12] / **GBR** - Mittal, R. - Gupta, M.K. - Chaplot, S.L. **In: Progress in Materials Science**: An International Review Journal. Oxford : Elsevier. Pergamon Press, 2018, Roč. 92, [online] [tlačená forma]. ISSN 0079-6425. ISSN (online) 1873-2208. - SCIE ; WOS CC, s. 360 - 445

2018 [01/12] / Singh, B. - Gupta, M.K. - Mittal, R. - Chaplot, S.L. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 27. - SCIE ; WOS CC, s. 15575 - 15581

2018 [01/12] / **USA** - Gupta, M.K. - Singh, B. - Mittal, R. - Chaplot, S.L. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 1, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 014301

2018 [01/12] / **USA** - Winter, I.S. - Montoya, J. - Persson, K.A. - Chrzan, D.C. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 2, č. 7, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 073601

2018 [01/12] / **CHE** - Singh, B. - Gupta, M.K. - Mittal, R. - Zbiri, M. - Hodgson, S.A. - Goodwin, A.L. - Schober, H. - Chaplot, S.L. **In: Frontiers in Chemistry**. Lausanne: Frontiers Media, 2018, Roč. 6, [online]. ISSN (online) 2296-2646. - SCIE ; WOS CC, s. Art. No. 544

2017 [01/12] / **USA** - Hester, B.R. - Hancock, J.C. - Lapidus, S.H. - Wilkinson, A.P. **In: Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2017, Roč. 29, č. 2, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCIE ; WOS CC, s. 823 - 831

2017 [01/12] / **USA** - Singh, B. - Gupta, M.K. - Mittal, R. - Zbiri, M. - Rols, S. - Patwe, S.J. - Achary, S.N. - Schober, H. - Tyagi, A.K. - Chaplot, S.L. **In: Journal of Applied Physics**. Melville: American Institute of Physics, 2017, Roč. 121, č. 8, [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCIE ; WOS CC, s. nestr.

2017 [01/12] / **USA** - Occhialini, C.A. - Handunkanda, S.U. - Curry, E.B. - Hancock, J.N. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 9, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 0941060

2017 [01/20] / **USA** - Hester, Brett R. - Hancock, Justin C. - Lapidus, Saul H. - Wilkinson, Angus P. **Composition, Response to Pressure, and Negative Thermal Expansion in MIIBIVF6 (M = Ca, Mg; B = Zr, Nb)** [elektronický dokument]. DOI 10.1021/acs.chemmater.6b04809 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2017, Roč. 29, č. 2, s. 823-831 [tlačená forma] [online]. ISSN 0897-

4756. ISSN (online) 1520-5002. - SCO, s. 823 - 831

2017 [01/20] / **USA** - Occhialini, Connor A. - Handunkanda, Sahan U. - Curry, Erin B. - Hancock, Jason N. **Classical, quantum, and thermodynamics of a lattice model exhibiting structural negative thermal expansion** [elektronický dokument]. DOI 10.1103/PhysRevB.95.094106 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 95, č. 9, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s.

2017 [01/20] / **USA** - Singh, Baltej - Gupta, Mayanak Kumar - Mittal, Ranjan - Zbiri, Mohamed - Rols, S. - Patwe, Sadequa Jahedkhan - Achary, Srungarpu Nagabhusan - Schober, Helmut - Tyagi, Avesh Kumar - Chaplot, Samrath Lal. **Role of phonons in negative thermal expansion and high pressure phase transitions in β-eucryptite: An ab-initio lattice dynamics and inelastic neutron scattering study** [elektronický dokument]. DOI 10.1063/1.4977244 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2017, Roč. 121, č. 8, art. no. 085106 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO, s. art. no. 085106

2016 [01/20] / **USA** - Handunkanda, Sahan U. - Occhialini, Connor A. - Said, Ayman H. - Hancock, Jason N. **Two-dimensional nanoscale correlations in the strong negative thermal expansion material ScF3** [elektronický dokument]. DOI 10.1103/PhysRevB.94.214102 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 21, art. no. 214102 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 214102

2016 [01/20] / **DEU** - Sanson, Andrea - Giarola, Marco - Mariotto, Gino - Hu, Lei - Chen, Jun - Xing, Xianran. **Lattice dynamics and anharmonicity of CaZrF6 from Raman spectroscopy and ab initio calculations** [elektronický dokument]. DOI 10.1016/j.matchemphys.2016.05.067 In: **Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2016, Roč. 180, s. 213-218 [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCO, s. 213 - 218

2016 [01/20] / **USA** - Van Roekeghem, Ambroise - Carrete, Jesús - Mingo, Natalio. **Anomalous thermal conductivity and suppression of negative thermal expansion in ScF3** [elektronický dokument]. DOI 10.1103/PhysRevB.94.020303 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 2, art. no. 020303 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 020303

2016 [01/20] / **USA** - Hu, Lei - Chen, Jun - Sanson, Andrea - Wu, Hui - Guglieri Rodriguez, Clara - Olivi, Luca - Ren, Yang - Fan, Longlong - Deng, Jinxia - Xing, Xianran. **New Insights into the Negative Thermal Expansion: Direct Experimental Evidence for the "guitar-String" Effect in Cubic ScF3** [elektronický dokument]. DOI 10.1021/jacs.6b02370 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 27, s. 8320-8323 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 8320 - 8323

2016 [01/20] / **USA** - Yang, C. - Tong, P. - Lin, J. C. - Guo, X. G. - Zhang, K. - Wang, M. - Wu, Y. - Lin, S. - Huang, P. C. - Xu, W. - Song, W. H. - Sun, Y. P. **Size effects on negative thermal expansion in cubic ScF3** [elektronický dokument]. DOI 10.1063/1.4959083 In: **Applied Physics Letters**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 109, č. 2, art. no. 023110 [tlačená forma] [online]. ISSN 0003-6951. ISSN (online) 1077-3118. - SCO, s. art. no. 023110

2016 [01/20] / **USA** - Bocharov, D. - Žguns, P. - Piskunov, S. - Kuzmin, A. - Purans, J. **Electronic structure of cubic ScF3 from first-principles calculations** [elektronický dokument]. DOI 10.1063/1.4959013 In: **Low Temperature Physics**. New York: American Institute of Physics. AIP Publishing, 2016, Roč. 42, č. 7, s. 556-560 [tlačená forma] [online]. ISSN 1063-777X. ISSN (online) 1090-6517. - SCO, s. 556 - 560

2016 [01/20] / **USA** - Schick, Joseph T. - Rappe, Andrew M. **Classical model of negative thermal expansion in solids**

with expanding bonds [elektronický dokument]. DOI 10.1103/PhysRevB.93.214304 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 21, art. no. 214304 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 214304

2016 [01/20] / **USA** - Piskunov, Sergei - Žguns, Pjotrs A. - Bocharov, Dmitry - Kuzmin, Alexei - Purans, Juris - Kalinko, Aleksandr - Evarestov, Robert A. - Ali, Shehab E. - Rocca, Francesco. **Interpretation of unexpected behavior of infrared absorption spectra of ScF3 beyond the quasiharmonic approximation** [elektronický dokument]. DOI 10.1103/PhysRevB.93.214101 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 21, art. no. 214101 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. 214101

2016 [01/20] / **USA** - Han, Fei - Chen, Jun - Hu, Lei - Ren, Yang - Rong, Yangchun - Pan, Zhao - Deng, Jinxia - Xing, Xianran. **The Distortion-Adjusted Change of Thermal Expansion Behavior of Cubic Magnetic Semiconductor (Sc1−xMx)F3 (M = Al, Fe)** [elektronický dokument]. DOI 10.1111/jace.14399 In: **Journal of the American Ceramic Society**: a monthly publication devoted to the arts and sciences related to ceramics. Westerville: American Ceramic Society, 2016, Roč. 99, č. 9, s. 2886-2888 [tlačená forma] [online]. ISSN 0002-7820. ISSN (online) 1551-2916. - SCO, s. 2886 - 2888

2016 [01/12] / **USA** - Bocharov, D. - Zguns, P. - Piskunov, S. - Kuzmin, A. - Purans, J. **In: Low Temperature Physics**. New York: American Institute of Physics. AIP Publishing, 2016, Roč. 42, č. 7, [tlačená forma] [online]. ISSN 1063-777X. ISSN (online) 1090-6517. - SCIE ; WOS CC, s. 556 - 560

2016 [01/12] / **USA** - Schick, J.T. - Rappe, A.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 214304

2016 [01/12] / **USA** - Piskunov, S. - Zguns, P.A. - Bocharov, D. - Kuzmin, A. - Purans, J. - Kalinko, A. - Evarestov, R.A. - Ali, S.E. - Rocca, F. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 93, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 214101

2016 [01/12] / **USA** - Yang, C. - Tong, P. - Lin, J.C. - Guo, X.G. - Zhang, K. - Wang, M. - Wu, Y. - Lin, S. - Huang, P.C. - Xu, W. - Song, W.H. - Sun, Y.P. **In: Applied Physics Letters**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 109, č. 2, [tlačená forma] [online]. ISSN 0003-6951. ISSN (online) 1077-3118. - SCIE ; WOS CC, s. Art. No. 023110

2016 [01/12] / **USA** - van Roekeghem, A. - Carrete, J. - Mingo, N. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 2, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 020303

2016 [01/12] / **USA** - Hu, L. - Chen, J. - Sanson, A. - Wu, H. - Rodriguez, C.G. - Olivi, L. - Ren, Y. - Fan, L.L. - Deng, J.X. - Xing, X.R. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 27, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 8320 - 8323

2016 [01/12] / Han, F. - Chen, J. - Hu, L. - Ren, Y. - Rong, Y.C. - Pan, Z. - Deng, J.X. - Xing, X.R. **In: Journal of the American Ceramic Society**, 2016, Roč. 99, č. 9. ISSN 0002-7220. - SCIE ; WOS CC, s. 2886 - 2888

2016 [01/12] / **DEU** - Sanson, A. - Giarola, M. - Mariotto, G. - Hu, L. - Chen, J. - Xing, X.R. **In: Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín:

Elsevier, 2016, Roč. 180, [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCIE ; WOS CC, s. 213 - 218

2016 [01/12] / **USA** - Handunkanda, S.U. - Occhialini, C.A. - Said, A.H. - Hancock, J.N. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2016, Roč. 94, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 214102

ADC_044: / Bučko, Tomáš (Autor) [UKOPRCFZ] (80%) - Hafner, Jürgen (Autor) (20%): **The role of spatial constraints and entropy in the adsorption and transformation of hydrocarbons catalyzed by zeolites**. – CCC ; SCO ; WOS CC.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – č. 329 (2015), s. 32-48 [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 2,174 - 2015
SJR: 2,668 - 2015
CiteScore: 11,7 - 2015

Ohlasy (57):
2025 [01/20] / **DEU** - Göltl, Florian. **Exploring Quality Criteria for the Computational Modeling of Heterogeneous Catalysts** [elektronický dokument]. DOI 10.1002/cphc.202401123 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 11, art. no. e202401123 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC, s.

2025 [01/20] / **USA** - Xiong, Danfeng - Lai, Zhuangzhuang - Chen, Jianfu - Yuan, Haiyang - Wang, Haifeng. **Ketene Conversion Chemistry within Mordenite Zeolite: Pore-Size-Dependent Reaction Mechanism, Product Selectivity, and Catalytic Activity** [elektronický dokument]. DOI 10.1021/jacs.5c03687 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2025, Roč. 147, č. 20, s. 17303-17314 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC ; SCIE, s. 17303 - 17314

2025 [01/20] / **GBR** - Karamanis, Ioannis - Dell'Angelo, David - Monnier, Hubert - Badawi, Michael. **Computational screening analysis of iron zeolites for selectively capturing NOx and CO over H2O and CO2** [elektronický dokument]. DOI 10.1039/d5me00003c In: **Molecular Systems Design and Engineering**. [s.l.]: The Royal Society of Chemistry, 2025, Roč. 10, č. 10, s. 855-867 [online]. ISSN (online) 20589689. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 855 - 867

2025 [01/20] / **GBR** - Mao, Yu - Wang, Ziyun - Waterhouse, Geoffrey I.N. **Understanding light olefin selectivity during Fischer-Tropsch syntheses over zeolites: A DFT exploration of the key role of ketene intermediates** [elektronický dokument]. DOI 10.1016/j.jece.2025.118822 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2025, Roč. 13, č. 5, art. no. 118822 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 118822

2024 [01/20] / **NLD** - Jiménez-Ruiz, Mónica - Lemishko, Tetiana - Rey, Fernando - Sastre, German. **Carbonylation of dimethyl ether in mordenite using Inelastic Neutron Scattering** [elektronický dokument]. DOI 10.1016/j.micromeso.2023.112850 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2024, Roč. 364, art. no. 112850 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO ; CCC ; WOS CC, s. art. no. 112850

2024 [01/20] / **CHE** - Khivantsev, Konstantin - Derewinski, Miroslaw A. - Kovarik, Libor - Bowden, Mark - Li, Xiaohong Shari - Jaegers, Nicholas R. - Boglaienko, Daria - Pereira-Hernandez, Xavier I. - Pearce, Carolyn - Wang, Yong - Szanyi, Janos. **Increasing Al-Pair Abundance in SSZ-13 Zeolite via Zeolite Synthesis in the Presence of Alkaline Earth Metal Hydroxide Produces Hydrothermally Stable Co-, Cu- and Pd-SSZ-13 Materials**. DOI 10.3390/catal14010056 In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 14, č. 1, art. no. 56 [online]. ISSN 2073-4344. - SCO ; CCC ; WOS CC, s. art. no. 56

2024 [01/20] / **GBR** - de Reviere, Arno - Verberckmoes, An - Sabbe, Maarten K. **Mechanistic origins for the enhanced ethanol dehydration kinetics in H-ZSM-5 by cofeeding n-butanol** [elektronický dokument]. DOI 10.1039/d4cy00532e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 15, s. 4319-4340 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4319 - 4340

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Wang, Mengen - Boscoboinik, Jorge Anibal - Lu, Deyu. **First-Principles Study of n-Butane Monomolecular Cracking and Dehydrogenation on Two-Dimensional-Zeolite Model Systems: Reaction Mechanisms and Effects of Spatial Confinement** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c01403 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 28, s. 13593-13600 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 13593 - 13600

2023 [01/20] / **GBR** - Cnudde, Pieter - Waroquier, Michel - Van Speybroeck, Veronique. **Universal descriptors for zeolite topology and acidity to predict the stability of butene cracking intermediates** [elektronický dokument]. DOI 10.1039/d3cy00642e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 16, s. 4857-4872 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4857 - 4872

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **GBR** - Hutton, Daniel J. - Göltl, Florian. **Free and internal energies for the adsorption of short alkanes into the zeolite SSZ-13 from ab initio molecular dynamics simulations** [elektronický dokument]. DOI 10.1039/d3cp02523c In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 39, s. 26604-26612 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 26604 - 26612

2022 [01/20] / **USA** - Chizallet, C. **Achievements and Expectations in the Field of Computational Heterogeneous Catalysis in an Innovation Context** [elektronický dokument] In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, č. 1-4, [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 69 - 81

2022 [01/20] / **USA** - De Wispelaere, K. - Plessow, P.N. - Studt, F. **Toward Computing Accurate Free Energies in Heterogeneous Catalysis: a Case Study for Adsorbed Isobutene in H-ZSM-5** [elektronický dokument] In: **ACS Physical Chemistry Au**. Washington: American Chemical Society, 2022, Roč. 2, č. 5, [online]. ISSN (online) 2694-2445. - SCO, s. 399 - 406

2022 [01/20] / **USA** - Lin, L.-C. **Computational Study of Alkane Adsorption in Bronsted Acid Zeolites for More Efficient Alkane Cracking** [elektronický dokument] In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2022, Roč. 38, č. 25, [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO, s. 7665 - 7677

2022 [01/20] / **GBR** - Ayadi, T. - Badawi, M. - Cantrel, L. - Lebegue, S. **Rational approach for an optimized formulation of silver-exchanged zeolites for iodine capture from first-principles calculations** [elektronický dokument] In: **Molecular Systems Design and Engineering**. [s.l.]: The Royal Society of Chemistry, 2022, Roč. 7, č. 5, [online]. ISSN (online) 20589689. - SCO, s. 422 - 433

2022 [01/20] / **USA** - Chizallet, Céline. **Achievements and Expectations in the Field of Computational Heterogeneous Catalysis in an Innovation Context** [elektronický dokument]. DOI 10.1007/s11244-021-01489-y In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, s. 69-81 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 69 - 81

2021 [01/20] / **USA** - Van der Mynsbrugge, J. - Bell, A.T. **Challenges for the theoretical description of the mechanism and kinetics of reactions catalyzed by zeolites** [elektronický dokument] In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 404, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 832 - 849

2021 [01/20] / **GBR** - Randrianandraina, J. - Badawi, M. - Cardey, B. - Grivet, M. - Groetz, J.-E. - Ramseyer, C. - Anzola, F.T. - Chambelland, C. - Ducret, D. **Adsorption of water in Na-LTA zeolites: An ab initio molecular dynamics investigation** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 34, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 19032 - 19042

2021 [01/20] / **USA** - Gutierrez-Acebo, E. - Rey, J. - Bouchy, C. - Schuurman, Y. - Chizallet, C. **Ethylcyclohexane Hydroconversion in EU-1 Zeolite: DFT-based Microkinetic Modeling Reveals the Nature of the Kinetically Relevant Intermediates** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2021, Roč. 13, č. 15, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 3434 - 3442

2021 [01/20] / **NLD** - Rubes, M. - Koudelkova, E. - Vaculik, J. - Trachta, M. - Bulanek, R. - Bludsky, O. **Analysis of the BAS OH band reveals a non-statistical incorporation of Al into the MOR framework** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2021, Roč. 317, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 110994

2020 [01/12] / Cabana, N.C. - Serra, R.R. - Boix, A.V. - Bolcatto, P.G. **Geometries and Interaction Energies of Toluene on CsxNa1-xMordenite** In: **Physica Status Solidi (B) Basic Research**, 2020, Roč. 257, č. 9. - SCO, s. Art. No. 2000131

2020 [01/12] / **USA** - Allen, M.C. - Hoffman, A.J. - Liu, T.-W. - Webber, M.S. - Hibbitts, D. - Schwartz, T.J. **Highly Selective Cross-Etherification of 5-Hydroxymethylfurfural with Ethanol** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 12, [online]. ISSN (online) 2155-5435. - SCO, s. 6771 - 6785

2020 [01/12] / **USA** - Chizallet, C. **Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 10, [online]. ISSN (online) 2155-5435. - SCO, s. 5579 - 5601

2020 [01/12] / **USA** - Ham, H. - Jung, H.S. - Kim, H.S. - Kim, J. - Cho, S.J. - Lee, W.B. - Park, M.-J. - Bae, J.W. **Gas-Phase Carbonylation of Dimethyl Ether on the Stable Seed-Derived Ferrierite** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 9, [online]. ISSN (online) 2155-5435. - SCO, s. 5135 - 5146

2020 [01/12] / **NLD** - Liu, M. - Vesely, O. - Eliasova, P. - Shamzhy, M. - Lyu, P. - Grajciar, L. **Identification of the most active sites for tetrahydropyranylation in zeolites: MFI as a test case** [elektronický dokument] In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 345, [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; SCIE ; WOS CC, s. 165 - 174

2019 [01/12] / **NLD** - Wang, S. - He, Y. - Jiao, W.Y. - Wang, J.G. - Fan, W.B. **In: Current opinion in chemical engineering**. Amsterdam: Elsevier, 2019, Roč. 23, [online]. ISSN (online) 2211-3398. - SCIE ; WOS CC, s. 146 - 154

2019 [01/12] / **USA** - Ramirez, A. - Chowdhury, A.D. - Dokania, A. - Cnudde, P. - Caglapn, M. - Yarulina, I. - Abou-Hamad, E. - Gevers, L. - Ould-Chikh, S. - De Wispelaere, K. - van Speybroeck, V. - Gascon, J. **In: ACS Catalysis**. Washington: American Chemical Society, 2019, Roč. 9, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 6320 - 6334

2019 [01/12] / **NLD** - Jabraoui, H. - Hessou, E.P. - Chibani, S. - Cantrel, L. - Lebegue, S. - Badawi, M. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2019, Roč. 485, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. 56 - 63

2019 [01/12] / **USA** - Bailleul, S. - Rogge, S.M.J. - Vanduyfhuys, L. - Van Speybroeck, V. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 16, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 3993 - 4010

2019 [01/12] / **CHE** - Hessou, E.P. - Ponce-Vargas, M. - Mensah, J.B. - Tielens, F. - Santos, J.C. - Badawi, M. **In: Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 5, [online]. ISSN (online) 2079-4991. - SCIE ; WOS CC, s. Art. No. 715

2018 [01/12] / **GBR** - Chibani, S. - Badawi, M. - Loiseau, T. - Volkringer, C. - Cantrel, L. - Paul, J.F. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 24, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 16770 - 16776

2018 [01/12] / Yang, C.T. - Janda, A. - Bell, A.T. - Lin, L.C. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 17. - SCIE ; WOS CC, s. 9397 - 9410

2018 [01/12] / Van der Mynsbrugge, J. - Janda, A. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ChemPhysChem**, 2018, Roč. 19, č. 4. - SCIE ; WOS CC, s. 341 - 358

2018 [01/12] / **USA** - Chen, L. - Falsig, H. - Janssens, T.V.W. - Gronbeck, H. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2018, Roč. 358, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCIE ; WOS CC, s. 179 - 186

2018 [01/12] / **USA** - Cnudde, P. - De Wispelaere, K. - Vanduyfhuys, L. - Demuynck, R. - Van der Mynsbrugge, J. - Waroquier, M. - Van Speybroeck, V. **In: ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 10, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 189 - 228

2018 [01/12] / Li, G.N. - Liu, C. - Rohling, R. - Hensen, E.J.M. - Pidko, E.A. **In: Modelling and Simulation in the Science of Micro- and Meso-Porous Materials**, 2018. - SCIE ; WOS CC, s. 229 - 263

2018 [01/12] / **GBR** - Grajciar, L. - Heard, C.J. - Bondarenko, A.A. - Polynski, M.V. - Meeprasert, J. - Pidko, E.A. - Nachtigall, P. **In: Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 47, č. 22, [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCIE ; WOS CC, s. 8307 - 8348

2018 [01/12] / **USA** - Rybicki, M. - Sauer, J. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2018, Roč. 140, č. 51, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 18151 - 18161

2018 [01/12] / De Wispelaere, K. - Vanduyfhuys, L. - Van Speybroeck, V. **In: Modelling and Simulation in the Science of Micro- and Meso-Porous Materials**, 2018, Roč. 2018. - SCIE ; WOS CC, s. 189 - 228

2018 [01/12] / Li, G.N. - Liu, C. - Rohling, R. - Hensen, E.J.M. - Pidko, E.A. **In: Modelling and Simulation in the Science of Micro- and Meso-Porous Materials**, 2018, Roč. 2018. - SCIE ; WOS CC, s. 229 - 263

2017 [01/12] / John, M. - Alexopoulos, K. - Reyniers, M.F. - Marin, G.B. **In: Catalysis Science & Technology**, 2017, Roč. 7, č. 14. - SCIE ; WOS CC, s. 2978 - 2997

2017 [01/12] / Janda, A. - Vlaisavljevich, B. - Smit, B. - Lin, L.C. - Bell, A.T. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 3. - SCIE ; WOS CC, s. 1618 - 1638

2017 [01/12] / Rasmussen, D.B. - Christensen, J.M. - Temel, B. - Studt, F. - Moses, P.G. - Rossmeisl, J. - Riisager, A. - Jensen, A.D. **In: Catalysis Science & Technology**, 2017, Roč. 7, č. 5. - SCIE ; WOS CC, s. 1141 - 1152

2017 [01/12] / John, M. - Alexopoulos, K. - Reyniers, M.F. - Marin, G.B. **In: Catalysis Science & Technology**, 2017, Roč. 7, č. 5. - SCIE ; WOS CC, s. 1055 - 1072

2017 [01/12] / **USA** - Van der Mynsbrugge, J. - Janda, A. - Sharada, S.M. - Lin, L.C. - Van Speybroeck, V. - Head-Gordon, M. - Bell, A.T. **In: ACS Catalysis**. Washington: American Chemical Society, 2017, Roč. 7, č. 4, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 2685 - 2697

2017 [01/12] / Chibani, S. - Medlej, I. - Lebegue, S. - Angyan, J.G. - Cantrel, L. - Badawi, M. **In: ChemPhysChem**, 2017, Roč. 18, č. 12. - SCIE ; WOS CC, s. 1642 - 1652

2016 [01/12] / De Wispelaere, K. - Bailleul, S. - Van Speybroeck, V. **In: Catalysis Science & Technology**, 2016, Roč. 6, č. 8. - SCIE ; WOS CC, s. 2686 - 2705

2016 [01/12] / **USA** - De Wispelaere, K. - Wondergem, C.S. - Ensing, B. - Hemelsoet, K. - Meijer, E.J. - Weckhuysen, B.M. - Van Speybroeck, V. - Ruiz-Martinez, J. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 3, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 1991 - 2002

2016 [01/12] / Alexopoulos, K. - Lee, M.S. - Liu, Y. - Zhi, Y.C. - Liu, Y.S. - Reyniers, M.F. - Marin, G.B. - Glezakou, V.A. - Rousseau, R. - Lercher, J.A. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 13. - SCIE ; WOS CC, s. 7172 - 7182

2016 [01/12] / **USA** - Janda, A. - Vlaisavljevich, B. - Lin, L.C. - Smit, B. - Bell, A.T. **In: Journal of the American Chemical Society**. Washington: American Chemical Society, 2016, Roč. 138, č. 14, [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCIE ; WOS CC, s. 4739 - 4756

2016 [01/12] / **USA** - Zhao, Z.J. - Kulkarni, A. - Vilella, L. - Norskov, J.K. - Studt, F. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 6, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 3760 - 3766

2016 [01/12] / **USA** - John, M. - Alexopoulos, K. - Reyniers, M.F. - Marin, G.B. **In: ACS Catalysis**. Washington: American Chemical Society, 2016, Roč. 6, č. 7, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 4081 - 4094

2016 [01/12] / **NLD** - Shang, J. - Li, G. - Webley, P.A. - Liu, J.Z. **In: Computational Materials Science**. Amsterdam: Elsevier, 2016, Roč. 122, [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCIE ; WOS CC, s. 307 - 313

2016 [01/12] / **GBR** - Chibani, S. - Chebbi, M. - Lebegue, S. - Cantrel, L. - Badawi, M. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2016, Roč. 18, č. 36, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 25574 - 25581

2015 [01/12] / **USA** - John, M. - Alexopoulos, K. - Reyniers, M.-F. - Marin, G.B. **In: Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2015, Roč. 330, [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. Art. No. 11809

2015 [01/12] / Zhang, Y.W. - Yu, J.Y. - Yeh, Y.H. - Gorte, R.J. - Rangarajan, S. - Mavrikakis, M. **In: Journal of Physical Chemistry C**, 2015, Roč. 119, č. 52. - SCIE ; WOS CC, s. 28970 - 28978

2016 - spolu : **6**

ADC_045: / Chibani, Siwar (Autor) (40%) - Chebbi, Mouheb (Autor) (10%) - Lebegue, Sebastien (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (20%) - Badawi, Michael (Autor) (20%): **A DFT investigation of the adsorption of iodine compounds and water in H-, Na-, Ag-, and Cu- mordenite**. – text, tab., obr. – [recenzované]. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 144, č. 24 (2016), art. no. 244705, s. [1-10] [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 65
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 2,965 - 2016
SNIP: 0,978 - 2016
SJR: 1,486 - 2016
CiteScore: 5,4 - 2016
Nordic List: 1 - 2016

Ohlasy (32):
2025 [01/20] / **GBR** - Mao, Yu - Wang, Ziyun - Waterhouse, Geoffrey I.N. **Understanding light olefin selectivity during Fischer-Tropsch syntheses over zeolites: A DFT exploration of the key role of ketene intermediates** [elektronický dokument]. DOI 10.1016/j.jece.2025.118822 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2025, Roč. 13, č. 5, art. no. 118822 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 118822

2025 [01/20] / **USA** - Xiong, Danfeng - Lai, Zhuangzhuang - Chen, Jianfu - Yuan, Haiyang - Wang, Haifeng. **Ketene Conversion Chemistry within Mordenite Zeolite: Pore-Size-Dependent Reaction Mechanism, Product Selectivity, and Catalytic Activity** [elektronický dokument]. DOI 10.1021/jacs.5c03687 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2025, Roč. 147, č. 20, s. 17303-17314 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC ; SCIE, s. 17303 - 17314

2025 [01/20] / **GBR** - Wang, Zijian - Ke, Ming - Song, Zhaozheng. **Exploration on the mechanism of crystal morphology**

transformation in mordenite [elektronický dokument]. DOI 10.1039/d5ra00666j In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 15, č. 11, s. 8696-8706 [online]. ISSN (online) 2046-2069. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 8696 - 8706

2025 [01/20] / **RUS** - Shelyapina, M. G. - Zvereva, I. A. - Kryuchkova, T. A. - Sheshko, T. F. - Akhmina, P. V. - Yafarova, L. V. - Antunez-Garcia, J. - Petranovskii, V. **Selective Dehydration of Glycerol to Hydroxyacetone over Cu-, Ag-, and AgFe-Mordenites** [elektronický dokument]. DOI 10.1134/S0023158425600038 In: **Kinetics and catalysis**. [Moscow]: Nauka Publishers. MAIK Nauka/Interperiodica, 2025, Roč. 66, č. 1, s. 43-53 [tlačená forma] [online]. ISSN 0023-1584. ISSN (online) 1608-3210. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 43 - 53

2024 [01/20] / **NLD** - Yu, Rui Li - Li, Qian Fan - Sun, Hao Ran - Li, Zhen Le - Xia, Liang Zhi. **Investigating the impact of amine-functionalized ZSM-5 with varying Si/Al ratios on the adsorption of radioactive gaseous iodine** [elektronický dokument]. DOI 10.1016/j.micromeso.2023.112893 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2024, Roč. 365, art. no. 112893 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO ; CCC ; WOS CC, s. art. no. 112893

2024 [01/20] / **CHE** - Elmekawy, Ahmed - Quach, Qui - Abdel-Fattah, Tarek M. **Synthesis and Characterization of Silver-Modified Nanoporous Silica Materials for Enhanced Iodine Removal** [elektronický dokument]. DOI 10.3390/nano14131143 In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 14, č. 13, art. no. 1143 [online]. ISSN (online) 2079-4991. - SCO ; CCC ; WOS CC, s. art. no. 1143

2024 [01/20] / **NLD** - Ma, Juncheng - Xu, Shuangping - Wang, Xintian - Zhang, Mingyu - Qu, Yanqing - Cao, Qiping - Jia, Hongge - Xu, Jingyu - Wang, Xing. **Biomass derived porous carbon for efficient iodine adsorption from vapor and solution** [elektronický dokument]. DOI 10.1016/j.seppur.2024.127613 In: **Separation and Purification Technology**. Amsterdam: Elsevier. Elsevier Science, 2024, Roč. 347, art. no. 127613 [tlačená forma] [online]. ISSN 1383-5866. ISSN (online) 1873-3794. - SCO ; CCC ; WOS CC, s. art. no. 127613

2023 [01/20] / **DEU** - Ahad, Jawaria - Ahmad, Masroor - Farooq, Amjad - Waheed, Khalid - Irfan, Naseem. **Removal of iodine by dry adsorbents in filtered containment venting system after 10 years of Fukushima accident** [elektronický dokument]. DOI 10.1007/s11356-023-27485-1 In: **Environmental science and pollution research**. Heidelberg: Springer Nature. Springer International Publishing AG, 2023, Roč. 30, č. 30, s. 74628-74670 [tlačená forma] [online]. ISSN 0944-1344. ISSN (online) 1614-7499. - SCO ; CCC ; WOS CC, s. 74628 - 74670

2023 [01/20] / **NLD** - Li, Yuanzhong - Li, Liling - Feng, Yufa - Wang, Huize - Liao, Jinyun - Ren, Jianwei - Zhou, Weiyou - He, Mingyang - Li, Hao. **Rattle-structured CuO/Co3O4@C microspheres, a potent bifunctional catalyst for hydrogen production from ammonia borane hydrolysis and methanolysis** [elektronický dokument]. DOI 10.1016/j.apsusc.2023.157840 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2023, Roč. 636, art. no. 157840 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 157840

2023 [01/20] / **USA** - Lin, Yue Qun - Tian, Xiao Mao - Zhu, Bi Xue - Chen, Dong Mei - Huang, Chao. **Five Porous Complexes Constructed from a Racemic Ligand: Synthesis, Chiral Self-Assembly, Iodine Adsorption, and Desorption Properties** [elektronický dokument]. DOI 10.1021/acs.inorgchem.3c01646 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2023, Roč. 62, č. 30, s. 12099-12110 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 12099 - 12110

2023 [01/20] / **USA** - Zhao, Jiabao - Qian, Weixin - Ma, Hongfang - Ying, Weiyong - Yuan, Peiqing - Zhang, Haitao. **Theoretical Study for Adsorption-Diffusion on H-MOR and Pyridine Pre-adsorbed H-MOR of Dimethyl Ether Carbonylation** [elektronický dokument]. DOI 10.1021/acsomega.3c02127 In: **ACS Omega**. Washington: American Chemical Society, 2023, Roč. 8, č. 24, s. 22067-22076 [online]. ISSN (online) 2470-1343. - SCO ; CCC ; WOS CC, s. 22067 - 22076

2023 [01/20] / **PRK** - Vaidya, Tejaswini - Stanford, John P. - van Rooyen, Nicolene - Raja, Krishnan - Utgikar, Vivek - Sabharwall, Piyush. **Capture of Volatile Organic Iodine Species Using Mordenites** [elektronický dokument]. DOI 10.7733/jnfcwt.2023.016 In: **Journal of Nuclear Fuel Cycle and Waste Technology**. Daejeon: Korean Radioactive Waste Society, 2023, Roč. 21, č. 2, s. 205-224 [tlačená forma] [online]. ISSN 1738-1894. ISSN (online) 2288-5471. - SCO ; WOS CC, s. 205 - 224

2023 [01/20] / **NLD** - Li, Qian Fan - Yu, Rui Li - Li, Zhen Le - Xia, Liang Zhi. **Iodine capture by ZSM-5 with different Si/Al ratios: An experimental and molecular simulation investigation** [elektronický dokument]. DOI 10.1016/j.micromeso.2023.112536 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2023, Roč. 354, art. no. 112536 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO ; CCC ; WOS CC, s. art. no. 112536

2022 [01/20] / **GBR** - Bahrani-Pour, M. - Beheshti, A. - Sedaghat, T. - Hoveizi, E. - Naseri, N. - Mayer, P. - Centore, R. **New Hg(ii) coordination polymers based on a thioimidazole ligand with good performance to detoxify Hg(ii) and reversibly capture iodine** [elektronický dokument] In: **Dalton Transactions**. Londýn: The Royal Society of Chemistry, 2022, Roč. 52, č. 3, [tlačená forma] [online]. ISSN 1477-9226. ISSN (online) 1477-9234. - SCO, s. 683 - 695

2022 [01/20] / **AUT** - Su, Y. - Hessou, E.P. - Colombo, E. - Belletti, G. - Moussadik, A. - Lucas, I.T. - Frochot, V. - Daudon, M. - Rouziere, S. - Bazin, D. - Li, K. - Quaino, P. - Tielens, F. **Crystalline structures of l-cysteine and l-cystine: a combined theoretical and experimental characterization** [elektronický dokument] In: **Amino Acids**: The Forum for Amino Acid, Peptide and Protein Research. Viedeň: Springer Nature. Springer Verlag, 2022, Roč. 54, č. 8, [tlačená forma] [online]. ISSN 0939-4451. ISSN (online) 1438-2199. - SCO, s. 1123 - 1133

2022 [01/20] / **USA** - Beheshti, A. - Bahrani-Pour, M. - Sedaghat, T. - Salahshournia, B. - Arefi-Nasab, H. - Mayer, P. - Centore, R. - Parisi, E. **Synthesis, Crystal Structures, H2S, and Iodine Uptake Properties of Four New Coordination Polymers Constructed from Group 12 Transition Metal Ions and a Bidentate Sulfur Donor Ligand** In: **Crystal Growth and Design**, 2022, Roč. 22, č. 7. - SCO, s. 4343 - 4356

2022 [01/20] / **DEU** - Yu, Y.-N. - Yin, Z. - Cao, L.-H. - Ma, Y.-M. **Organic porous solid as promising iodine capture materials** [elektronický dokument] In: **Journal of Inclusion Phenomena and Macrocyclic Chemistry**. Berlín: Springer Nature, 2022, Roč. 102, č. 5-6, [tlačená forma] [online]. ISSN 1388-3127. ISSN (online) 1573-1111. - SCO, s. 395 - 427

2021 [01/20] / **GBR** - Tong, D. - Zhao, Y. - Chen, Z. - Wang, Y. - Jia, Z. - Nie, X. - Xiao, S. **Theoretical insights into volatile iodine adsorption onto COF-DL229** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 44, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 25365 - 25373

2021 [01/20] / **CHN** - Wang, W. - Qian, W. - Ma, H. - Ying, W. - Zhang, H. **A theoretical study on adsorption-diffusion of dimethyl ether carbonylation on pyridine-modified H-MOR** In: **Huagong Xuebao/CIESC Journal**, 2021, Roč. 72, č. 9. - SCO, s. 4786 - 4795

2021 [01/20] / **USA** - Jung, Y.-E. - Kang, S.-W. - Yim, M.-S. **Feasibility Study of Using Bi-mna Metal-Organic Frameworks as Adsorbents for Radioiodine Capture at High Temperature** In: **Industrial and Engineering Chemistry Research**, 2021, Roč. 60, č. 16. - SCO, s. 5964 - 5975

2021 [01/20] / **GBR** - Rathi, A. - Basu, S. - Barman, S. **Structural framework effect of various CeO2-loaded zeolites on the adsorptive removal of fipronil** [elektronický dokument] In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2021, Roč. 9, č. 2, [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s. Art. No. 105167

2021 [01/20] / **GBR** - Wang, W. - Qian, W. - Ma, H. - Ying, W. - Zhang, H. **A theoretical study on the feed ratio of dimethyl ether carbonylation on H-MOR zeolites** [elektronický dokument] In: **Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2021, Roč. 119, č. 9, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCO, s. Art. No. e1896044

2020 [01/12] / **NLD** - Liu, J.W. - Yin, Y.R. - Fu, X.Z. - Luo, J.L. **Stability of C3-C6 carbonium ions inside zeolites: A first principles study** [elektronický dokument] In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 503, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. Art. No. UNSP

2020 [01/12] / **USA** - Khalil, I. - Celis-Cornejo, C.M. - Thomas, K. - Bazin, P. - Travert, A. - Perez-Martinez, D.J. - Baldovino-Medrano, V.G. - Paul, J.F. - Mauge, F. **In Situ IR-ATR Study of the Interaction of Nitrogen Heteroaromatic Compounds with HY Zeolites: Experimental and Theoretical Approaches** [elektronický dokument] In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2020, Roč. 12, č. 4, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO, s. 1095 - 1108

2020 [01/12] / **NLD** - Moloney, M.P. - Massoni, N. - Egodawatte, S. - zur Loye, H.-C. - Grandjean, A. **A Solvent Free Approach for the Preparation of Silver Modified Mesoporous Silica for Iodine Entrapment** [elektronický dokument] In: **Journal of Inorganic and Organometallic Polymers and Materials**. Amsterdam: Springer Nature, 2020, Roč. 30, č. 7, [tlačená forma] [online]. ISSN 1574-1443. ISSN (online) 1574-1451. - SCO, s. 2756 - 2763

2020 [01/12] / **NLD** - Bulanek, R. - Koudelkova, E. - Trachta, M. - Bludsky, O. - Rubes, M. **Re-examining the interpretation of CO adsorbed on Lewis acid sites of alkali metal-exchanged MOR zeolite** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2020, Roč. 296, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 110007

2020 [01/12] / **NLD** - Park, S. - An, H. - Park, M.B. - Lee, J. **Adsorption behavior of methyl iodide on a silver ion-exchanged ZSM-5** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2020, Roč. 294, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 109842

2019 [01/12] / **NLD** - Vorontsov, A.V. - Valdes, H. - Smirniotis, P.G. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2019, Roč. 1166, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. Art. No. UNSP

2018 [01/12] / Chun, H. - Kang, J. - Han, B. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 22. - SCIE ; WOS CC, s. 11799 - 11806

2018 [01/12] / **USA** - Cantrel, L. - Albiol, T. - Bosland, L. - Colombani, J. - Cousin, F. - Gregoire, A.C. - Leroy, O. - Morin, S. **In: Journal of nuclear engineering and radiation science**. United States: American Society of Mechanical Engineers, 2018, Roč. 4, č. 2, [tlačená forma] [online]. ISSN 2332-8983. ISSN (online) 2332-8975. - SCIE ; WOS CC, s. Art. No. UNSP

2018 [01/12] / **USA** - Nan, Y. - Liu, J.X. - Tang, S.Q. - Lin, R.H. - Tavlarides, L.L. **In: Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2018, Roč. 57, č. 3, [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCIE ; WOS CC, s. 1048 - 1058

2018 [01/12] / **GBR** - Huve, J. - Ryzhikov, A. - Nouali, H. - Lalia, V. - Auge, G. - Daou, T.J. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 8, č. 51, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 29248 - 29273

ADC_046: / Gould, Tim (Autor) (40%) - Lebegue, Sebastien (Autor) (10%) - Ángyán, János G. (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%): **A Fractionally Ionic Approach to Polarizability and van der Waals Many-Body Dispersion Calculations**. – text, ilustr., graf. – [recenzované]. – DOI 10.1021/acs.jctc.6b00925. – CCC ; SCO ; WOS CC ; SCIE.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 12, č. 12 (2016), s. 5920-5930 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 78
[OV 120 Chémia, chemická technológia a biotechnológie]
[ŠO 1420 chémia]
Indikátor časopisu:
SNIP: 1,505 - 2016
SJR: 2,711 - 2016
CiteScore: 9,6 - 2016

Ohlasy (34):
2025 [01/20] / **USA** - Palos, Etienne - Zhao, Heng - Daas, Kimberly J. - Fabiano, Eduardo - Paesani, Francesco - Vuckovic, Stefan. **Moller-Plesset Adiabatic Connection Theory for Diverse Noncovalent Interactions** [elektronický dokument]. DOI 10.1021/acs.jpclett.5c01304 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2025, Roč. 16, č. 31, s. 7898-7908 [online]. ISSN (online) 1948-7185. - WOS CC ; CCC ; SCO, s. 7898 - 7908

2025 [01/20] / **NLD** - Dang, Diem Thi Xuan - Le, Dai Nam - Woods, Lilia M. **Dissecting van der Waals interactions with density functional theory – Wannier-basis approach** [elektronický dokument]. DOI 10.1016/j.cpc.2025.109525 In: **Computer Physics Communications**: An International Journal and Program Library for Computational Physics and Physical Chemistry. Amsterdam: Elsevier, 2025, Roč. 310, art. no. 109525 [tlačená forma] [online]. ISSN 0010-4655. ISSN (online) 1879-2944. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 109525

2025 [01/20] / **USA** - Muhli, Heikki - Ala-Nissila, Tapio - Caro, Miguel A. **Atom-wise formulation of the many-body dispersion problem for linear-scaling van der Waals corrections** [elektronický dokument]. DOI 10.1103/PhysRevB.111.054103 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 111, č. 5, art. no. 054103 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 054103

2025 [01/20] / **GBR** - Matveev, Andrei T. - Kovalskii, Andrey M. - Antipina, Liubov Y. - Klimchuk, Daria O. - Manakhov, Anton M. - Al-Qasim, Abdulaziz S. - Shtansky, Dmitry V. **Experimental and theoretical insights into enhanced hydrogen uptake by H2-activated BNOC nanomaterials** [elektronický dokument]. DOI 10.1016/j.ijhydene.2024.11.399 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 97, s. 787-797 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC ; SCIE, s. 787 - 797

2025 [01/20] / **USA** - Jang, Taehwan - Shin, Seung Jae - Lim, Hyung Kyu - Goddard, William A. - Kim, Hyungjun. **DFT-CES2: Quantum Mechanics Based Embedding for Mean-Field QM/MM of Solid-Liquid Interfaces** [elektronický dokument]. DOI 10.1021/jacsau.5c00176 In: **JACS Au**. Washington: American Chemical Society, 2025, Roč. 5, č. 4, s. 2047-2058 [online]. ISSN (online) 2691-3704. - SCO ; WOS CC ; ESCI ; OA, s. 2047 - 2058

2025 [01/20] / **USA** - Hariharan, Seenivasan - Kinge, Sachin - Visscher, Lucas. **Modeling Heterogeneous Catalysis Using Quantum Computers: An Academic and Industry Perspective** [elektronický dokument]. DOI 10.1021/acs.jcim.4c01212

In: **Journal of Chemical Information and Modeling**. Washington, D.C.: American Chemical Society, 2025, Roč. 65, č. 2, s. 472-511 [tlačená forma] [online]. ISSN 1549-9596. ISSN (online) 1549-960X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 472 - 511

2025 [01/20] / **GBR** - Liu, Jiaxuan - Fang, Zhong - Weng, Hongming - Wu, Quansheng. **DPmoire: a tool for constructing accurate machine learning force fields in moiré systems** [elektronický dokument]. DOI 10.1038/s41524-025-01740-0 In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 11, č. 1, art. no. 248 [online]. ISSN (online) 2057-3960. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 248

2025 [01/20] / **USA** - Rajbanshi, Abhinna - Xing, Jie - Gong, Dongliang - Shelton, Williams A. - Jin, Rongying. **An alternative ground state of MnBi2Te4 obtained by magnetic annealing** [elektronický dokument]. DOI 10.1063/5.0284832 In: **APL materials**. Melville: ACA and AIP Publishing, 2025, Roč. 13, č. 10, art. no. 101110 [online]. ISSN (online) 2166-532X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101110

2025 [01/20] / **USA** - Khabibrakhmanov, Almaz - Fedorov, Dmitry V. - Ambrosetti, Alberto - Crain, Jason - Hunt, Katharine L.C. - Johnson, Erin R. - Jordan, Kenneth D. - Góger, Szabolcs - Gori, Matteo - Karimpour, Mohammad Reza - Maurer, Reinhard J. - Sadhukhan, Mainak - Stöhr, Martin - Tkatchenko, Alexandre. **Accurate noncovalent interactions in atomistic systems via quantum Drude oscillators** [elektronický dokument]. DOI 10.1063/5.0281913 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 15, art. no. 151001 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 151001

2025 [01/20] / **GBR** - Joshy, Abin - Wang, Fei - Younus, Sidra - Bai, Keyuan - Larionov, Konstantin V. - Antipina, Liubov Yu - Sorokin, Pavel B. - Ling, Yun - Wei, Jiang. **Scalable synthesis of millimeter-long single crystal Ta2Ni3Se8 Van der Waals nanowires** [elektronický dokument]. DOI 10.1038/s41598-025-03238-7 In: **Scientific reports**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 15, č. 1, art. no. 19535 [online]. ISSN (online) 2045-2322. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 19535

2025 [01/20] / **CHE** - Herbert, John M. - Gray, Montgomery - Liu, Kuan Yu - Carter-Fenk, Kevin. **Extended Symmetry-Adapted Perturbation Theory (XSAPT): A Cubic-Scaling Platform for Computing Accurate Intermolecular Interaction Energies and ab Initio Energy Decomposition Analysis** [elektronický dokument]. DOI 10.1007/430_2025_98 In: **Structure and Bonding Computational Methods for the Analysis of Non-Covalent Interactions**. Cham: Springer Nature, 2025, s. 137-222 [tlačená forma] [online]. ISBN 978-3-032-01542-6. ISBN (online) 978-3-032-01543-3. ISSN 00815993. ISSN (online) 16168550. - SCO, s. 137 - 222

2025 [01/20] / **USA** - Gao, Xiang - Ouyang, Wengen - Kronik, Leeor - Urbakh, Michael - Hod, Oded. **Anisotropic interlayer force fields for van der Waals interfaces: Development and applications** [elektronický dokument]. DOI 10.1063/5.0273079 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 4, art. no. 041001 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 041001

2025 [01/20] / **NLD** - Chepkasov, Ilya V. - Baidyshev, Viktor S. - Kvashnin, Alexander G. **Polyaromatic hydrocarbons as prospective anode materials for metal ion battery** [elektronický dokument]. DOI 10.1016/j.est.2025.116831 In: **Journal of Energy Storage**. Amsterdam: Elsevier, 2025, Roč. 125, art. no. 116831 [tlačená forma] [online]. ISSN 2352-152X. ISSN (online) 2352-1538. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 116831

2025 [01/20] / **GBR** - Garrido Aldea, Jaime - Esteras, Dorye L. - Roche, Stephan - Garcia, Jose H. **Challenges and strategies for first-principles simulations of two-dimensional magnetic phenomena** [elektronický dokument]. DOI 10.1039/d4nr05503a In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 43, s. 24955-24989 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 24955 - 24989

2025 [01/20] / **USA** - Carneiro Queiroz da Silva, G. - Salazar, J. Marcos. **Emergence of an Icosahedral (H2)13 Cluster inside a Pure Silica Faujasite** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c08679 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 14, s. 7031-7039 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 7031 - 7039

2024 [01/20] / **USA** - Shi, Benjamin X. - Wales, David J. - Michaelides, Angelos - Myung, Chang Woo. **Going for Gold(-Standard): Attaining Coupled Cluster Accuracy in Oxide-Supported Nanoclusters** [elektronický dokument]. DOI 10.1021/acs.jctc.4c00379 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 12, s. 5306-5316 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 5306 - 5316

2024 [01/20] / **USA** - Hoja, Johannes - List, Alexander - Boese, A. Daniel. **Multimer Embedding Approach for Molecular Crystals up to Harmonic Vibrational Properties** [elektronický dokument]. DOI 10.1021/acs.jctc.3c01082 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 1, s. 357-367 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 357 - 367

2024 [01/20] / **USA** - Cossu, F. - Nafday, D. - Palotás, K. - Biderang, M. - Kim, H. S. - Akbari, A. - Di Marco, I. **Stacking of charge-density waves in 2 H-NbSe2 bilayers**. DOI 10.1103/PhysRevResearch.6.043111 In: **Physical Review Research**. New York: American Institute of Physics. American Physical Society, 2024, Roč. 6, č. 4, art. no. 043111 [online]. ISSN 2643-1564. - SCO ; WOS CC, s. art. no. 043111

2023 [01/20] / **GBR** - Gori, Matteo - Kurian, Philip - Tkatchenko, Alexandre. **Second quantization of many-body dispersion interactions for chemical and biological systems** [elektronický dokument]. DOI 10.1038/s41467-023-43785-z In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2023, Roč. 14, č. 1, art. no. 8218 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s. art. no. 8218

2023 [01/20] / **USA** - Nickerson, Cameron J. - Bryenton, Kyle R. - Price, Alastair J.A. - Johnson, Erin R. **Comparison of Density-Functional Theory Dispersion Corrections for the DES15K Database** [elektronický dokument]. DOI 10.1021/acs.jpca.3c04332 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2023, Roč. 127, č. 41, s. 8712-8722 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO ; CCC ; WOS CC, s. 8712 - 8722

2023 [01/20] / **USA** - Cheng, Ying Xing - Verstraelen, Toon. **The significance of fluctuating charges for molecular polarizability and dispersion coefficients** [elektronický dokument]. DOI 10.1063/5.0163842 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 9, art. no. 094111 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 094111

2023 [01/20] / **USA** - Zhang, Yue Jiao - Ren, Yin Ti - Lv, Xiao Huan - Zhao, Xiao Lin - Yang, Rui - Wang, Nie Wei - Jin, Chen Dong - Zhang, Hu - Lian, Ru Qian - Gong, Peng Lai - Wang, Rui Ning - Wang, Jiang Long - Shi, Xing Qiang. **Momentum matching and band-alignment type in van der Waals heterostructures: Interfacial effects and materials screening** [elektronický dokument]. DOI 10.1103/PhysRevB.107.235420 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 107, č. 23, art. no. 235420 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 235420

2023 [01/20] / **GBR** - Tu, Nguyen Thien Phuc - Rezajooei, Nazanin - Johnson, Erin R. - Rowley, Christopher N. **A neural network potential with rigorous treatment of long-range dispersion** [elektronický dokument]. DOI 10.1039/d2dd00150k In: **Digital Discovery**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 2, č. 3, s. 718-727. ISSN (online) 2635098X. - SCO ; WOS CC, s. 718 - 727

2023 [01/20] / **USA** - Feng, Chaoqiang - Xi, Jin - Zhang, Yaolong - Jiang, Bin - Zhou, Yong. **Accurate and Interpretable Dipole Interaction Model-Based Machine Learning for Molecular Polarizability** [elektronický dokument]. DOI 10.1021/acs.jctc.2c01094 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2023, Roč. 19, č. 4, s. 1207-1217 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 1207 - 1217

2023 [01/20] / **USA** - Adeleke, Adebayo A. - Johnson, Erin R. **Effects of dispersion corrections on the theoretical description of bulk metals** [elektronický dokument]. DOI 10.1103/PhysRevB.107.064101 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 107, č. 6, art. no. 064101 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 064101

2023 [01/20] / **USA** - Dobson, John F. - Ambrosetti, Alberto. **MBD + C: How to Incorporate Metallic Character into Atom-Based Dispersion Energy Schemes** [elektronický dokument]. DOI 10.1021/acs.jctc.3c00353 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2023, Roč. 19, č. 18, s. 6434-6451 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; WOS CC, s. 6434 - 6451

2023 [01/20] / **CHE** - Valenti, Sofia - Cazorla, Claudio - Romanini, Michela - Tamarit, Josep Lluís - Macovez, Roberto. **Eutectic Mixture Formation and Relaxation Dynamics of Coamorphous Mixtures of Two Benzodiazepine Drugs** [elektronický dokument]. DOI 10.3390/pharmaceutics15010196 In: **Pharmaceutics**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 15, č. 1, art. no. 196 [online]. ISSN (online) 1999-4923. - SCO ; WOS CC, s. art. no. 196

2023 [01/20] / **USA** - Poier, Pier Paolo - Adjoua, Olivier - Lagardère, Louis - Piquemal, Jean Philip. **Generalized Many-Body Dispersion Correction through Random-Phase Approximation for Chemically Accurate Density Functional Theory** [elektronický dokument]. DOI 10.1021/acs.jpclett.2c03722 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 6, s. 1609-1617 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 1609 - 1617

2023 [01/20] / **USA** - Chepkasov, Ilya V. - Baidyshev, Viktor S. - Kvashnin, Alexander G. **Structure-driven tuning of O and CO adsorption on AuCu nanoparticles: A density functional theory study** [elektronický dokument]. DOI 10.1103/PhysRevB.108.205414 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 108, č. 20, art. no. 205414 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 205414

2023 [01/20] / **GBR** - Delachaux, F. - Hessou, E. P. - Vallières, C. - Monnier, H. - Badawi, M. **A dispersion-corrected DFT method for zeolite-based CO2/N2separation: Assessment and application** [elektronický dokument]. DOI 10.1016/j.jece.2022.109052 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2023, Roč. 11, č. 1, art. no. 109052 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s.

2023 [01/20] / **USA** - Poier, Pier Paolo - Lagardère, Louis - Piquemal, Jean Philip. **Smooth particle mesh Ewald-integrated stochastic Lanczos many-body dispersion algorithm** [elektronický dokument]. DOI 10.1063/5.0166476 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 15, art. no. 154109 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 154109

2023 [01/20] / **USA** - Hermann, Jan - Stöhr, Martin - Góger, Szabolcs - Chaudhuri, Shayantan - Aradi, Bálint - Maurer, Reinhard J. - Tkatchenko, Alexandre. **libMBD: A general-purpose package for scalable quantum many-body dispersion calculations** [elektronický dokument]. DOI 10.1063/5.0170972 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 17, art. no. 174802 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 174802

2023 [01/20] / **GBR** - Manz, Thomas A. **Density-Derived Electrostatic and Chemical Methods** [elektronický dokument]. DOI 10.1016/B978-0-12-821978-2.00072-6 In: **Comprehensive Computational Chemistry**. Oxford: Elsevier, 2023, s.

362-405 [tlačená forma] [online]. ISBN 978-0-12-821978-2. ISBN (online) 978-0-12-823256-9. ISBN (chybné) 978-0-12-823256-9. - SCO, s. 362 - 405

2023 [01/20] / **USA** - Bryenton, Kyle R. - Johnson, Erin R. **Many-body dispersion in model systems and the sensitivity of self-consistent screening** [elektronický dokument]. DOI 10.1063/5.0142465 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 20, art. no. 204110 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 204110

ADC_047: / Gould, Tim (Autor) (60%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%): **C-6 Coefficients and Dipole Polarizabilities for All Atoms and Many Ions in Rows 1-6 of the Periodic Table**. – text, tab., obr. – [recenzované]. – DOI 10.1021/acs.jctc.6b00361. – CCC ; SCO ; OA ; WOS CC.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 12, č. 8 (2016), s. 3603-3613 [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
Lit.: 55
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,505 - 2016
SJR: 2,711 - 2016
CiteScore: 9,6 - 2016

Ohlasy (116):
2025 [01/20] / **USA** - Cheng, Ying Xing. **Relativistic and Electron-Correlation Effects in Static Dipole Polarizabilities for Group 11 Elements** [elektronický dokument]. DOI 10.1021/acs.jpca.4c07189 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2025, Roč. 129, č. 7, s. 1830-1840 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO ; WOS CC, s. 1830 - 1840

2025 [01/20] / **GBR** - Cheng, Ying Xing. **Relativistic and electron-correlation effects in static dipole polarizabilities for group 12 elements** [elektronický dokument]. DOI 10.1039/d4cp04754k In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 6, s. 3430-3441 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 3430 - 3441

2025 [01/20] / **NLD** - Davis, Megan C. - Kort-Kamp, Wilton J.M. - Holby, Edward F. - Zelenay, Piotr - Matanovic, Ivana. **Computational screening of transition metal-nitrogen-carbon materials as electrocatalysts for CO2 reduction** [elektronický dokument]. DOI 10.1016/j.electacta.2024.145357 In: **Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2025, Roč. 510, art. no. 145357 [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 145357

2025 [01/20] / **USA** - Koots, Rian - Ding, Grace - Pérez-Ríos, Jesús. **Direct three-body atom recombination: Halogen atoms** [elektronický dokument]. DOI 10.1063/5.0275410 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 163, č. 2, art. no. 024307 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 024307

2025 [01/20] / **GBR** - Mitev, Georgi B. - Bowesman, Charles A. - Zhang, Jingxin - Yurchenko, Sergei N. - Tennyson, Jonathan. **ExoMol line lists – LXI. A trihybrid line list for rovibronic transitions of the hydroxyl radical (OH)**

[elektronický dokument]. DOI 10.1093/mnras/stae2803 In: **Monthly Notices of the Royal Astronomical Society**: a journal of the Royal Astronomical Society. Oxford: Oxford University Press, 2025, Roč. 536, č. 4, s. 3401-3420 [tlačená forma] [online]. ISSN 0035-8711. ISSN (online) 1365-2966. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 3401 - 3420

2025 [01/20] / **GBR** - Matveev, Andrei T. - Kovalskii, Andrey M. - Antipina, Liubov Y. - Klimchuk, Daria O. - Manakhov, Anton M. - Al-Qasim, Abdulaziz S. - Shtansky, Dmitry V. **Experimental and theoretical insights into enhanced hydrogen uptake by H2-activated BNOC nanomaterials** [elektronický dokument]. DOI 10.1016/j.ijhydene.2024.11.399 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2025, Roč. 97, s. 787-797 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO ; CCC ; WOS CC ; SCIE, s. 787 - 797

2025 [01/20] / **USA** - Kelsall, Jack - Radić, Aleksandar - Ellis, John - Ward, David J. - Jardine, Andrew P. **Minimizing interference in low-pressure supersonic beam sources** [elektronický dokument]. DOI 10.1063/5.0247870 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2025, Roč. 162, č. 9, art. no. 094304 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 094304

2025 [01/20] / **USA** - Jang, Taehwan - Shin, Seung Jae - Lim, Hyung Kyu - Goddard, William A. - Kim, Hyungjun. **DFT-CES2: Quantum Mechanics Based Embedding for Mean-Field QM/MM of Solid-Liquid Interfaces** [elektronický dokument]. DOI 10.1021/jacsau.5c00176 In: **JACS Au**. Washington: American Chemical Society, 2025, Roč. 5, č. 4, s. 2047-2058 [online]. ISSN (online) 2691-3704. - SCO ; WOS CC ; ESCI ; OA, s. 2047 - 2058

2025 [01/20] / **USA** - He, Xin - Liu, Wenjian - Ayers, Paul W. - Liu, Shubin. **Distinguishing Aromaticity from Antiaromaticity with Information-Theoretic and Energetic Information Quantities and Their Links to Molecular Properties** [elektronický dokument]. DOI 10.1021/acs.jpca.5c06745 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2025, Roč. 129, č. 51, s. 11820-11833 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO ; CCC ; WOS CC ; SCIE, s. 11820 - 11833

2025 [01/20] / **USA** - Heikkinen, Niko - Keskiväli, Laura - Kuutti, Krista - Ikonen, Rasmus - Baraiya, Bhumi A. - Korpelin, Ville - Lahtinen, Manu - Kanervo, Jaana - Heikkilä, Mikko J. - Ye, Xinwei - Weckhuysen, Bert M. - Honkala, Karoliina - Lehtonen, Juha - Reinikainen, Matti. **Production of Isobutylene from Syngas – Isosynthesis Over Zirconia-Based Catalysts** [elektronický dokument]. DOI 10.1007/s11244-025-02184-y In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2025, Roč. 68, č. 20, s. 2418-2432 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 2418 - 2432

2025 [01/20] / **GBR** - Shaidu, Yusuf - Naik, Mit H. - Louie, Steven G. - Neaton, Jeffrey B. **Transferable dispersion-aware machine learning interatomic potentials for multilayer transition metal dichalcogenide heterostructures** [elektronický dokument]. DOI 10.1038/s41524-025-01761-9 In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 11, č. 1, art. no. 273 [online]. ISSN (online) 2057-3960. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 273

2025 [01/20] / **USA** - Flores Alfaro, Gabriel M. - Shneider, Mikhail N. - Gerakis, Alexandros. **Coherent Brillouin scattering in weakly ionized plasmas** [elektronický dokument]. DOI 10.1063/5.0285222 In: **Physics of Plasmas**. Melville: American Institute of Physics, 2025, Roč. 32, č. 11, art. no. 113513 [tlačená forma] [online]. ISSN 1070-664X. ISSN (online) 1089-7674. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 113513

2025 [01/20] / **NLD** - Kaur, Harpreet - Jyoti - Shukla, Neelam - Arora, Bindiya. **Two- and three-body dispersion coefficients for interaction of Cu and Ag atoms with Group I, II, and XII elements** [elektronický dokument]. DOI 10.1016/j.chemphys.2025.112731 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2025, Roč. 596, art. no. 112731 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 112731

2025 [01/20] / **GBR** - Liu, Jiaxuan - Fang, Zhong - Weng, Hongming - Wu, Quansheng. **DPmoire: a tool for constructing accurate machine learning force fields in moiré systems** [elektronický dokument]. DOI 10.1038/s41524-025-01740-0 In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 11, č. 1, art. no. 248 [online]. ISSN (online) 2057-3960. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 248

2025 [01/20] / **USA** - Rajbanshi, Abhinna - Xing, Jie - Gong, Dongliang - Shelton, Williams A. - Jin, Rongying. **An alternative ground state of MnBi2Te4 obtained by magnetic annealing** [elektronický dokument]. DOI 10.1063/5.0284832 In: **APL materials**. Melville: ACA and AIP Publishing, 2025, Roč. 13, č. 10, art. no. 101110 [online]. ISSN (online) 2166-532X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101110

2025 [01/20] / **GBR** - Garrido Aldea, Jaime - Esteras, Dorye L. - Roche, Stephan - Garcia, Jose H. **Challenges and strategies for first-principles simulations of two-dimensional magnetic phenomena** [elektronický dokument]. DOI 10.1039/d4nr05503a In: **Nanoscale**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 17, č. 43, s. 24955-24989 [tlačená forma] [online]. ISSN 2040-3364. ISSN (online) 2040-3372. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 24955 - 24989

2024 [01/20] / **USA** - Koots, R. - Brown, G. - Pérez-Ríos, J. **Sulfur recombination: A direct approach** [elektronický dokument]. DOI 10.1063/5.0222273 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2024, Roč. 161, č. 8, art. no. 084302 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 084302

2024 [01/20] / **NLD** - Zare, Mehdi - Kots, Pavel A. - Hinton, Zachary R. - Epps, Thomas H. - Korley, La Shanda T.J. - Caratzoulas, Stavros - Vlachos, Dionisios G. **Effect of reaction media on hydrogenolysis of polyethylene plastic waste: Polymer-surface interactions in small alkane/polymer blends**. DOI 10.1016/j.apcatb.2024.123969 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2024, Roč. 351, art. no. 123969 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s. art. no. 123969

2024 [01/20] / **GBR** - Venkatramana, Vishwesh - Carvalho, Patricia Almeida. **Accurate space-group prediction from composition** [elektronický dokument]. DOI 10.1107/S1600576724004497 In: **Journal of applied crystallography**. Chester: International Union of Crystallography, 2024, Roč. 57, č. Pt 4, s. 975-985 [tlačená forma] [online]. ISSN 0021-8898. ISSN (online) 1600-5767. - SCO ; CCC ; WOS CC, s. 975 - 985

2024 [01/20] / **GBR** - Rehr, J. J. - Kas, J. J. **Real-space multiple-scattering approach to the van der Waals interaction** [elektronický dokument]. DOI 10.1088/2516-1075/ad3591 In: **Electronic Structure**. Bristol: Institute of Physics. IOP Publishing, 2024, Roč. 6, č. 1, art. no. 017002. ISSN (online) 2516-1075. - SCO ; WOS CC, s. art. no. 017002

2024 [01/20] / **GBR** - Yang, Chongyao - Wu, Wei - Choy, Kwang Leong. **First-principles studies of oxygen interstitial dopants in RbPbI3 halide for perovskite solar cells** [elektronický dokument]. DOI 10.1088/1361-651X/ad104f In: **Modelling and simulation in materials science and engineering**. Bristol: Institute of Physics. IOP Publishing, 2024, Roč. 32, č. 1, art. no. 015007 [online] [tlačená forma]. ISSN 0965-0393. ISSN (online) 1361-651X. - SCO ; CCC ; WOS CC, s. art. no. 015007

2024 [01/20] / **RUS** - Sokurov, Aslan A. **Numerical calculation of integrals in the density functional theory in the electron gas approximation using CUDA technology** [elektronický dokument]. DOI 10.21638/spbu10.2024.303 In: **Vestnik Sankt-Peterburgskogo Universiteta, Prikladnaya Matematika, Informatika, Protsessy Upravleniya**, 2024, Roč. 20, č. 3, s. 335-349. ISSN 18119905. ISSN (online) 25422251. - SCO, s. 335 - 349

2024 [01/20] / **USA** - Góger, Szabolcs - Karimpour, Mohammad Reza - Tkatchenko, Alexandre. **Four-Dimensional Scaling of Dipole Polarizability: From Single-Particle Models to Atoms and Molecules** [elektronický dokument]. DOI 10.1021/acs.jctc.4c00582 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society,

2024, Roč. 20, č. 15, s. 6621-6631 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; WOS CC, s. 6621 - 6631

2024 [01/20] / **USA** - Cheng, Ying Xing. **Relativistic and electron-correlation effects in static dipole polarizabilities for main-group elements** [elektronický dokument]. DOI 10.1103/PhysRevA.110.042805 In: **Physical Review A**. Maryland: American Institute of Physics, 2024, Roč. 110, č. 4., art. no. 042805 [tlačená forma] [online]. ISSN 2469-9926. ISSN (online) 2469-9934. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Dobson, John F. - Ambrosetti, Alberto. **MBD + C: How to Incorporate Metallic Character into Atom-Based Dispersion Energy Schemes** [elektronický dokument]. DOI 10.1021/acs.jctc.3c00353 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2023, Roč. 19, č. 18, s. 6434-6451 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; WOS CC, s. 6434 - 6451

2023 [01/20] / **USA** - Kusaba, Minoru - Hayashi, Yoshihiro - Liu, Chang - Wakiuchi, Araki - Yoshida, Ryo. **Representation of materials by kernel mean embedding** [elektronický dokument]. DOI 10.1103/PhysRevB.108.134107 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2023, Roč. 108, č. 13, art. no. 134107 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC, s. art. no. 134107

2023 [01/20] / **USA** - Dochain, A. - Andrianarijaona, V. M. - Urbain, X. **Isotope effect for the mutual neutralization reaction at low collision energies: He++ H-** [elektronický dokument]. DOI 10.1103/PhysRevA.108.042809 In: **Physical Review A**. Maryland: American Institute of Physics, 2023, Roč. 108, č. 4, art. no. 042809 [tlačená forma] [online]. ISSN 2469-9926. ISSN (online) 2469-9934. - SCO, s. art. no. 042809

2023 [01/20] / **USA** - Battard, T. - Lahs, S. - Crépin, C. - Comparat, D. **Cesium atoms in a cryogenic argon matrix** [elektronický dokument]. DOI 10.1103/PhysRevA.108.042820 In: **Physical Review A**. Maryland: American Institute of Physics, 2023, Roč. 108, č. 4, art. no. 042820 [tlačená forma] [online]. ISSN 2469-9926. ISSN (online) 2469-9934. - SCO ; CCC ; WOS CC, s. art. no. 042820

2023 [01/20] / **USA** - Góger, Szabolcs - Khabibrakhmanov, Almaz - Vaccarelli, Ornella - Fedorov, Dmitry V. - Tkatchenko, Alexandre. **Optimized Quantum Drude Oscillators for Atomic and Molecular Response Properties** [elektronický dokument]. DOI 10.1021/acs.jpclett.3c01221 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 27, s. 6217-6223 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 6217 - 6223

2023 [01/20] / **CHN** - Sharipov, Alexander S. - Loukhovitski, Boris I. **A simple semiempirical model for the static polarizability of ions** [elektronický dokument]. DOI 10.1088/1674-1056/acd2b2 In: **Chinese Physics B**. Peking: Chinese Physical Society, 2023, Roč. 32, č. 8, art. no. 083301 [tlačená forma] [online]. ISSN 1674-1056. ISSN (online) 2058-3834. - SCO ; CCC ; WOS CC, s. art. no. 083301

2023 [01/20] / **USA** - Saeedimasine, Marzieh - Grote, Fredrik - Lyubartsev, Alexander P. **Ab Initio Derived Classical Force Field for Molecular Dynamics Simulations of ZnO Surfaces in Biological Environment** [elektronický dokument]. DOI 10.1021/acs.jpca.3c00424 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2023, Roč. 127, č. 25, s. 5446-5457 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO ; CCC ; WOS CC, s. 5446 - 5457

2023 [01/20] / **GBR** - Yan, Pei Gen - Babb, James F. **Fine-structure transitions of Si and S induced by collisions with atomic hydrogen** [elektronický dokument]. DOI 10.1093/mnras/stad1050 In: **Monthly Notices of the Royal Astronomical Society**: a journal of the Royal Astronomical Society. Oxford: Oxford University Press, 2023, Roč. 522, č. 1, s. 1265-1269 [tlačená forma] [online]. ISSN 0035-8711. ISSN (online) 1365-2966. - SCO ; CCC ; WOS CC, s. 1265 - 1269

2023 [01/20] / **USA** - Korpelin, Ville - Sahoo, Gokarneswar - Ikonen, Rasmus - Honkala, Karoliina. **ReOx as a Bronsted acidic modifier in glycerol hydrodeoxygenation: Computational insight into the balance between acid and metal catalysis** [elektronický dokument]. DOI 10.1016/j.jcat.2023.03.032 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2023, Roč. 422, s. 12-23 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 12 - 23

2023 [01/20] / **USA** - Mendonça, João P. - Jachymski, Krzysztof. **Quantum simulation of extended electron-phonon-coupling models in a hybrid Rydberg atom setup** [elektronický dokument]. DOI 10.1103/PhysRevA.107.032808 In: **Physical Review A**. Maryland: American Institute of Physics, 2023, Roč. 107, č. 3, art. no. 032808 [tlačená forma] [online]. ISSN 2469-9926. ISSN (online) 2469-9934. - SCO ; CCC ; WOS CC, s. art. no. 032808

2023 [01/20] / **GBR** - Silvestrelli, Pier Luigi - Subashchandrabose, S. - Seif, Abdolvahab - Ambrosetti, Alberto. **Screening and antiscreening in fullerene-like cages: Dipole-field amplification with ionic nanocages** [elektronický dokument]. DOI 10.1016/j.cartre.2022.100242 In: **Carbon trends**. [Oxford]: Elsevier, 2023, Roč. 10, art. no. 100242 [online]. ISSN (online) 2667-0569. - SCO ; WOS CC, s. art. no. 100242

2023 [01/20] / **USA** - Sohail, B. - Blowey, P. J. - Rochford, L. A. - Ryan, P. T.P. - Duncan, D. A. - Lee, T. L. - Starrs, P. - Costantini, G. - Woodruff, D. P. - Maurer, R. J. **Donor-Acceptor Co-Adsorption Ratio Controls the Structure and Electronic Properties of Two-Dimensional Alkali-Organic Networks on Ag(100)** [elektronický dokument]. DOI 10.1021/acs.jpcc.2c08688 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 5, s. 2716-2727 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; WOS CC, s. 2716 - 2727

2023 [01/20] / **CHN** - Sharipov, Alexander S. - Pelevkin, Alexey V. - Loukhovitski, Boris I. **A simple semiempirical model for the static polarizability of electronically excited atoms and molecules** [elektronický dokument]. DOI 10.1088/1674-1056/ac8342 In: **Chinese Physics B**. Peking: Chinese Physical Society, 2023, Roč. 32, č. 4, art. no. 043301 [tlačená forma] [online]. ISSN 1674-1056. ISSN (online) 2058-3834. - SCO ; WOS CC, s.

2022 [01/20] / **GBR** - Shin, S.-J. - Kim, D.H. - Bae, G. - Ringe, S. - Choi, H. - Lim, H.-K. - Choi, C.H. - Kim, H. **On the importance of the electric double layer structure in aqueous electrocatalysis** [elektronický dokument] In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2022, Roč. 13, č. 1, [online]. ISSN (online) 2041-1723. - SCO, s. Art. No. 174

2022 [01/20] / **GBR** - Sheng, X. - Tang, K.T. - Toennies, J.P. **A semiempirical potential for alkali halide diatoms with damped interactions I. Rittner potential** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 40, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 24823 - 24833

2022 [01/20] / **USA** - Ricci, M. - Silvestrelli, P.L. - Dobson, J.F. - Ambrosetti, A. **Exact Sum-Rule Approach to Polarizability and Asymptotic van der Waals Functionals-Derivation of Exact Single-Particle Benchmarks** In: **Journal of Physical Chemistry Letters**, 2022, Roč. 13, č. 35. - SCO, s. 8298 - 8304

2022 [01/20] / **USA** - Abella, L. - Autschbach, J. **Density Functional Response Calculations of Dispersion Coefficients C6and C9of Closed- and Open-Shell Systems** In: **Journal of Physical Chemistry A**, 2022, Roč. 126, č. 34. - SCO, s. 5821 - 5831

2022 [01/20] / **USA** - Florez, E. - Smits, O.R. - Mewes, J.-M. - Jerabek, P. - Schwerdtfeger, P. **From the gas phase to the solid state: The chemical bonding in the superheavy element flerovium** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2022, Roč. 157, č. 6, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 064304

2022 [01/20] / **NLD** - da Silva, R.S. - Ballester, M.Y. **Radiative lifetimes of the doublet states of 107Ag16O: A configuration interaction study** [elektronický dokument] In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2022, Roč. 557, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO, s. Art. No. 111480

2022 [01/20] / **USA** - Mahato, D. - Sharma, L. - Srivastava, R. **Fully relativistic study on electron impact elastic scattering from Nq+ (q = 1-3), Na+, Arq+ (q = 1-3, 7-8), and Xeq+ (q = 2-6, 8)** In: **: International journal of quantum chemistry,** 2022, Roč. 122, č. 1. - SCO, s. Art. No. e26815

2022 [01/20] / **GBR** - da Silva, R.S. - Ballester, M.Y. **Multireference configuration interaction calculations on the FeS molecule** [elektronický dokument] In: **Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2022, Roč. 120, č. 13, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCO, s. Art. No. e2096142

2022 [01/20] / **NLD** - Shukla, N. - Kaur, H. - Arora, B. - Srivastava, R. **Two-dipole and three-dipole interaction coefficients of group XII elements** In: **Physica B: Condensed Matter**, 2022, Roč. 624. - SCO, s. Art. No. 413422

2022 [01/20] / **USA** - Braeckevelt, T. - Goeminne, R. - Vandenhaute, S. - Borgmans, S. - Verstraelen, T. - Steele, J.A. - Roeffaers, M.B.J. - Hofkens, J. - Rogge, S.M.J. - van Speybroeck, V. **Accurately Determining the Phase Transition Temperature of CsPbI3via Random-Phase Approximation Calculations and Phase-Transferable Machine Learning Potentials** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 19, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 8561 - 8576

2022 [01/20] / **GBR** - Holland, J. - Bhandari, A. - Kramer, D. - Milman, V. - Hanke, F. - Skylaris, C.-K. **Ab initio study of lithium intercalation into a graphite nanoparticle** [elektronický dokument] In: **Materials advances**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 3, č. 23, [online]. ISSN (online) 2633-5409. - SCO, s. 8469 - 8484

2022 [01/20] / **USA** - Chepkasov, I.V. - Smet, J.H. - Krasheninnikov, A.V. **Single- and Multilayers of Alkali Metal Atoms inside Graphene/MoS2Heterostructures: A Systematic First-Principles Study** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 37. - SCO, s. 15558 - 15564

2022 [01/20] / **DEU** - Emrem, B. - Kempt, R. - Finzel, K. - Heine, T. **London Dispersion-Corrected Density Functionals Applied to van der Waals Stacked Layered Materials: Validation of Structure, Energy, and Electronic Properties** [elektronický dokument] In: **Advanced theory and simulations**. Weinheim: John Wiley & Sons. Wiley-VCH, 2022, Roč. 5, č. 7, [online]. ISSN (online) 2513-0390. - SCO, s. Art. No. 2200055

2022 [01/20] / **USA** - Gray, M. - Herbert, J.M. **Comprehensive Basis-Set Testing of Extended Symmetry-Adapted Perturbation Theory and Assessment of Mixed-Basis Combinations to Reduce Cost** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 4, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 2308 - 2330

2022 [01/20] / **USA** - Liu, X. - Chen, F. - Guo, W. **Ionic contribution to van der Waals interaction of polar compounds** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 105, č. 12, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 125411

2021 [01/20] / **USA** - Burrows, A. - Cooper, S. - Schwerdtfeger, P. **Instability of the body-centered cubic lattice within the sticky hard sphere and Lennard-Jones model obtained from exact lattice summations** [elektronický dokument] In: **Physical Review E**: Statistical, nonlinear, biological, and soft matter physics. College Park: American Institute of Physics.

American Physical Society, 2021, Roč. 104, č. 3, [tlačená forma] [online] [CD-ROM]. ISSN 2470-0045. ISSN (online) 2470-0053. - SCO, s. Art. No. 035306

2021 [01/20] / **USA** - Hellgren, M. - Baguet, L. **Random phase approximation with exchange for an accurate description of crystalline polymorphism** In: **Physical Review Research**. New York: American Institute of Physics. American Physical Society, 2021, Roč. 3, č. 3, [online]. ISSN 2643-1564. - SCO, s. Art. No. 033263

2021 [01/20] / **USA** - Vaccarelli, O. - Fedorov, D.V. - Stohr, M. - Tkatchenko, A. **Quantum-mechanical force balance between multipolar dispersion and Pauli repulsion in atomic van der Waals dimers** In: **Physical Review Research**. New York: American Institute of Physics. American Physical Society, 2021, Roč. 3, č. 3, [online]. ISSN 2643-1564. - SCO, s. Art. No. 033181

2021 [01/20] / **USA** - Kaur, H. - Shukla, N. - Srivastava, R. - Arora, B. **Dispersion coefficients for physisorption of heavy ions and atoms with graphene and carbon nanotubes** [elektronický dokument] In: **Physical Review A**: Atomic, molecular, and optical physics and quantum information. College Park: American Institute of Physics, 2021, Roč. 104, č. 1, [tlačená forma] [online]. ISSN 1050-2947. ISSN (online) 1094-1622. - SCO, s. Art. No. 012806

2021 [01/20] / **GBR** - Rouse, I. - Power, D. - Brandt, E.G. - Schneemilch, M. - Kotsis, K. - Quirke, N. - Lyubartsev, A.P. - Lobaskin, V. **First principles characterisation of bio-nano interface** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 24, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 13473 - 13482

2021 [01/20] / **USA** - Irikura, K.K. **Polarizability of atomic Pt, Pt+, and Pt-** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 174302

2021 [01/20] / **USA** - Kooi, D.P. - Weckman, T. - Gori-Giorgi, P. **Dispersion without Many-Body Density Distortion: Assessment on Atoms and Small Molecules** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 4, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 2283 - 2293

2021 [01/20] / **USA** - Welsh, I.D. - Crittenden, D.L. **New atoms-in-molecules dispersion models for use in ab initio derived force fields** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 0037157

2021 [01/20] / **NLD** - Cassar, D.R. **ViscNet: Neural network for predicting the fragility index and the temperature-dependency of viscosity** [elektronický dokument] In: **Acta Materialia**. Amsterdam: Acta Materialia, 2021, Roč. 206, [tlačená forma] [online]. ISSN 1359-6454. ISSN (online) 1873-2453. - SCO, s. Art. No. 116602

2021 [01/20] / **USA** - Ehn, L. - Cernusak, I. **Atomic and ionic polarizabilities of B, C, N, O, and F** In: **: International journal of quantum chemistry,** 2021, Roč. 121, č. 4. - SCO, s. Art. No. e26467

2021 [01/20] / **USA** - Vazquez-Fernandez, I. - Druzbicki, K. - Fernandez-Alonso, F. - Mukhopadhyay, S. - Nockemann, P. - Parker, S.F. - Rudic, S. - Stana, S.-M. - Tomkinson, J. - Yeadon, D.J. - Seddon, K.R. - Plechkova, N.V. **Spectroscopic Signatures of Hydrogen-Bonding Motifs in Protonic Ionic Liquid Systems: Insights from Diethylammonium Nitrate in the Solid State** In: **Journal of Physical Chemistry C**, 2021, Roč. 125, č. 44. - SCO, s. 24463 - 24476

2021 [01/20] / **USA** - Ouyang, W. - Sofer, R. - Gao, X. - Hermann, J. - Tkatchenko, A. - Kronik, L. - Urbakh, M. - Hod, O. **Anisotropic interlayer force field for transition metal dichalcogenides: The case of molybdenum disulfide** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society,

2021, Roč. 17, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 7237 - 7245

2021 [01/20] / **CHE** - Annies, S. - Panosetti, C. - Voronenko, M. - Mauth, D. - Rahe, C. - Scheurer, C. **Accessing structural, electronic, transport and mesoscale properties of li-gics via a complete dftb model with machine-learned repulsion potential** In: M**aterials**, 2021, Roč. 14, č. 21. - SCO, s. Art. No. 6633

2021 [01/20] / **USA** - Jana, S. - Myneni, H. - Smiga, S. - Constantin, L.A. - Samal, P. **Benchmark test of a dispersion corrected revised Tao-Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 155, č. 11, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 114102

2021 [01/20] / **USA** - Price, A.J.A. - Bryenton, K.R. - Johnson, E.R. **Requirements for an accurate dispersion-corrected density functional** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 23, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 230902

2021 [01/20] / **USA** - Rossi, M. **Progress and challenges in ab initio simulations of quantum nuclei in weakly bonded systems** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 170902

2021 [01/20] / **GBR** - Hofmann, O.T. - Zojer, E. - Hormann, L. - Jeindl, A. - Maurer, R.J. **First-principles calculations of hybrid inorganic-organic interfaces: From state-of-the-art to best practice** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 8132 - 8180

2020 [01/12] / **NLD** - Berro, Y. - Badawi, M. - El Haj Hassan, F. - Kassir, M. - Tielens, F. **Water-silanol interactions on the amorphous silica surface: A dispersion-corrected DFT investigation** [elektronický dokument] In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2020, Roč. 320, [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. Art. No. 114496

2020 [01/12] / **USA** - Otero-De-La-Roza, A. - Johnson, E.R. **Application of XDM to ionic solids: The importance of dispersion for bulk moduli and crystal geometries** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 054121

2020 [01/12] / **USA** - Tang, H. - Chowdhury, S.T.U.R. - Tao, J. - Perdew, J.P. **Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 101, č. 19, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 195426

2020 [01/12] / **GBR** - Caldeweyher, E. - Mewes, J.-M. - Ehlert, S. - Grimme, S. **Extension and evaluation of the D4 London-dispersion model for periodic systems** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 16, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 8499 - 8512

2020 [01/12] / **GBR** - Rehak, F.R. - Piccini, G. - Alessio, M. - Sauer, J. **Including dispersion in density functional theory for adsorption on flat oxide surfaces, in metal-organic frameworks and in acidic zeolites** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 14, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 7577 - 7585

2020 [01/12] / **USA** - Hermann, J. - Tkatchenko, A. **Density Functional Model for van der Waals Interactions: Unifying Many-Body Atomic Approaches with Nonlocal Functionals** [elektronický dokument] In: **Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 124, č. 14, [tlačená forma] [online]. ISSN 0031-9007. ISSN (online) 1079-7114. - SCO, s. Art. No. 146401

2020 [01/12] / Otero-De-La-Roza, A. - Leblanc, L.M. - Johnson, E.R. **Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately** In: **Journal of Physical Chemistry Letters**, 2020, Roč. 11, č. 6. - SCO, s. 2298 - 2302

2020 [01/12] / **USA** - Liu, X. - Yang, J. - Guo, W. **Semiempirical van der Waals method for two-dimensional materials with incorporated dielectric functions** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 101, č. 4, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 045428

2020 [01/12] / **USA** - Hourahine, B. - Aradi, B. - Blum, V. - Bonafe, F. - Buccheri, A. - Camacho, C. - Cevallos, C. - Deshaye, M.Y. - Dumitric, T.A. - Dominguez, A. - Ehlert, S. - Elstner, M. **DFTB+, a software package for efficient approximate density functional theory based atomistic simulations** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 152, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 124101

2020 [01/12] / **USA** - Jana, S. - Patra, A. - Smiga, S. - Constantin, L.A. - Samal, P. **Insights from the density functional performance of water and water-solid interactions: SCAN in relation to other meta-GGAs** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 21, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 214116

2020 [01/12] / **USA** - Pendse, A. - Shirol, S. - Tiwari, S. - Wuster, S. **Generation and decoherence of soliton spatial superposition states** [elektronický dokument] In: **Physical Review A**: Atomic, molecular, and optical physics and quantum information. College Park: American Institute of Physics, 2020, Roč. 102, č. 5, [tlačená forma] [online]. ISSN 1050-2947. ISSN (online) 1094-1622. - SCO, s. Art. No. 053322

2020 [01/12] / Chen, J. - Hariharan, S. - Meyer, J. - Guo, H. **Potential Energy Landscape of CO Adsorbates on NaCl(100) and Implications in Isomerization of Vibrationally Excited CO** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 35. - SCO, s. 19146 - 19156

2020 [01/12] / **USA** - Visentin, G. - Kalinina, I.S. - Buchachenko, A.A. **Extended combination rule for like-atom dipole dispersion coefficients** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2020, Roč. 153, č. 6, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 064110

2020 [01/12] / **USA** - Cutini, M. - Maschio, L. - Ugliengo, P. **Exfoliation Energy of Layered Materials by DFT-D: Beware of Dispersion!** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 5244 - 5252

2020 [01/12] / **USA** - Shukla, N. - Arora, B. - Sharma, L. - Srivastava, R. **Two-dipole and three-dipole dispersion coefficients for interaction of alkaline-earth-metal atoms with alkaline-earth-metal atoms and alkaline-earth-metal ions** [elektronický dokument] In: **Physical Review A**: Atomic, molecular, and optical physics and quantum information. College Park: American Institute of Physics, 2020, Roč. 102, č. 2, [tlačená forma] [online]. ISSN 1050-2947. ISSN (online) 1094-1622. - SCO, s. Art. No. 022817

2020 [01/12] / **CHE** - Oleynichenko, A.V. - Zaitsevskii, A. - Skripnikov, L.V. - Eliav, E. **Relativistic fock space coupled cluster method for many-electron systems: Non-perturbative account for connected triple excitations** [elektronický dokument] In: **Symmetry**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 12, č. 7, [online]. ISSN (online) 2073-8994. - SCO, s. Art. No. 1101

2020 [01/12] / **USA** - Blowey, P.J. - Blowey, P.J. - Sohail, B. - Rochford, L.A. - Lafosse, T. - Duncan, D.A. - Ryan, P.T.P. - Ryan, P.T.P. - Warr, D.A. - Lee, T.-L. - Costantini, G. - Maurer, R.J. - Woodruff, D.P. **Alkali Doping Leads to Charge-Transfer Salt Formation in a Two-Dimensional Metal-Organic Framework** [elektronický dokument] In: **ACS Nano**. Washington: American Chemical Society, 2020, Roč. 14, č. 6, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCO, s. 7475 - 7483

2020 [01/12] / **USA** - Maxwell, C.I. - Saoudi, M. - Pencer, J. **Development of a Polarizable Interatomic Potential for Molten Lithium, Sodium, and Potassium Nitrate** [elektronický dokument] In: **Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2020, Roč. 124, č. 23, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCO, s. 4751 - 4761

2020 [01/12] / **USA** - Yan, P.-G. - Tang, L.-Y. - Yan, Z.-C. - Babb, J.F. **Long-range interaction of Li(2 S 2)-Li(2 S 2)-Li+(1 S 1)** [elektronický dokument] In: **Physical Review A**: Atomic, molecular, and optical physics and quantum information. College Park: American Institute of Physics, 2020, Roč. 101, č. 3, [tlačená forma] [online]. ISSN 1050-2947. ISSN (online) 1094-1622. - SCO, s. Art. No. 032702

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. - Cole, D.J. - Limas, N.G. - Fiszbein, B. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 34, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 19297 - 19324

2019 [01/12] / **GBR** - Schwerdtfeger, P. - Nagle, J.K. **In: Molecular Physics**: an International Journal at the Interface Between Chemistry and Physics . Londýn: Taylor & Francis Group, 2019, Roč. 117, č. 9-12, [tlačená forma] [online]. ISSN 0026-8976. ISSN (online) 1362-3028. - SCIE ; WOS CC, s. 1200 - 1225

2019 [01/12] / **USA** - Fischer, M. - Kim, W.J. - Badawi, M. - Lebegue, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 150, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094102

2019 [01/12] / **USA** - Cawkwell, M.J. - Perriot, R. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 150, č. 2, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 024107

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 57, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 33310 - 33336

2019 [01/12] / **USA** - Yang, J.H. - Kitchaev, D.A. - Ceder, G. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 3, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 035132

2019 [01/12] / Salazar, J.M. - Badawi, M. - Radola, B. - Macaud, M. - Simon, J.M. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 38. - SCIE ; WOS CC, s. 23455 - 23463

2019 [01/12] / **USA** - Terentjev, A.V. - Constantin, L.A. - Artacho, E. - Pitarke, J.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 100, č. 23, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 235439

2018 [01/12] / **USA** - Hesselmann, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP

Publishing, 2018, Roč. 149, č. 4, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 044103

2018 [01/12] / **NLD** - Hesselmann, A. - Meitei, O.R. **In: Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2018, Roč. 1129, [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCIE ; WOS CC, s. 57 - 69

2018 [01/12] / **USA** - Tao, J.M. - Perdew, J.P. - Tang, H. - Shahi, C. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 148, č. 7, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 074110

2018 [01/12] / **USA** - Bedoya-Martinez, N. - Giunchi, A. - Salzillo, T. - Venuti, E. - Della Valle, R.G. - Zojer, E. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4380 - 4390

2018 [01/12] / **USA** - Srour, J. - Badawi, M. - Hassan, F.E. - Postnikov, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 054106

2018 [01/12] / **USA** - Loboda, O.A. - Dolgonos, G.A. - Boese, A.D. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124104

2018 [01/12] / **GBR** - Wieme, J. - Lejaeghere, K. - Kresse, G. - Van Speybroeck, V. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2018, Roč. 9, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 4899

2018 [01/12] / **USA** - Terentjev, A.V. - Constantin, L.A. - Pitarke, J.M. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 21, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 214108

2018 [01/12] / **USA** - Jerabek, P. - Schwerdtfeger, P. - Nagle, J.K. **In: Physical Review A**: Atomic, molecular, and optical physics and quantum information. College Park: American Institute of Physics, 2018, Roč. 98, č. 1, [tlačená forma] [online]. ISSN 1050-2947. ISSN (online) 1094-1622. - SCIE ; WOS CC, s. Art. No. 012508

2018 [01/12] / Heidar-Zadeh, F. - Ayers, P.W. - Verstraelen, T. - Vinogradov, I. - Vohringer-Martinez, E. - Bultinck, P. **In: Journal of Physical Chemistry A**, 2018, Roč. 122, č. 17. - SCIE ; WOS CC, s. 4219 - 4245

2018 [01/12] / **USA** - Alderman, O.L.G. - Benmore, C.J. - Neuefeind, J. - Coillet, E. - Mermet, A. - Martinez, V. - Tamalonis, A. - Weber, R. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 2, č. 4, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 043602

2018 [01/12] / Bueno-Perez, R. - Balestra, S.R.G. - Camblor, M.A. - Min, J.G. - Hong, S.B. - Merkling, P.J. - Calero, S. **In: Chemistry-A European Journal**, 2018, Roč. 24, č. 16. - SCIE ; WOS CC, s. 4121 - 4132

2018 [01/12] / Riquelme, M. - Lara, A. - Mobley, D.L. - Verstraelen, T. - Matamala, A.R. - Vohringer-Martinez, E. **In: Journal of Chemical Information and Modeling**, 2018, Roč. 58, č. 9. - SCIE ; WOS CC, s. 1779 - 1797

2018 [01/12] / **USA** - Fedorov, D.V. - Sadhukhan, M. - Stohr, M. - Tkatchenko, A. **In: Physical Review Letters**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 121, č. 18, [tlačená forma] [online]. ISSN 0031-

9007. ISSN (online) 1079-7114. - SCIE ; WOS CC, s. Art. No. 183401

2018 [01/12] / **USA** - Berwanger, J. - Huber, F. - Stilp, F. - Giessibl, F.J. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 19, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 195409

2017 [01/12] / **GBR** - Goulart, M. - Kuhn, M. - Rasul, B. - Postler, J. - Gatchell, M. - Zettergren, H. - Scheier, P. - Echt, O. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 41, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 27968 - 27973

2017 [01/12] / **USA** - Tao, J.M. - Zheng, F. - Gebhardt, J. - Perdew, J.P. - Rappe, A.M. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2017, Roč. 1, č. 2, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 020802

2017 [01/12] / Iskra, A. - Gentleman, A.S. - Kartouzian, A. - Kent, M.J. - Sharp, A.P. - Mackenzie, S.R. **In: Journal of Physical Chemistry A**, 2017, Roč. 121, č. 1. - SCIE ; WOS CC, s. 133 - 140

2017 [01/12] / **USA** - Fransson, T. - Rehn, D.R. - Dreuw, A. - Norman, P. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094301

2016 [01/12] / **USA** - Verstraelen, T. - Vandenbrande, S. - Heidar-Zadeh, F. - Vanduyfhuys, L. - Van Speybroeck, V. - Waroquier, M. - Ayers, P.W. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 3894 - 3912

ADC_048: / Baltrušaitis, Jonas (Autor) (50%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%) - Michaels, W. (Autor) (4%) - Makkee, M. (Autor) (3%) - Mul, G. (Autor) (3%): **Catalytic methyl mercaptan coupling to ethylene in chabazite: DFT study of the first C-C bond formation**. – DOI 10.1016/j.apcatb.2016.01.021. – CCC ; WOS CC ; SCO.
In: *Applied Catalysis B: Environmental* [textový dokument (print)] . – Amsterdam (Holandsko) : Elsevier. – ISSN 0926-3373. – č. 187 (2016), s. 195-203 [tlačená forma]
Počet všetkých autorov: 5
[článok]
Lit.: 77
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 2,206 - 2016
SJR: 2,693 - 2016
CiteScore: 14,9 - 2016

Ohlasy (12):
2025 [01/20] / **USA** - Chen, Wei - Sobalska, Julia - Fu, Wenqian - Tarach, Karolina A. - Bocus, Massimo - Tang, Tiandi - Góra-Marek, Kinga - Van Speybroeck, Veronique. **Formaldehyde-Mediated Initial Carbon–Carbon Bond Formation in Zeolite-Catalyzed Methanol-to-Hydrocarbon Conversion** [elektronický dokument]. DOI 10.1021/jacs.5c06141 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2025, Roč. 147, č. 28, s. 24719-24733 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 24719 - 24733

2024 [01/20] / **NLD** - Bayout, Abdelilah - Cammarano, Claudia - Gimello, Olinda - Medeiros Costa, Izabel - Veryasov, Gleb - Hulea, Vasile. **Methyl mercaptan-to-hydrocarbons: Effect of topology of zeolite catalysts** [elektronický dokument]. DOI 10.1016/j.mcat.2024.114541 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2024, Roč. 569, art. no. 114541 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO ; CCC ; WOS CC, s. art. no. 114541

2024 [01/20] / **USA** - Gaumard, Robin - Guesmi, Hazar - Calaminici, Patrizia - Köster, Andreas - Samaniego Rojas, Juan Diego - Mineva, Tzonka. **Benzene Methylation by Methyl Mercaptan over Acidic Chabazite: Concerted or Stepwise Mechanism?** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c01048 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 17, s. 7115-7126 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO, s. 7115 - 7126

2023 [01/20] / **GBR** - Watanabe, Ryo - Oba, Natsu - Smith, Suchada - Oshima, Kazumasa - Kishida, Masahiro - Miyake, Koji - Nishiyama, Norikazu - Verma, Priyanka - Fukuhara, Choji. **Effect of Ga substitution with Al in ZSM-5 zeolite in methanethiol-to-hydrocarbon conversion** [elektronický dokument]. DOI 10.1039/d3ra01852k In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 31, s. 21441-21447 [online]. ISSN (online) 2046-2069. - SCO ; CCC ; WOS CC, s. 21441 - 21447

2022 [01/20] / **NLD** - Xu, F. - Li, Z. - Zhu, R. - Chu, Y. - Pan, Z. - Xia, S. - Fu, J. - Xiao, Z. - Ji, X. - Liu, M. - Weng, B. **Narrow band-gapped perovskite oxysulfide for CO2 photoreduction towards ethane** In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2022, Roč. 316, [tlačená forma]. ISSN 0926-3373. - SCO, s. Art. No. 121615

2021 [01/20] / **GBR** - Ren, S. - Liang, W. - Fang, H. - Zhu, Y. **Performance and poisoning analysis of organic sulfur resistance of Pd-Ce catalyst in catalytic oxidation of VOCs** [elektronický dokument] In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2021, Roč. 9, č. 6, [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s. Art. No. 106640

2021 [01/20] / **CHE** - Yan, J.-K. - Liu, X.-P. - Mao, J. - Li, K. - Luo, Y.-M. - Mei, Y. - He, D.-D. **Research Progress of Catalytic Reaction Mechanism of Methyl Mercaptan to Olefins** [elektronický dokument] In: **Journal of molecular catalysis**. Lausanne: Elsevier, 2021, Roč. 35, č. 4, [tlačená forma]. ISSN 0304-5102. ISSN (online) 1873-3131. - SCO, s. 353 - 364

2021 [01/20] / **GBR** - Yu, M. - Tormene, N. - Bolshakov, A. - Mezari, B. - Liutkova, A. - Kosinov, N. - Hensen, E.J.M. **Selective methanethiol-to-olefins conversion over HSSZ-13 zeolite** [elektronický dokument] In: **Chemical Communications**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 57, č. 27, [tlačená forma] [online]. ISSN 1359-7345. ISSN (online) 1364-548X. ISSN (zrušené) 0009-241X. - SCO, s. 3323 - 3326

2020 [01/12] / Xie, X. - Xu, S. - Xu, Z. - Zhao, W. **Synthesis Technique and Methods of Mercaptan Compounds** In: **Cailiao Daobao/Materials Reports**, 2020, Roč. 34, č. 4. - SCO, s. 7168 - 7176

2018 [01/12] / **NLD** - Li, Q.M. - Zhang, M. - Wang, C.M. - Zhu, Y.A. - Zhou, X.G. - Xie, Z.K. **In: Molecular Catalysis**. Amsterdam: Elsevier, 2018, Roč. 446, [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCIE ; WOS CC, s. 106 - 114

2017 [01/12] / Bermejo-Deval, R. - Walter, R.M.H. - Gutierrez, O.Y. - Lercher, J.A. **In: Catalysis Science & Technology**, 2017, Roč. 7, č. 19. - SCIE ; WOS CC, s. 4437 - 4443

2017 [01/12] / **USA** - Reina, M. - Martinez, A. - Cammarano, C. - Leroi, C. - Hulea, V. - Mineva, T. **In: ACS Omega**. Washington: American Chemical Society, 2017, Roč. 2, č. 8, [online]. ISSN (online) 2470-1343. - SCIE ; WOS CC, s. 4647 - 4656

ADC_049: / Bučko, Tomáš (Autor) [UKOPRCFZ] (70%) - Lebegue, Sebastien (Autor) (10%) - Gould, Tim (Autor) (10%) - Ángyán, János G. (Autor) (10%): **Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation**. – [recenzované]. – DOI 10.1088/0953-8984/28/4/045201. – CCC ; SCO ; WOS CC.
In: *Journal of Physics* [textový dokument (print)] [elektronický dokument] : Condensed Matter. – Bristol (Veľká Británia) : Institute of Physics. IOP Publishing. – ISSN 0953-8984. – ISSN (online) 1361-648X. – Roč. 28, č. 4 (2016), s. [1-13] [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 50
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 2,678 - 2016
SNIP: 0,923 - 2016
SJR: 1,553 - 2016
CiteScore: 4,5 - 2016
Kvartil Q:
2016, JIF - Physics, condensed matter - Q2

Ohlasy (87):
2025 [01/20] / **NLD** - Dang, Diem Thi Xuan - Le, Dai Nam - Woods, Lilia M. **Dissecting van der Waals interactions with density functional theory – Wannier-basis approach** [elektronický dokument]. DOI 10.1016/j.cpc.2025.109525 In: **Computer Physics Communications**: An International Journal and Program Library for Computational Physics and Physical Chemistry. Amsterdam: Elsevier, 2025, Roč. 310, art. no. 109525 [tlačená forma] [online]. ISSN 0010-4655. ISSN (online) 1879-2944. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 109525

2025 [01/20] / **USA** - Muhli, Heikki - Ala-Nissila, Tapio - Caro, Miguel A. **Atom-wise formulation of the many-body dispersion problem for linear-scaling van der Waals corrections** [elektronický dokument]. DOI 10.1103/PhysRevB.111.054103 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2025, Roč. 111, č. 5, art. no. 054103 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 054103

2025 [01/20] / **USA** - Thakur, Vikas Singh - Banerjee, Swastika. **Ion-Specific Storage and Diffusion Mechanisms in Cross-Linked Layered Phosphorus Electrodes: From Clustering to Correlated Dynamics** [elektronický dokument]. DOI 10.1021/acs.jpcc.5c06846 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 48, s. 21355-21363 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE, s. 21355 - 21363

2025 [01/20] / **NLD** - Dmitruk, Kirill A. - Podolyako, Ignat A. - Shlyapin, Dmitry A. - Shubin, Aleksandr A. - Netskina, Olga V. **Adsorption of CO2 on N-doped carbon materials: the effect of the subsurface layer** [elektronický dokument]. DOI 10.1016/j.susc.2025.122819 In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2025, Roč. 762, art. no. 122819 [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 122819

2025 [01/20] / **USA** - Sulaiman, Nura M. - Weikun, Liu - Yunhan, Zhen - Douxing, Pan. **Lennard-Jones Potential Parameters and Cut-Off Modifications for Layered Transition Metal Dichalcogenides** [elektronický dokument]. DOI 10.1115/1.4068957 In: **Journal of applied mechanics**. NewYork: American Society of Mechanical Engineers, 2025, Roč. 92, č. 10, art. no. 101010 [tlačená forma]. ISSN 0021-8936. ISSN (online) 1528-9036. - SCO ; CCC ; WOS CC ; SCIE, s.

art. no. 101010

2025 [01/20] / **USA** - Jinghan, Li - Yutian, Li - Sulaiman, Nura M. - Douxing, Pan. **Lennard-Jones interfacial parameters and cut-off modifications for layered buckled honeycomb bi-elemental crystals** [elektronický dokument]. DOI 10.1063/5.0277888 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2025, Roč. 138, č. 7, art. no. 075303 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 075303

2024 [01/20] / **USA** - Pan, Douxing - Li, Jinghan - Voon, Lok C.Lew Yan - Wei, Peijun. **Determination of Lennard-Jones potential parameters for interfacial interaction in elemental layered crystals** [elektronický dokument]. DOI 10.1063/5.0213582 In: **Journal of Applied Physics**. Melville: American Institute of Physics, 2024, Roč. 135, č. 20, art. no. 204301 [tlačená forma] [online]. ISSN 0021-8979. ISSN (online) 1089-7550. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Osestad, Eivind Kristen - Zossimova, Ekaterina - Walter, Michael - Holst, Bodil - Fiedler, Johannes. **Atomic diffraction by nanoholes in hexagonal boron nitride** [elektronický dokument]. DOI 10.1039/d4na00322e In: **Nanoscale Advances**. Londýn: The Royal Society of Chemistry, 2024, Roč. 6, č. 21, s. 5337-5347 [online]. ISSN (online) 2516-0230. - SCO ; CCC ; WOS CC, s. 5337 - 5347

2024 [01/20] / **USA** - Ying, Penghua - Hod, Oded - Urbakh, Michael. **Superlubric Graphullerene** [elektronický dokument]. DOI 10.1021/acs.nanolett.4c02794 In: **Nano letters**. Washington: American Chemical Society, 2024, Roč. 24, č. 34, s. 10599-10604 [tlačená forma] [online]. ISSN 1530-6984. ISSN (online) 1530-6992. - SCO ; CCC ; WOS CC, s. 10599 - 10604

2024 [01/20] / **NLD** - Liang, Chaoping - Liu, Zhe - Wang, Feilong - Zhou, Haojie - Luo, Guangxiong - Ding, Fei. **Unravelling K intercalation on graphene and its variants through two-dimensional cluster expansion modeling** [elektronický dokument]. DOI 10.1016/j.apsusc.2024.160218 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2024, Roč. 663, art. no. 160218 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC, s. art. no. 160218

2024 [01/20] / **USA** - Ravichandran, Siddharth - Najafi, Mahsa - Goeminne, Ruben - Denayer, Joeri F.M. - Van Speybroeck, Veronique - Vanduyfhuys, Louis. **Reaching Quantum Accuracy in Predicting Adsorption Properties for Ethane/Ethene in Zeolitic Imidazolate Framework-8 at Low Pressure Regime** [elektronický dokument]. DOI 10.1021/acs.jctc.4c00293 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 12, s. 5225-5240 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 5225 - 5240

2024 [01/20] / **USA** - Thakur, Vikas Singh - Banerjee, Swastika. **Inducing Rigidity in Layered Structures for Improved Anodic Performance in Magnesium-Ion Battery: A Computational Design** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c07951 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 19, s. 7865-7875 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 7865 - 7875

2024 [01/20] / **USA** - Sheldon, Christopher - Paier, Joachim - Usvyat, Denis - Sauer, Joachim. **Hybrid RPA:DFT Approach for Adsorption on Transition Metal Surfaces: Methane and Ethane on Platinum (111)** [elektronický dokument]. DOI 10.1021/acs.jctc.3c01308 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 5, s. 2219-2227 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 2219 - 2227

2024 [01/20] / **USA** - Novotný, Michal - Dubecký, Matúš - Karlický, František. **Toward accurate modeling of structure and energetics of bulk hexagonal boron nitride** [elektronický dokument]. DOI 10.1002/jcc.27222 In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2024, Roč. 45, č. 2, s. 115-121 [tlačená forma] [online]. ISSN

0192-8651. ISSN (online) 1096-987X. - SCO ; CCC ; WOS CC, s. 115 - 121

2023 [01/20] / **GBR** - Delachaux, F. - Hessou, E. P. - Vallières, C. - Monnier, H. - Badawi, M. **A dispersion-corrected DFT method for zeolite-based CO2/N2separation: Assessment and application** [elektronický dokument]. DOI 10.1016/j.jece.2022.109052 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2023, Roč. 11, č. 1, art. no. 109052 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO, s.

2023 [01/20] / **USA** - Poier, Pier Paolo - Lagardère, Louis - Piquemal, Jean Philip. **Smooth particle mesh Ewald-integrated stochastic Lanczos many-body dispersion algorithm** [elektronický dokument]. DOI 10.1063/5.0166476 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 15, art. no. 154109 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Hermann, Jan - Stöhr, Martin - Góger, Szabolcs - Chaudhuri, Shayantan - Aradi, Bálint - Maurer, Reinhard J. - Tkatchenko, Alexandre. **libMBD: A general-purpose package for scalable quantum many-body dispersion calculations** [elektronický dokument]. DOI 10.1063/5.0170972 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 17, art. no. 174802 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Thodkar, Kishan - Cazade, Pierre - Thompson, Damien. **Theoretical and Experimental Characterization of Molecular Self-Assembly on Graphene Films**. DOI 10.1002/9783527843374.ch9 In: **Graphene Field-Effect Transistors: Advanced Bioelectronic Devices for Sensing Applications**. Hoboken: John Wiley & Sons, 2023, s. 185-206. ISBN 9783527843374. ISBN 9783527349906. - SCO, s. 185 - 206

2023 [01/20] / **USA** - Szaro, Nicholas A. - Bello, Mubarak - Fricke, Charles H. - Bamidele, Olajide H. - Heyden, Andreas. **Benchmarking the Accuracy of Density Functional Theory against the Random Phase Approximation for the Ethane Dehydrogenation Network on Pt(111)** [elektronický dokument]. DOI 10.1021/acs.jpclett.3c02723 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2023, Roč. 14, č. 48, s. 10769-10778 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 10769 - 10778

2023 [01/20] / **USA** - Hill, Adam - Kras, Weronika - Theodosiou, Fragkoulis - Wanat, Monika - Lee, Daniel - Cruz-Cabeza, Aurora J. **Polymorphic Solid Solutions in Molecular Crystals: Tips, Tricks, and Switches** [elektronický dokument]. DOI 10.1021/jacs.3c07105 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2023, Roč. 145, č. 37, s. 20562-20577 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC, s. 20562 - 20577

2023 [01/20] / **GBR** - Murata, Hidenobu. **DFT-D3 study of two-dimensional polymerization of C60 crystal under high pressure** [elektronický dokument]. DOI 10.35848/1347-4065/acb74d In: **Japanese Journal of Applied Physics**. Tokyo: Japan Society of Applied Physics, 2023, Roč. 62, č. 2, art. no. 021002 [tlačená forma] [online]. ISSN 0021-4922. ISSN (online) 1347-4065. - SCO ; CCC ; WOS CC, s. art. no. 021002

2022 [01/20] / **USA** - Zhang, T.-T. - Tang, Q.-L. - Zhang, X. - Duan, X.-X. - Yang, Y.-H. - Zhang, M.-L. - Qu, Z.-Y. **Ab Initio Microkinetics of H2S Interactions with Clean and Sulfided Au(110) at Low Temperature: A Strong Assistance in Partial Dissociation from Single Sulfur Atoms** In: **Journal of Physical Chemistry C**, 2022, Roč. 126, č. 51. - SCO, s. 21585 - 21595

2022 [01/20] / **CHE** - Dubskikh, V.A. - Kovalenko, K.A. - Nizovtsev, A.S. - Lysova, A.A. - Samsonenko, D.G. - Dybtsev, D.N. - Fedin, V.P. **Enhanced Adsorption Selectivity of Carbon Dioxide and Ethane on Porous Metal-Organic Framework Functionalized by a Sulfur-Rich Heterocycle** [elektronický dokument] In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 12, č. 23, [online]. ISSN (online) 2079-4991. - SCO, s. Art. No. 4281

2022 [01/20] / **USA** - Myneni, H. - Jonsson, E.O. - Jonsson, H. - Dohn, A.O. **Polarizable Force Field for Acetonitrile Based on the Single-Center Multipole Expansion** [elektronický dokument] In: **Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2022, Roč. 126, č. 45, [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCO, s. 9339 - 9348

2022 [01/20] / **USA** - Braeckevelt, T. - Goeminne, R. - Vandenhaute, S. - Borgmans, S. - Verstraelen, T. - Steele, J.A. - Roeffaers, M.B.J. - Hofkens, J. - Rogge, S.M.J. - van Speybroeck, V. **Accurately Determining the Phase Transition Temperature of CsPbI3via Random-Phase Approximation Calculations and Phase-Transferable Machine Learning Potentials** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 19, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 8561 - 8576

2022 [01/20] / **NLD** - Loncaric, I. - Alducin, M. - Juaristi, J.I. **O2 on Ag(110): A puzzle for exchange-correlation functionals** [elektronický dokument] In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2022, Roč. 554, [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO, s. Art. No. 111424

2022 [01/20] / **USA** - Wang, Y. - Fan, Z. - Qian, P. - Ala-Nissila, T. - Caro, M.A. **Structure and Pore Size Distribution in Nanoporous Carbon** [elektronický dokument] In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 2, [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 617 - 628

2022 [01/20] / **USA** - Zhang, Tian Tian - Tang, Qian Lin - Zhang, Xian - Duan, Xiao Xuan - Yang, Yi Hang - Zhang, Mao Lin - Qu, Zhi Yuan. **Ab Initio Microkinetics of H<inf>2</inf>S Interactions with Clean and Sulfided Au(110) at Low Temperature: A Strong Assistance in Partial Dissociation from Single Sulfur Atoms** [elektronický dokument]. DOI 10.1021/acs.jpcc.2c05363 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2022, Roč. 126, č. 51, s. 21585-21595 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO, s. 21585 - 21595

2022 [01/20] / **CHE** - Dubskikh, Vadim A. - Kovalenko, Konstantin A. - Nizovtsev, Anton S. - Lysova, Anna A. - Samsonenko, Denis G. - Dybtsev, Danil N. - Fedin, Vladimir P. **Enhanced Adsorption Selectivity of Carbon Dioxide and Ethane on Porous Metal–Organic Framework Functionalized by a Sulfur-Rich Heterocycle** [elektronický dokument]. DOI 10.3390/nano12234281 In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2022, Roč. 12, č. 23, art. no. 4281 [online]. ISSN (online) 2079-4991. - SCO, s. art. no. 4281

2022 [01/20] / **USA** - Myneni, Hemanadhan - Jónsson, Elvar Örn - Jónsson, Hannes - Dohn, Asmus Ougaard. **Polarizable Force Field for Acetonitrile Based on the Single-Center Multipole Expansion** [elektronický dokument]. DOI 10.1021/acs.jpcb.2c04255 In: **Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2022, Roč. 126, č. 45, s. 9339-9348 [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCO, s. 9339 - 9348

2022 [01/20] / **USA** - Braeckevelt, Tom - Goeminne, Ruben - Vandenhaute, Sander - Borgmans, Sander - Verstraelen, Toon - Steele, Julian A. - Roeffaers, Maarten B.J. - Hofkens, Johan - Rogge, Sven M.J. - Van Speybroeck, Veronique. **Accurately Determining the Phase Transition Temperature of CsPbI3 via Random-Phase Approximation Calculations and Phase-Transferable Machine Learning Potentials** [elektronický dokument]. DOI 10.1021/acs.chemmater.2c01508 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 19, s. 8561-8576 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 8561 - 8576

2022 [01/20] / **NLD** - Lončarić, Ivor - Alducin, Maite - Juaristi, J. Iñaki. **O2 on Ag(110): A puzzle for exchange-correlation functionals** [elektronický dokument]. DOI 10.1016/j.chemphys.2021.111424 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2022, Roč. 554, art.

no. 111424 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO, s. art. no. 111424

2022 [01/20] / **USA** - Wang, Yanzhou - Fan, Zheyong - Qian, Ping - Ala-Nissila, Tapio - Caro, Miguel A. **Structure and Pore Size Distribution in Nanoporous Carbon** [elektronický dokument]. DOI 10.1021/acs.chemmater.1c03279 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2022, Roč. 34, č. 2, s. 617-628 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO, s. 617 - 628

2021 [01/20] / **USA** - Ouyang, W. - Sofer, R. - Gao, X. - Hermann, J. - Tkatchenko, A. - Kronik, L. - Urbakh, M. - Hod, O. **Anisotropic interlayer force field for transition metal dichalcogenides: The case of molybdenum disulfide** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 11, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 7237 - 7245

2021 [01/20] / **USA** - Sheldon, C. - Paier, J. - Sauer, J. **Adsorption of CH4on the Pt(111) surface: Random phase approximation compared to density functional theory** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 155, č. 17, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 174702

2021 [01/20] / **USA** - Jana, S. - Myneni, H. - Smiga, S. - Constantin, L.A. - Samal, P. **Benchmark test of a dispersion corrected revised Tao-Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 155, č. 11, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 114102

2021 [01/20] / **CHN** - Li, K. - Wang, J. - Blatov, V.A. - Gong, Y. - Umezawa, N. - Tada, T. - Hosono, H. - Oganov, A.R. **Crystal and electronic structure engineering of tin monoxide by external pressure** [elektronický dokument] In: **Journal of Advanced Ceramics**. Peking: Tsinghua University Press, 2021, Roč. 10, č. 3, [tlačená forma] [online]. ISSN 2226-4108. ISSN (online) 2227-8508. - SCO, s. 565 - 577

2021 [01/20] / **USA** - Sun, G. - Liu, X. - Abramov, Y.A. - Nilsson Lill, S.O. - Chang, C. - Burger, V. - Broo, A. **Current State-of-the-art In-house and Cloud-Based Applications of Virtual Polymorph Screening of Pharmaceutical Compounds: A Challenging Case of AZD1305** In: **Crystal Growth and Design**, 2021, Roč. 21, č. 4. - SCO, s. 1972 - 1983

2021 [01/20] / **NLD** - Tunega, D. - Zaoui, A. **Adsorption of polycyclic aromatic hydrocarbons on FeOOH polymorphs: A theoretical study** [elektronický dokument] In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2021, Roč. 706, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO, s. Art. No. 121795

2021 [01/20] / **GBR** - Melissen, S.T.A.G. - Le Bahers, T. - Sautet, P. - Steinmann, S.N. **What does graphitic carbon nitride really look like?** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 4, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 2853 - 2859

2021 [01/20] / **USA** - Li, X. - Qiang, X. - Gong, Z. - Zhang, Y. - Gong, P. - Chen, L. **Tunable negative poisson's ratio in Van der Waals superlattice** [elektronický dokument] In: **Research**: a science partner journal. [Washington]: American Association for the Advancement of Science, 2021, Roč. 2021, [online]. ISSN (online) 2639-5274. - SCO, s. Art. No. 1904839

2020 [01/12] / **NLD** - Berro, Y. - Badawi, M. - El Haj Hassan, F. - Kassir, M. - Tielens, F. **Water-silanol interactions on the amorphous silica surface: A dispersion-corrected DFT investigation** [elektronický dokument] In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2020, Roč. 320, [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. Art. No. 114496

2020 [01/12] / **USA** - Duan, X. - Liu, Z. - Hanrahan, B.M. - Zhu, W. - Liu, S. **Designing xenes with two-dimensional triangular lattice** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 12, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 124003

2020 [01/12] / **GBR** - Jagielski, J. - Solari, S.F. - Jordan, L. - Scullion, D. - Blulle, B. - Li, Y.-T. - Krumeich, F. - Chiu, Y.-C. - Ruhstaller, B. - Santos, E.J.G. - Shih, C.-J. **Scalable photonic sources using two-dimensional lead halide perovskite superlattices** [elektronický dokument] In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2020, Roč. 11, č. 1, [online]. ISSN (online) 2041-1723. - SCO, s. Art. No. 387

2020 [01/12] / **USA** - Kim, J. - Gulans, A. - Draxl, C. **Work-function modification of PEG(thiol) adsorbed on the Au(111) surface: A first-principles study** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 11, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 116001

2020 [01/12] / **USA** - Li, H. - Shi, W. - Guo, Y. - Guo, W. **Nonmonotonic interfacial friction with normal force in two-dimensional crystals** [elektronický dokument] In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 102, č. 8, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. Art. No. 085427

2020 [01/12] / Yuan, D. - Zhang, Y. - Ho, W. - Wu, R. **Effects of van der Waals Dispersion Interactions in Density Functional Studies of Adsorption, Catalysis, and Tribology on Metals** In: **Journal of Physical Chemistry C**, 2020, Roč. 124, č. 31. - SCO, s. 16926 - 16942

2020 [01/12] / **USA** - Morales-Garcia, A. - Illas, F. **Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids** [elektronický dokument] In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2020, Roč. 4, č. 7, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO, s. Art. No. 73601

2020 [01/12] / **NLD** - Truyens, A.-J. - Vekeman, J. - Tielens, F. **A subtle balance between interchain interactions and surface reconstruction at the origin of the alkylthiol/Au(111) self-assembled monolayer geometry** [elektronický dokument] In: **Surface Science**: (including Surface Science Letters). Amsterdam: Elsevier, 2020, Roč. 696, [tlačená forma]. ISSN 0039-6028. ISSN (online) 1879-2758. - SCO, s. Art. No. 121597

2020 [01/12] / **GBR** - Li, X. - Huang, C. - Hu, S. - Deng, B. - Chen, Z. - Han, W. - Chen, L. **Negative and near-zero Poisson's ratios in 2D graphene/MoS2 and graphene/h-BN heterostructures** [elektronický dokument] In: **Journal of Materials Chemistry C**: Materials for Optical, Magnetic and Electronic Devices. Londýn: The Royal Society of Chemistry, 2020, Roč. 8, č. 12, [tlačená forma] [online]. ISSN 2050-7526. ISSN (online) 2050-7534. - SCO, s. 4021 - 4029

2020 [01/12] / **DEU** - Asher, M. - Angerer, D. - Korobko, R. - Diskin-Posner, Y. - Egger, D.A. - Yaffe, O. **Anharmonic Lattice Vibrations in Small-Molecule Organic Semiconductors** [elektronický dokument] In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2020, Roč. 32, č. 10, [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO, s. Art. No. 1908028

2020 [01/12] / **USA** - Ouyang, W. - Azuri, I. - Mandelli, D. - Tkatchenko, A. - Kronik, L. - Urbakh, M. - Hod, O. **Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2020, Roč. 16, č. 1, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 666 - 676

2020 [01/12] / **GBR** - Jiao, Z. - Chen, X. - Fang, C. - Xu, G. - Zhang, C. - Fan, L. - Liu, B. **DFT study of Cs/Sr/Ag adsorption on defective matrix graphite** [elektronický dokument] In: **Science and Technology of Nuclear Installations**. london: Hindawi Publishing Corporation, 2020, Roč. 2020, [tlačená forma] [online]. ISSN 16876075. ISSN (online) 16876083. - SCO, s. Art. No. 4921623

2019 [01/12] / **USA** - Beck, H. - Gehrmann, C. - Egger, D.A. **In: APL materials**. Melville: ACA and AIP Publishing, 2019, Roč. 7, č. 2, [online]. ISSN (online) 2166-532X. - SCIE ; WOS CC, s. Art. No. 021108

2019 [01/12] / **NLD** - Dolgonos, G.A. - Boese, A.D. **In: Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2019, Roč. 718, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCIE ; WOS CC, s. 7 - 11

2019 [01/12] / **GBR** - Kiruthika, S. - Fjellvag, H. - Ravindran, P. **In: Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2019, Roč. 7, č. 11, [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCIE ; WOS CC, s. 6228 - 6240

2019 [01/12] / DeBenedetti, W.J.I. - Hines, M.A. **In: Journal of Physical Chemistry C**, 2019, Roč. 123, č. 14. - SCIE ; WOS CC, s. 8836 - 8842

2019 [01/12] / **USA** - Caldeweyher, E. - Ehlert, S. - Hansen, A. - Neugebauer, H. - Spicher, S. - Bannwarth, C. - Grimme, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2019, Roč. 150, č. 15, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 154122

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. - Cole, D.J. - Limas, N.G. - Fiszbein, B. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 34, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 19297 - 19324

2019 [01/12] / **DEU** - Mio, A.M. - Konze, P.M. - Meledin, A. - Kpers, M. - Pohlmann, M. - Kaminski, M. - Dronskowski, R. - Mayer, J. - Wuttig, M. **In: Advanced Functional Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2019, Roč. 29, č. 37, [tlačená forma] [online]. ISSN 1616-301X. ISSN (online) 1616-3028. - SCIE ; WOS CC, s. Art. No. 1902332

2019 [01/12] / **GBR** - Manz, T.A. - Chen, T.Y. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 57, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 33310 - 33336

2019 [01/12] / **GBR** - Yuan, D.W. - Liao, H.T. - Hu, W.Y. **In: Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 37, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCIE ; WOS CC, s. 21049 - 21056

2019 [01/12] / **GBR** - Liu, J. - Lu, H.G. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2019, Roč. 9, č. 59, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 34481 - 34485

2019 [01/12] / **CHE** - Stein, M. - Heimsaat, M. **In: Crystals**. Bazilej: Multidisciplinary Digital Publishing Institute, 2019, Roč. 9, č. 12, [online]. ISSN (online) 2073-4352. - SCIE ; WOS CC, s. Art. No. 665

2018 [01/12] / **USA** - Hesselmann, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 4, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 044103

2018 [01/12] / **USA** - Varga, S. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 148, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 051102

2018 [01/12] / **USA** - Bedoya-Martinez, N. - Giunchi, A. - Salzillo, T. - Venuti, E. - Della Valle, R.G. - Zojer, E. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 8, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 4380 - 4390

2018 [01/12] / **USA** - Srour, J. - Badawi, M. - Hassan, F.E. - Postnikov, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 5, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 054106

2018 [01/12] / **USA** - Loboda, O.A. - Dolgonos, G.A. - Boese, A.D. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2018, Roč. 149, č. 12, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 124104

2018 [01/12] / Tawfik, S.A. - Reimers, J.R. - Stampfl, C. - Ford, M.J. **In: Journal of Physical Chemistry C**, 2018, Roč. 122, č. 39. - SCIE ; WOS CC, s. 22675 - 22687

2018 [01/12] / **USA** - Gruber, T. - Gruneis, A. **In: Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2018, Roč. 98, č. 13, [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCIE ; WOS CC, s. Art. No. 134108

2018 [01/12] / **GBR** - Wieme, J. - Lejaeghere, K. - Kresse, G. - Van Speybroeck, V. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2018, Roč. 9, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 4899

2018 [01/12] / **GBR** - Reimers, J.R. - Tawfik, S.A. - Ford, M.J. **In: Chemical Science**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 9, č. 39, [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCIE ; WOS CC, s. 7620 - 7627

2017 [01/12] / **GBR** - Li, X.H. - Wang, B.J. - Cai, X.L. - Zhang, L.W. - Wang, G.D. - Ke, S.H. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2017, Roč. 7, č. 45, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 28393 - 28398

2017 [01/12] / **USA** - Kebede, G.G. - Spangberg, D. - Mitev, P.D. - Broqvist, P. - Hermansson, K. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 6, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 064703

2017 [01/12] / **USA** - Al-Hamdani, Y.S. - Alfe, D. - Michaelides, A. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2017, Roč. 146, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094701

2017 [01/12] / **USA** - Karlicky, F. - Otyepkova, E. - Lo, R. - Pitonak, M. - Jurecka, P. - Pykal, M. - Hobza, P. - Otyepka, M. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2017, Roč. 13, č. 3, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 1328 - 1340

2017 [01/12] / **USA** - Ghedjatti, A. - Magnin, Y. - Fossard, F. - Wang, G. - Amara, H. - Flahaut, E. - Lauret, J.S. - Loiseau, A. **In: ACS Nano**. Washington: American Chemical Society, 2017, Roč. 11, č. 5, [tlačená forma] [online]. ISSN 1936-0851. ISSN (online) 1936-086X. - SCIE ; WOS CC, s. 4840 - 4847

2017 [01/12] / **GBR** - Falin, A. - Cai, Q.R. - Santos, E.J.G. - Scullion, D. - Qian, D. - Zhang, R. - Yang, Z. - Huang, S.M. - Watanabe, K. - Taniguchi, T. - Barnett, M.R. - Chen, Y. - Ruoff, R.S. - Li, L.H. **In: Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2017, Roč. 8, [online]. ISSN (online) 2041-1723. - SCIE ; WOS CC, s. Art. No. 15815

2017 [01/12] / Bedoya-Martinez, N. - Schrode, B. - Jones, A.O.F. - Salzillo, T. - Ruzie, C. - Demitri, N. - Geerts, Y.H. - Venuti, E. - Della Valle, R.G. - Zojer, E. - Resel, R. **In: Journal of Physical Chemistry Letters**, 2017, Roč. 8, č. 15. - SCIE ; WOS CC, s. 3690 - 3695

2017 [01/12] / Kupers, M. - Konze, P.M. - Maintz, S. - Steinberg, S. - Mio, A.M. - Cojocaru-Miredin, O. - Zhu, M. - Muller, M. - Luysberg, M. - Mayer, J. - Wuttig, M. - Dronskowski, R. **In: Angewandte Chemie-International Edition**, 2017, Roč. 56, č. 34. - SCIE ; WOS CC, s. 10204 - 10208

2017 [01/12] / **USA** - Demuynck, R. - Rogge, S.M.J. - Vanduyfhuys, L. - Wieme, J. - Waroquier, M. - Van Speybroeck, V. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2017, Roč. 13, č. 12, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 5861 - 5873

2016 [01/12] / Brandenburg, J.G. - Grimme, S. **In: Acta Crystallographica Section B-Structural Science Crystal Engineering**, 2016, Roč. 72. - SCIE ; WOS CC, s. 502 - 513

2016 [01/12] / **USA** - Cutini, M. - Civalleri, B. - Corno, M. - Orlando, R. - Brandenburg, J.G. - Maschio, L. - Ugliengo, P. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 7, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 3340 - 3352

2016 [01/12] / **USA** - Klimes, J. **In: Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2016, Roč. 145, č. 9, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCIE ; WOS CC, s. Art. No. 094506

2016 [01/12] / Deringer, V.L. - Csanyi, G. **In: Journal of Physical Chemistry C**, 2016, Roč. 120, č. 38. - SCIE ; WOS CC, s. 21552 - 21560

2016 [01/12] / **USA** - Leven, I. - Maaravi, T. - Azuri, I. - Kronik, L. - Hod, O. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2016, Roč. 12, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2896 - 2905

ADC_050: / Bučko, Tomáš (Autor) [UKOPRCFZ] (80%) - Šimko, František (Autor) (20%): **On the structure of crystalline and molten cryolite: Insights from the ab initio molecular dynamics in NpT ensemble**. – text, tab., obr. – [recenzované]. – DOI 10.1063/1.4941333. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 144, č. 6 (2016), art. no. 064502, s. [1-10] [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
Lit.: 50
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 2,965 - 2016
SNIP: 0,978 - 2016
SJR: 1,486 - 2016
CiteScore: 5,4 - 2016
Nordic List: 1 - 2016

Ohlasy (14):

2025 [01/20] / **USA** - Betsis, Konstantinos - Karalis, Konstantinos - Xenidis, Anthimos. **Ab Initio Molecular Dynamics Simulation Study on the Molten Structure of Cryolite to the Cryolitic Bath, Na3AlF6–AlF3–Al2O3–CaF2** [elektronický dokument]. DOI 10.1021/acsomega.5c05781 In: **ACS Omega**. Washington: American Chemical Society, 2025, Roč. 10, č. 36, s. 41820-41827 [online]. ISSN (online) 2470-1343. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 41820 - 41827

2025 [01/20] / **GBR** - Yan, Haiyan - Chen, Lei - Zhang, Yun - Cao, Xuanyu - Zhang, Meiguang - Wei, Qun. **Temperature-dependent structural stability, mechanical strength, and thermodynamics of pyrite-type silicon pernitride** [elektronický dokument]. DOI 10.1039/d5cp03090k In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 45, s. 24558-24568 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 24558 - 24568

2023 [01/20] / **DEU** - Zhang, Yifan - Hu, Xianwei - Zhang, Wendi - Yang, Jiaxin - Chen, Liyu - Tang, Shuai - Liu, Aimin - Shi, Zhongning - Wang, Zhaowen. **Study on Decomposition Mechanism of K3AlF6 by Quantum Chemical Calculations** [elektronický dokument]. DOI 10.1134/S0036024423050308 In: **Russian Journal of Physical Chemistry A**. Cham: Springer Nature, 2023, Roč. 97, č. 5, s. 997-1006 [tlačená forma] [online]. ISSN 0036-0244. ISSN (online) 1531-863X. - SCO ; CCC ; WOS CC, s. 997 - 1006

2023 [01/20] / **USA** - Tian, Hongyang - Zhang, Houjun - Zhang, Jinli - Han, You. **Nucleation Mechanism of Nano-Iron Oxide in a Supercritical Water Reaction** [elektronický dokument]. DOI 10.1021/acs.jpcc.2c07151 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 3, s. 1507-1518 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; WOS CC, s. 1507 - 1518

2022 [01/20] / **DEU** - Zhang, Y. - Hu, X. - Lin, M. - Liu, A. - Shi, Z. - Wang, Z. **Quantum Chemical Calculation on the Decomposition Mechanism of Na3AlF6** [elektronický dokument] In: **Russian Journal of Physical Chemistry A**. Cham: Springer Nature, 2022, Roč. 96, č. 5, [tlačená forma] [online]. ISSN 0036-0244. ISSN (online) 1531-863X. - SCO, s. 1035 - 1043

2022 [01/20] / **GBR** - Patra, I. - Abdulhadi, A.M. - Fahim, F.S. - Bashar, B.S. - Alawsi, T. - Salmani, M. **The Effects of Temperature and Impact Velocity on the Shock Wave Response of Pore-Embedded Metallic Glasses** In: **Advances in Materials Science and Engineering**, 2022, Roč. 2022. ISSN 1687-6822. - SCO, s. Art. No. 6111294

2020 [01/12] / **USA** - Raynor, S. - Song, H.H. **Development of a Cyclic Periodic Wave Function Approach for the Study of Infinitely Periodic Solid-State Systems** [elektronický dokument] In: **ACS Omega**. Washington: American Chemical Society, 2020, Roč. 5, č. 48, [online]. ISSN (online) 2470-1343. - SCO, s. 31060 - 31068

2020 [01/12] / **GBR** - Parker, S.F. - Ramirez-Cuesta, A.J. - Daemen, L.L. **The structure and vibrational spectroscopy of cryolite, Na3AlF6** [elektronický dokument] In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 10, č. 43, [online]. ISSN (online) 2046-2069. - SCO, s. 25856 - 25863

2020 [01/12] / Li, X. - Li, N. - Liu, W. - Tang, Z. - Wang, J. **Unrevealing the thermophysical properties and microstructural evolution of MgCl2-NaCl-KCl eutectic: FPMD simulations and experimental measurements** In: **Solar Energy Materials and Solar Cells**, 2020, Roč. 210. - SCO, s. Art. No. 110504

2020 [01/12] / **NLD** - Lin, M. - Hu, X. - Shi, Z. - Gao, B. - Yu, J. - Wang, Z. **Existence of Al2F7− in molten MF-AlF3 (M=K, Cs) systems as determined by Raman spectroscopy and structural simulation** In: **Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 44, [tlačená forma] [online]. ISSN 2095-4956. - SCO, s. 19 - 23

2019 [01/12] / **USA** - Filippov, S. - Klarbring, J. - Haussermann, U. - Simak, S.I. **In: Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2019, Roč. 3, č. 2, [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCIE ; WOS CC, s. Art. No. 023602

2018 [01/12] / **NLD** - Gheribi, A.E. - Machado, K. - Zanghi, D. - Bessada, C. - Salanne, M. - Chartrand, P. **In: Electrochimica Acta**: The official journal of the International Society of Electrochemistry (ISE). Amsterdam: Elsevier, 2018, Roč. 274, [tlačená forma] [online]. ISSN 0013-4686. ISSN (online) 1873-3859. - SCIE ; WOS CC, s. 266 - 273

2017 [01/12] / Udovenko, A.A. - Karabtsov, A.A. - Laptash, N.M. **In: Acta Crystallographica Section B-Structural Science Crystal Engineering**, 2017, Roč. 73. - SCIE ; WOS CC, s. 1 - 9

2017 [01/12] / Machado, K. - Zanghi, D. - Sarou-Kanian, V. - Cadars, S. - Burbano, M. - Salanne, M. - Bessada, C. **In: Journal of Physical Chemistry C**, 2017, Roč. 121, č. 19. - SCIE ; WOS CC, s. 10289 - 10297

2017 - **spolu** : **4**

ADC_051: / Kubota, Yoshiyuki (Autor) (40%) - Ohnuma, Toshiharu (Autor) (30%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (30%): **Carbon dioxide capture in 2-aminoethanol aqueous solution from ab initio molecular dynamics simulations**. – text, tab., obr. – [recenzované]. – DOI 10.4467/16890027AP.17.004.6968. – CCC ; SCO ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 146, č. 9 (2017), art. no. 094303, s. [1-9] [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 55
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 2.843 - 2017
SNIP: 0,955 - 2017
SJR: 1,252 - 2017
CiteScore: 5,4 - 2017
Nordic List: 1 - 2017

Ohlasy (9):
2024 [01/20] / **CHE** - Hafizi Yazdabadi, Sahar - Mihrin, Dmytro - Feilberg, Karen Louise - Wugt Larsen, René. **Spectroscopic and Quantum Chemical Evidence of Amine–CO2 and Alcohol–CO2 Interactions: Confirming an Intriguing Affinity of CO2 to Monoethanolamine (MEA)** [elektronický dokument]. DOI 10.3390/molecules29235521 In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 29, č. 23, art. no. 5521 [online]. ISSN (online) 1420-3049. - SCO ; CCC ; WOS CC, s. art. no. 5521

2024 [01/20] / **GBR** - Kechoindi, S. - Ben Yaghlane, S. - Mogren Al Mogren, M. - Bodi, A. - Hochlaf, M. **Photoelectron spectrum and breakdown diagram of ethanolamine: conformers, excited states, and thermochemistry** [elektronický dokument]. DOI 10.1039/d4cp03015j In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2024, Roč. 26, č. 37, s. 24656-24666 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 24656 - 24666

2024 [01/20] / **USA** - Martins-Costa, Marilia T.C. - Ruiz-López, Manuel F. **Reactivity of Monoethanolamine at the Air-Water Interface and Implications for CO2 Capture** [elektronický dokument]. DOI 10.1021/acs.jpcb.3c06856 In: **Journal**

of Physical Chemistry B: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 5, s. 1289-1297 [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCO ; CCC ; WOS CC, s. 1289 - 1297

2023 [01/20] / **USA** - He, Xin - Gao, Yangyan - Shi, Yunlei - Zhang, Xiaowen - Liang, Zhiwu - Zhang, Riguang - Song, Xingfei - Lai, Qinghua - Adidharma, Hertanto - Russell, Armistead G. - Eddings, Eric G. - Fei, Weiyang - Cheng, Fangqin - Tsang, Shik Chi Edman - Wang, Jianji - Fan, Maohong. **[EMmim][NTf2]—a Novel Ionic Liquid (IL) in Catalytic CO2 Capture and ILs' Applications** [elektronický dokument]. DOI 10.1002/advs.202205352 In: **Advanced Science**. Hoboken: John Wiley & Sons. Wiley Blackwell, 2023, Roč. 10, č. 3, art. no. 2205352 [online]. ISSN (online) 2198-3844. - SCO, s.

2023 [01/20] / **DEU** - Xie, Fan - Sun, Wenhao - Pinacho, Pablo - Schnell, Melanie. **CO2 Aggregation on Monoethanolamine: Observations from Rotational Spectroscopy** [elektronický dokument]. DOI 10.1002/anie.202218539 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2023, Roč. 62, č. 14, art. no. e202218539 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Ma, Xinyou - Bryantsev, Vyacheslav S. - Roy, Santanu. **An ab initio free energy study of the reaction mechanism and rate-limiting steps of CO2 capture by aqueous glycine** [elektronický dokument]. DOI 10.1016/j.xcrp.2023.101642 In: **Cell Reports Physical Science**. Cambridge: Elsevier. Cell Press, 2023, Roč. 4, č. 11, art. no. 101642 [tlačená forma] [online]. ISSN (online) 2666-3864. - SCO ; CCC ; WOS CC, s.

2021 [01/20] / **GBR** - Govoni, M. - Whitmer, J. - de Pablo, J. - Gygi, F. - Galli, G. **Code interoperability extends the scope of quantum simulations** [elektronický dokument] In: **npj Computational Materials**. Londýn: Springer Nature. Nature Publishing Group, 2021, Roč. 7, č. 1, [online]. ISSN (online) 2057-3960. - SCIE ; SCO ; WOS CC, s. Art. No. 32

2020 [01/12] / Sakti, A.W. - Nishimura, Y. - Nakai, H. **Recent advances in quantum-mechanical molecular dynamics simulations of proton transfer mechanism in various water-based environments** In: **Wiley Interdisciplinary Reviews: Computational Molecular Science**, 2020, Roč. 10, č. 1. - SCO, s. Art. No. e1419

2018 [01/12] / **USA** - Sevgen, E. - Giberti, F. - Sidky, H. - Whitmer, J.K. - Galli, G. - Gygi, F. - de Pablo, J.J. **In: Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2018, Roč. 14, č. 6, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCIE ; WOS CC, s. 2881 - 2888

ADC_052: / Taifan, William E. (Autor) (40%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (30%) - Baltrušaitis, Jonas (Autor) (30%): **Catalytic conversion of ethanol to 1,3-butadiene on MgO: A comprehensive mechanism elucidation using DFT calculations**. – [recenzované]. – CCC ; SCO ; WOS CC.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – č. 346 (2017), s. 78-91 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 97
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
SNIP: 1,865 - 2017
SJR: 2,397 - 2017
CiteScore: 11,4 - 2017

Ohlasy (94):

2025 [01/20] / **DEU** - Ghoshal, Sourav - Carnegie, Nathaniel - Ezeakunne, Chidozie - Dangi, Beni B. - Kattel, Shyam. **Deciphering Mg-Surface Interactions with Unsaturated Hydrocarbons: An Integrated Experimental-Theoretical Study** [elektronický dokument]. DOI 10.1002/cphc.202401061 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 7, art. no. e202401061 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **USA** - Fung, Victor - Janik, Michael - Crossley, Steven - Chin, Ya Huei Cathy - Savara, Aditya. **Unimolecular and bimolecular reactions of organic intermediates on metal oxide catalysts: an update** [elektronický dokument]. DOI 10.1080/01614940.2024.2354699 In: **Catalysis Reviews - Science and Engineering**. Philadelphia: Taylor & Francis Group, 2025, Roč. 67, č. 4, s. 1060-1125 [tlačená forma] [online]. ISSN 0161-4940. ISSN (online) 1520-5703. - SCO ; CCC ; WOS CC ; SCIE, s. 1060 - 1125

2025 [01/20] / **CHN** - Liu, Na - Wang, Mingkai - Zhou, Yijun - Shao, Lishu - Zhang, Lin - Zhan, Peng - Wu, Zhiping. **Developments of catalysts for the direct conversion of aqueous ethanol to butadiene** [elektronický dokument]. DOI 10.1016/j.greenca.2024.11.008 In: **Green Carbon**. Qingdao : Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, 2025, Roč. 3, č. 3, s. 246-259 [online]. ISSN (online) 29501555. - SCO ; WOS CC ; ESCI ; OA, s. 246 - 259

2025 [01/20] / **USA** - Tian, Song - Lu, Jian - Faria Albanese, Jimmy A. **Fluorination modulates the interaction of water with MgO catalysts during propylene glycol dehydrogenation** [elektronický dokument]. DOI 10.1016/j.jcat.2025.116167 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2025, Roč. 448, art. no. 116167 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 116167

2025 [01/20] / **GBR** - Qi, Xinyu - Geng, Jinglong - Zhao, Siyuan - Ma, Xiaoxun - Dai, Chengyi. **Zr-containing deboronated beta zeolite as a catalyst for the 1,3-butadiene obtaining process from an ethanol-acetaldehyde mixture** [elektronický dokument]. DOI 10.1016/j.fuel.2025.134395 In: **Fuel**: the science and technology of fuel and energy. Oxford: Elsevier, 2025, Roč. 387, art. no. 134395 [tlačená forma] [online]. ISSN 0016-2361. ISSN (online) 1873-7153. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 134395

2025 [01/20] / **USA** - Moskowitz, Benjamin M. - Moon, Jisue - Li, Yuanyuan - Cheng, Yongqiang - Daemen, Luke L. - Lee, Lane - Fung, Victor - Savara, Aditya - Frenkel, Anatoly I. - Wu, Zili - Wachs, Israel E. **Structure–Activity Relationships for Ethanol Dehydrogenation to Acetaldehyde by Silica-Supported Zinc Oxide Catalysts** [elektronický dokument]. DOI 10.1021/acscatal.5c03430 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, s. 17225-17240 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 17225 - 17240

2024 [01/20] / **DEU** - Ishikawa, Wakako - Sato, Shunichi. **Mechanical Interatomic Bond Formation in Ethanol and Methanol–Ethanol Mixture by Laser-Driven Shock Waves** [elektronický dokument]. DOI 10.1002/cphc.202400164 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 25, č. 16, art. no. e202400164 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Wang, Kangzhou - Zhang, Weijie - Gao, Weizhe - Liu, Zhihao - Gao, Xinhua - Ma, Qingxiang - Zhang, Jianli - Zhao, Tian Sheng - Tsubaki, Noritatsu. **Recent advances in tailor-made catalysts for the direct conversion of ethanol to butadiene** [elektronický dokument]. DOI 10.1016/j.fuel.2024.131872 In: **Fuel**: the science and technology of fuel and energy. Oxford: Elsevier, 2024, Roč. 370, [tlačená forma] [online]. ISSN 0016-2361. ISSN (online) 1873-7153. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **NLD** - Chung, Sang–Ho –H - de Miguel, Juan Carlos Navarro - Li, Teng - Lavrik, Polina - Komaty, Sarah - Yuan, Youyou - Poloneeva, Daria - Anbari, Wejdan H. - Hedhili, Mohamed Nejib - Zaarour, Moussa - Martín, Cristina -

Shoinkhorova, Tuiana - Abou–Hamad, Edy - Gascon, Jorge - Ruiz–Martínez, Javier. **Core–shell structured magnesia–silica as a next generation catalyst for one-step ethanol-to-butadiene Lebedev process**. DOI 10.1016/j.apcatb.2023.123628 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2024, Roč. 344, art. no. 123628 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s. art. no. 123628

2024 [01/20] / **NLD** - Ballesteros Plata, D. - Balestra, G. - Cecilia, J. A. - Barroso Martín, I. - Infantes-Molina, A. - Tabanelli, T. - Cavani, F. - López Nieto, J. M. - Montaña, M. - Rodríguez Castellón, E. **On the selective transformation of ethanol over Mg- and/or La-containing mixed oxides catalysts** [elektronický dokument]. DOI 10.1016/j.cattod.2023.114470 In: **Catalysis Today**. Amsterdam: Elsevier. Elsevier Science, 2024, Roč. 429, art. no. 114470 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO ; CCC ; WOS CC, s. art. no. 114470

2024 [01/20] / **GBR** - Wang, Peng - Hou, Shaowen - Tu, Pengxiang - Xue, Bing - Guan, Weixin - Wang, Dong - Zhou, Danfeng - He, Yajun - Chen, Xinhui - Wang, Yixing - Fang, Kegong - Li, Xiaonian - Ni, Jun. **Coordinating the interaction of ZnO and ZrO2 for an efficient ethanol-to-butadiene process** [elektronický dokument]. DOI 10.1039/d3cy01242e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 7, s. 1822-1836 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 1822 - 1836

2024 [01/20] / **GBR** - Xia, Wei - Wang, Xue - Li, Shuangshuang - Jiang, Zhenhua - Chen, Kun - Liu, Dong. **Multiple synergistic roles of Zr modification on ZSM-5 in performant and stable catalyst for ethanol conversion to propene** [elektronický dokument]. DOI 10.1016/j.energy.2023.129910 In: **Energy**: the International Journal. Londýn: Elsevier, 2024, Roč. 288, art. no. 129910 [tlačená forma] [online]. ISSN 0360-5442. ISSN (online) 1873-6785. - SCO ; CCC ; WOS CC, s. art. no. 129910

2024 [01/20] / **CHE** - He, Zhihao - Huang, Teng - Gao, Meiben - Kong, Desong - Li, Meng. **Effect of the Side-Chain Length in Polycarboxylic Superplasticizer on the Competition Adsorption in the Presence of Montmorillonite: A Density Functional Theory Study** [elektronický dokument]. DOI 10.3390/molecules29040752 In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 29, č. 4, art. no. 752 [online]. ISSN (online) 1420-3049. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Fung, Victor - Janik, Michael - Crossley, Steven - Chin, Ya Huei Cathy - Savara, Aditya. **Toward Understanding and Controlling Organic Reactions on Metal Oxide Catalysts** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c02470 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 28, s. 13451-13465 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 13451 - 13465

2023 [01/20] / **DEU** - Chung, Sang Ho - Li, Teng - Shoinkhorova, Tuiana - Komaty, Sarah - Ramirez, Adrian - Mukhambetov, Ildar - Abou-Hamad, Edy - Shterk, Genrikh - Telalovic, Selvedin - Dikhtiarenko, Alla - Sirks, Bart - Lavrik, Polina - Tang, Xinqi - Weckhuysen, Bert M. - Bruijnicx, Pieter C.A. - Gascon, Jorge - Ruiz-Martínez, Javier. **Origin of active sites on silica–magnesia catalysts and control of reactive environment in the one-step ethanol-to-butadiene process** [elektronický dokument]. DOI 10.1038/s41929-023-00945-0 In: **Nature Catalysis**. Berlín: Springer Nature, 2023, Roč. 6, č. 4, s. 363-376. ISSN (online) 2520-1158. - SCO ; CCC ; WOS CC, s. 363 - 376

2023 [01/20] / **CHE** - Bojang, Adama A. - Wu, Ho Shing. **1,3-Butadiene Production Using Ash-Based Catalyst**. DOI 10.3390/catal13020258 In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 2, art. no. 258 [online]. ISSN 2073-4344. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Dochain, Denis D. - Van Den Daelen, Antoine - Styskalik, Ales - Vykoukal, Vit - Debecker, Damien P. **Aerosol-Assisted sol-gel synthesis of mesoporous Ag-Ta-SiO2catalysts for the direct upgrading of ethanol to butadiene** [elektronický dokument]. DOI 10.1039/d2su00080f In: **RSC Sustainability**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 1, č. 3, s. 599-608 [online]. ISSN (online) 2753-8125. - SCO, s. 599 - 608

2022 [01/20] / **GBR** - Zhang, Minhua - Zhou, Baofeng - Chen, Yifei - Gong, Hao. **A multiscale simulation on the formation mechanism of crotonaldehyde and the influence of operating parameters on the process during the production of vinyl acetate from acetylene** [elektronický dokument]. DOI 10.1039/d2re00251e In: **Reaction chemistry & engineering**. Londýn: The Royal Society of Chemistry, 2022, Roč. 44, č. 55, [online]. ISSN (online) 2058-9883. - SCO, s.

2022 [01/20] / **DEU** - Kayanuma, Megumi - Shinke, Yu - Miyazawa, Tomohisa - Fujitani, Tadahiro - Choe, Yoong Kee. **Theoretical study of the side reactions of ethanol-to-butadiene conversion on MgO catalyst: formation of diethyl ether, ethyl acetal, 1,3-butanediol, methyl ethyl ketone, n-butanol, butanal, and acetone** [elektronický dokument]. DOI 10.1007/s00214-022-02927-0 In: **Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2022, Roč. 141, č. 11, art. no. 63 [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCO, s. art. no. 63

2022 [01/20] / **NLD** - Vieira, José Lucas - Destro, Priscila - Laier, Leticia O. - Marques, Clelia M.P. - Gallo, Jean Marcel R. - Bueno, José Maria C. **MgO/SiO2 prepared by wet-kneading as a catalyst for ethanol conversion to 1,3-butadiene: Prins condensation as the predominant mechanism** [elektronický dokument]. DOI 10.1016/j.mcat.2022.112718 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2022, Roč. 532, art. no. 112718 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO, s. art. no. 112718

2022 [01/20] / **NLD** - Chagas, Luciano H. - Zonetti, Priscila C. - Souza, Eugenio F. - Pandoli, Omar G. - Alves, Odivaldo C. - Rabello, Carlos R.K. - Moreira, Carla R. - Silveira, Erika B. - Mendes, Fabiana M.T. - Gaspar, Alexandre B. - Appel, Lucia G. **Sugar-cane based biorefineries: The butadiene synthesis from ethanol employing ZnZr/SiO2 catalyst** [elektronický dokument]. DOI 10.1016/j.mcat.2022.112690 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2022, Roč. 531, art. no. 112690 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO, s. art. no. 112690

2022 [01/20] / **USA** - Rasmussen, Mathew J. - Najmi, Sean - Innocenti, Giada - Medford, Andrew J. - Sievers, Carsten - Medlin, J. Will. **Supported molybdenum oxides for the aldol condensation reaction of acetaldehyde** [elektronický dokument]. DOI 10.1016/j.jcat.2022.03.002 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2022, Roč. 408, s. 216-226 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 216 - 226

2022 [01/20] / **NLD** - Huang, Hengbo - Fang, Ting - Liu, Hui - Zhou, Hao - Chen, Dongfang - Jia, Wenzhi - Liu, Min - Li, Junhui - Zhu, Zhirong. **Ethanol-to-hydrocarbons reaction over HZSM-5: Enhanced ethanol/ethylene into C<inf>3+</inf> hydrocarbons conversion by pristine external Brönsted acid sites** [elektronický dokument]. DOI 10.1016/j.micromeso.2022.111824 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 335, art. no. 111824 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. art. no. 111824

2022 [01/20] / **NLD** - Vieira, J.L. - Destro, P. - Laier, L.O. - Marques, C.M.P. - Gallo, J.M.R. - Bueno, J.M.C. **MgO/SiO2 prepared by wet-kneading as a catalyst for ethanol conversion to 1,3-butadiene: Prins condensation as the predominant mechanism** [elektronický dokument] In: **Molecular Catalysis**. Amsterdam: Elsevier, 2022, Roč. 532, [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO, s. Art. No. 112718

2022 [01/20] / **NLD** - Chagas, L.H. - Zonetti, P.C. - Souza, E.F. - Pandoli, O.G. - Alves, O.C. - Rabello, C.R.K. - Moreira, C.R. - Silveira, E.B. - Mendes, F.M.T. - Gaspar, A.B. - Appel, L.G. **Sugar-cane based biorefineries: The butadiene synthesis from ethanol employing ZnZr/SiO2 catalyst** [elektronický dokument] In: **Molecular Catalysis**. Amsterdam: Elsevier, 2022, Roč. 531, [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO, s. Art. No. 112690

2022 [01/20] / **NLD** - Huang, H. - Fang, T. - Liu, H. - Zhou, H. - Chen, D. - Jia, W. - Liu, M. - Li, J. - Zhu, Z. **Ethanol-to-hydrocarbons reaction over HZSM-5: Enhanced ethanol/ethylene into C3+ hydrocarbons conversion by pristine external Bronsted acid sites** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2022, Roč. 335, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 111824

2021 [01/20] / **USA** - Anpo, M. - Costentin, G. - Giamello, E. - Lauron-Pernot, H. - Sojka, Z. **Characterisation and reactivity of oxygen species at the surface of metal oxides** [elektronický dokument]. DOI 10.1016/j.jcat.2020.10.011 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 393, s. 259-280 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. 259 - 280

2021 [01/20] / **GBR** - Metzker, Gustavo - Vargas, Jorge Andrés Mora - Boscolo, Mauricio. **Heterogeneous catalytic ethanol transformation into chemicals: Some Brazilian contributions**. DOI 10.1016/bs.adioch.2021.02.005 In: **Catalysis in Biomass Conversion**. Londýn: Elsevier. Academic Press, 2021, s. 343-375 [tlačená forma]. ISBN 978-0-323-85058-2. - SCO, s. 343 - 375

2021 [01/20] / **NLD** - Xia, W. - Wang, J. - Wang, L. - Qian, C. - Ma, C. - Huang, Y. - Fan, Y. - Hou, M. - Chen, K. **Ethylene and propylene production from ethanol over Sr/ZSM-5 catalysts: A combined experimental and computational study** In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2021, Roč. 294, [tlačená forma]. ISSN 0926-3373. - SCO, s. Art. No. 120242

2021 [01/20] / **NLD** - Huo, X. - Conklin, D.R. - Zhou, M. - Vorotnikov, V. - Assary, R.S. - Purdy, S.C. - Page, K. - Li, Z. - Unocic, K.A. - Balderas, R.I. - Richards, R.M. - Vardon, D.R. **Catalytic activity and water stability of the MgO(111) surface for 2-pentanone condensation** In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2021, Roč. 294, [tlačená forma]. ISSN 0926-3373. - SCO, s. Art. No. 120234

2021 [01/20] / **NLD** - Tiewcharoen, S. - Maihom, T. - Sittiwong, J. - Limtrakul, J. **The influence of cation exchange and tetravalent metal substitutions in Lewis acidic BEA zeolites for phenol adsorption and Tautomerization: A computational study** [elektronický dokument] In: **Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2021, Roč. 780, [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCO, s. Art. No. 138886

2021 [01/20] / **GBR** - Tian, X. - Tian, H. **Roles of ethanol and Si-OH in the aldol condensation of ethyl acetate over a Cs/SBA-15 catalyst** In: **Reaction Chemistry and Engineering**, 2021, Roč. 6, č. 6. - SCO, s. 1002 - 1015

2021 [01/20] / **NLD** - Cabello Gonzalez, G.M. - Villanueva Perales, A.L. - Campoy, M. - Lopez Beltran, J.R. - Martinez, A. - Vidal-Barrero, F. **Kinetic modelling of the one-step conversion of aqueous ethanol into 1,3-butadiene over a mixed hemimorphite-HfO2/SiO2 catalyst** [elektronický dokument] In: **Fuel Processing Technology**. Amsterdam: Elsevier, 2021, Roč. 216, [tlačená forma] [online]. ISSN 0378-3820. ISSN (online) 1873-7188. - SCO, s. Art. No. 106767

2021 [01/20] / **USA** - Khivantsev, K. - Vityuk, A. - Aleksandrov, H.A. - Vayssilov, G.N. - Alexeev, O.S. - Amiridis, M.D. **Catalytic conversion of ethene to butadiene or hydrogenation to ethane on HY zeolite-supported rhodium complexes: Cooperative support/Rh-center route** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 18, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 184706

2021 [01/20] / **USA** - Butera, V. - Tanabe, Y. - Shinke, Y. - Miyazawa, T. - Fujitani, T. - Kayanuma, M. - Choe, Y.-K. **Mechanistic investigation on ethanol-to-butadiene conversion reaction over metal oxide clusters** In: **: International journal of quantum chemistry,** 2021, Roč. 121, č. 5. - SCO, s. Art. No. e26494

2021 [01/20] / **CHE** - Chung, S.-H. - Ramirez, A. - Shoinkhorova, T. - Mukhambetov, I. - Abou-Hamad, E. - Telalovic, S. - Gascon, J. - Ruiz-Martinez, J. **The importance of thermal treatment on wet-kneaded silica-magnesia catalyst and lebedev ethanol-to-butadiene process** [elektronický dokument] In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 11, č. 3, [online]. ISSN (online) 2079-4991. - SCO, s. Art. No. 579

2021 [01/20] / **USA** - Zhang, M. - Li, R. - Wu, Y. - Yu, Y. **Mechanistic insights into the meerwein-ponndorf-verley reaction and relative side reactions over mgo in the process of ethanol to 1,3-butadiene: A DFT study** In: **Industrial**

and Engineering Chemistry Research, 2021, Roč. 60, č. 7. - SCO, s. 2871 - 2880

2021 [01/20] / **NLD** - Metzker, G. - Vargas, J.A.M. - Boscolo, M. **Heterogeneous catalytic ethanol transformation into chemicals: Some Brazilian contributions** In: **Advances in Inorganic Chemistry**. Amsterdam: Elsevier, 2021. - SCO, s. 343 - 375

2021 [01/20] / **NLD** - Xia, Wei - Wang, Junguo - Wang, Longxiang - Qian, Chen - Ma, Chao - Huang, Yaxin - Fan, Yu - Hou, Mengda - Chen, Kun. **Ethylene and propylene production from ethanol over Sr/ZSM-5 catalysts: A combined experimental and computational study**. DOI 10.1016/j.apcatb.2021.120242 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2021, Roč. 294, art. no. 120242 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s. art. no. 120242

2021 [01/20] / **NLD** - Yan, Hao - Yao, Shuang - Zhao, Siming - Liu, Mengyuan - Zhang, Wenxiang - Zhou, Xin - Zhang, Guangyu - Jin, Xin - Liu, Yibin - Feng, Xiang - Chen, Xiaobo - Chen, De - Yang, Chaohe. **Insight into the basic strength-dependent catalytic performance in aqueous phase oxidation of glycerol to glyceric acid** [elektronický dokument]. DOI 10.1016/j.ces.2020.116191 In: **Chemical Engineering Science**. Amsterdam: Elsevier, 2021, č. 230, art. no. 116191 [tlačená forma]. ISSN 0009-2509. ISSN (online) 1873-4405. - SCO ; CCC ; WOS CC, s. art. no. 116191

2021 [01/20] / **USA** - Zhang, Minhua - Li, Ruishen - Wu, Yufei - Yu, Yingzhe. **Mechanistic insights into the meerwein-ponndorf-verley reaction and relative side reactions over mgo in the process of ethanol to 1,3-butadiene: A DFT study** [elektronický dokument]. DOI 10.1021/acs.iecr.0c05915 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2021, Roč. 60, č. 7, s. 2871-2880 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO ; CCC ; WOS CC, s. 2871 - 2880

2021 [01/20] / **CHE** - Chung, Sang Ho - Ramirez, Adrian - Shoinkhorova, Tuiana - Mukhambetov, Ildar - Abou-Hamad, Edy - Telalovic, Selevedin - Gascon, Jorge - Ruiz-Martínez, Javier. **The importance of thermal treatment on wet-kneaded silica–magnesia catalyst and lebedev ethanol-to-butadiene process** [elektronický dokument]. DOI 10.3390/nano11030579 In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 11, č. 3, s. 1-17 [online]. ISSN (online) 2079-4991. - SCO ; CCC ; WOS CC, s. 1 - 17

2021 [01/20] / **USA** - Butera, Valeria - Tanabe, Yusuke - Shinke, Yu - Miyazawa, Tomohisa - Fujitani, Tadahiro - Kayanuma, Megumi - Choe, Yoong Kee. **Mechanistic investigation on ethanol-to-butadiene conversion reaction over metal oxide clusters** [elektronický dokument]. DOI 10.1002/qua.26494 In: **International Journal of Quantum Chemistry**. Hoboken: John Wiley & Sons, 2021, Roč. 121, č. 5, art. no. e26494 [tlačená forma] [online]. ISSN 0020-7608. ISSN (online) 1097-461X. - SCO ; CCC ; WOS CC, s. art. no. e26494

2021 [01/20] / **USA** - Khivantsev, Konstantin - Vityuk, Artem - Aleksandrov, Hristiyan A. - Vayssilov, Georgi N. - Alexeev, Oleg S. - Amiridis, Michael D. **Catalytic conversion of ethene to butadiene or hydrogenation to ethane on HY zeolite-supported rhodium complexes: Cooperative support/Rh-center route** [elektronický dokument]. DOI 10.1063/5.0042322 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2021, Roč. 154, č. 18, art. no. 184706 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 184706

2021 [01/20] / **NLD** - Cabello González, G. M. - Villanueva Perales, A. L. - Campoy, M. - López Beltran, J. R. - Martínez, A. - Vidal-Barrero, F. **Kinetic modelling of the one-step conversion of aqueous ethanol into 1,3-butadiene over a mixed hemimorphite-HfO2/SiO2 catalyst** [elektronický dokument]. DOI 10.1016/j.fuproc.2021.106767 In: **Fuel Processing Technology**. Amsterdam: Elsevier, 2021, Roč. 216, art. no. 106767 [tlačená forma] [online]. ISSN 0378-3820. ISSN (online) 1873-7188. - SCO ; CCC ; WOS CC, s. art. no. 106767

2021 [01/20] / **GBR** - Tian, Xiang - Tian, Hengshui. **Roles of ethanol and Si-OH in the aldol condensation of ethyl acetate over a Cs/SBA-15 catalyst** [elektronický dokument]. DOI 10.1039/d1re00020a In: **Reaction chemistry & engineering**. Londýn: The Royal Society of Chemistry, 2021, Roč. 6, č. 6, s. 1002-1015 [online]. ISSN (online) 2058-9883.

- SCO ; CCC ; WOS CC, s. 1002 - 1015

2021 [01/20] / **NLD** - Tiewcharoen, Supakit - Maihom, Thana - Sittiwong, Jarinya - Limtrakul, Jumras. **The influence of cation exchange and tetravalent metal substitutions in Lewis acidic BEA zeolites for phenol adsorption and Tautomerization: A computational study** [elektronický dokument]. DOI 10.1016/j.cplett.2021.138886 In: **Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2021, Roč. 780, art. no. 138886 [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCO ; CCC ; WOS CC, s. art. no. 138886

2021 [01/20] / **NLD** - Huo, Xiangchen - Conklin, Davis R. - Zhou, Mingxia - Vorotnikov, Vassili - Assary, Rajeev S. - Purdy, Stephen C. - Page, Katharine - Li, Zhenglong - Unocic, Kinga A. - Balderas, Raiven I. - Richards, Ryan M. - Vardon, Derek R. **Catalytic activity and water stability of the MgO(111) surface for 2-pentanone condensation**. DOI 10.1016/j.apcatb.2021.120234 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2021, Roč. 294, art. no. 120234 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s. art. no. 120234

2021 [01/20] / **CHE** - Liu, Cheng - Li, Yan - Wu, Linlin - Geng, Zhongfeng. **Synthesis of 1,3-butadiene from ethanol/acetaldehyde over ZrO2-MgO-SiO2 catalyst: The thermodynamics and reaction kinetics analysis** [elektronický dokument]. DOI 10.1016/j.cej.2020.127861 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2021, č. 421, art. no. 127861 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 127861

2020 [01/20] / **NLD** - Li, Houqian - Pang, Jifeng - Jaegers, Nicholas R. - Kovarik, Libor - Engelhard, Mark - Savoy, Anthony W. - Hu, Jianzhi - Sun, Junming - Wang, Yong. **Conversion of ethanol to 1,3–butadiene over Ag–ZrO2/SiO2 catalysts: The role of surface interfaces**. DOI 10.1016/j.jechem.2020.05.038 In: **Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 54, s. 7-15 [tlačená forma] [online]. ISSN 2095-4956. - SCO, s. 7 - 15

2020 [01/20] / **DEU** - Bin Samsudin, Ismail - Zhang, Hongwei - Jaenicke, Stephan - Chuah, Gaik Khuan. **Recent Advances in Catalysts for the Conversion of Ethanol to Butadiene** [elektronický dokument]. DOI 10.1002/asia.202001023 In: **Chemistry - An Asian Journal**. Weinheim: John Wiley & Sons. Wiley-VCH, 2020, Roč. 15, č. 24, s. 4199-4214 [tlačená forma] [online]. ISSN 1861-4728. ISSN (online) 1861-471X. - SCO ; CCC ; WOS CC, s. 4199 - 5214

2020 [01/20] / **NLD** - Orazi, V. - Juan, A. - González, E. A. - Marchetti, Jorge M. - Jasen, P. V. **DFT study of ethanol adsorption on CaO(0 0 1) surface** [elektronický dokument]. DOI 10.1016/j.apsusc.2019.144254 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, č. 500, art. no. 144254 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. art. no. 144254

2020 [01/20] / **GBR** - Yan, Bing - Wang, Luyi - Wang, Bolong - Chen, Quanxin - Liu, Chunjing - Li, Jian - Jiang, Tao. **Carbon material-supported Fe<inf>7</inf>C<inf>3</inf>@FeO nanoparticles: A highly efficient catalyst for carbon dioxide reduction with 1-butene** [elektronický dokument]. DOI 10.1039/d0re00249f In: **Reaction chemistry & engineering**. Londýn: The Royal Society of Chemistry, 2020, Roč. 5, č. 11, s. 2101-2108 [online]. ISSN (online) 2058-9883. - SCO, s. 2101 - 2108

2020 [01/20] / **DEU** - Yan, Bing - Wang, Luyi - Chen, Quanxin - Dou, Hongxin - Liu, Chunjing - Li, Jian - Jiang, Tao. **Highly Selective Conversion of 1-Butene to 1,3-Butadiene under CO<inf>2</inf> Atmosphere over an Alumina-supported Iron-based Catalyst: The Role of Brønsted Acids and Lewis Acids** [elektronický dokument]. DOI 10.1002/slct.202003195 In: **Chemistry Select**. Weinheim: John Wiley & Sons. Wiley-VCH, 2020, Roč. 5, č. 36, s. 11237-11241 [online]. ISSN (online) 2365-6549. - SCO, s. 11237 - 11241

2020 [01/20] / **DEU** - Kyriienko, P. I. - Larina, O. V. - Soloviev, S. O. - Orlyk, S. M. **Catalytic Conversion of Ethanol Into 1,3-Butadiene: Achievements and Prospects: A Review** [elektronický dokument]. DOI 10.1007/s11237-020-09654-2 In: **Theoretical and Experimental Chemistry**. Berlín: Springer Nature, 2020, Roč. 56, č. 4, s. 213-242 [tlačená forma]

[online]. ISSN 0040-5760. ISSN (online) 1573-935X. - SCO, s. 213 - 242

2020 [01/20] / **NLD** - Yue, Chuan Jun - Chen, Huang Li - Gu, Li Ping - Zheng, Ji Wei - Zhuang, Ya Feng. **Synthesis of crotonic acid from ethanol by sequential catalysis** [elektronický dokument]. DOI 10.1016/j.scp.2020.100288 In: **Sustainable chemistry and pharmacy**. Amsterdam: Elsevier, 2020, Roč. 17, art. no. 100288 [online]. ISSN (online) 2352-5541. - SCO, s. art. no. 100288

2020 [01/20] / **GBR** - Pomalaza, Guillaume - Arango Ponton, Paola - Capron, Mickaël - Dumeignil, Franck. **Ethanol-to-butadiene: The reaction and its catalysts** [elektronický dokument]. DOI 10.1039/d0cy00784f In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 10, č. 15, s. 4860-4911 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 4860 - 4911

2020 [01/20] / **NLD** - Yang, Yao - Wang, Duo - Jiang, Pengfei - Gao, Wenliang - Cong, Rihong - Yang, Tao. **Structure-induced Lewis-base Ga4B2O9 and its superior performance in Knoevenagel condensation reaction** [elektronický dokument]. DOI 10.1016/j.mcat.2020.110914 In: **Molecular Catalysis**. Amsterdam: Elsevier, 2020, Roč. 490, art. no. 110914 [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO, s. art. no. 110914

2020 [01/20] / **USA** - Abdulrazzaq, Hussein T. - Rahmani Chokanlu, Amir - Frederick, Brian G. - Schwartz, Thomas J. **Reaction Kinetics Analysis of Ethanol Dehydrogenation Catalyzed by MgO-SiO<inf>2</inf>** [elektronický dokument]. DOI 10.1021/acscatal.0c00811 In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 11, s. 6318-6331 [online]. ISSN (online) 2155-5435. - SCO, s. 6318 - 6331

2020 [01/12] / **NLD** - Orazi, V. - Juan, A. - Gonzalez, E.A. - Marchetti, J.M. - Jasen, P.V. **In: Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2020, Roč. 500, [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCIE ; WOS CC, s. Art. No. UNSP

2020 [01/12] / **DEU** - Bin Samsudin, I. - Zhang, H. - Jaenicke, S. - Chuah, G.-K. **Recent Advances in Catalysts for the Conversion of Ethanol to Butadiene** [elektronický dokument] In: **Chemistry - An Asian Journal**. Weinheim: John Wiley & Sons. Wiley-VCH, 2020, Roč. 15, č. 24, [tlačená forma] [online]. ISSN 1861-4728. ISSN (online) 1861-471X. - SCO, s. 4199 - 4214

2020 [01/12] / **GBR** - Yan, B. - Wang, L. - Wang, B. - Chen, Q. - Liu, C. - Li, J. - Jiang, T. **Carbon material-supported Fe7C3@FeO nanoparticles: A highly efficient catalyst for carbon dioxide reduction with 1-butene** In: **Reaction Chemistry and Engineering**, 2020, Roč. 5, č. 11. - SCO, s. 2101 - 2108

2020 [01/12] / Yan, B. - Wang, L. - Chen, Q. - Dou, H. - Liu, C. - Li, J. - Jiang, T. **Highly Selective Conversion of 1-Butene to 1,3-Butadiene under CO2 Atmosphere over an Alumina-supported Iron-based Catalyst: The Role of Bronsted Acids and Lewis Acids** In: **ChemistrySelect**, 2020, Roč. 5, č. 36. - SCO, s. 11237 - 11241

2020 [01/12] / **NLD** - Yue, C.-J. - Chen, H.-L. - Gu, L.-P. - Zheng, J.-W. - Zhuang, Y.-F. **Synthesis of crotonic acid from ethanol by sequential catalysis** [elektronický dokument] In: **Sustainable chemistry and pharmacy**. Amsterdam: Elsevier, 2020, Roč. 17, [online]. ISSN (online) 2352-5541. - SCO, s. Art. No. 100288

2020 [01/12] / Kyriienko, P.I. - Larina, O.V. - Soloviev, S.O. - Orlyk, S.M. **Catalytic Conversion of Ethanol Into 1,3-Butadiene: Achievements and Prospects: A Review** In: **Theoretical and Experimental Chemistry**, 2020, Roč. 56, č. 4. - SCO, s. 213 - 242

2020 [01/12] / **GBR** - Pomalaza, G. - Arango Ponton, P. - Capron, M. - Dumeignil, F. **Ethanol-to-butadiene: The reaction and its catalysts** [elektronický dokument] In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2020, Roč. 10, č. 15, [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 4860 - 4911

2020 [01/12] / **NLD** - Yang, Y. - Wang, D. - Jiang, P. - Gao, W. - Cong, R. - Yang, T. **Structure-induced Lewis-base Ga4B2O9 and its superior performance in Knoevenagel condensation reaction** [elektronický dokument] In: **Molecular Catalysis**. Amsterdam: Elsevier, 2020, Roč. 490, [tlačená forma] [online]. ISSN 2468-8274. ISSN (online) 2468-8231. - SCO, s. Art. No. 110914

2020 [01/12] / **USA** - Abdulrazzaq, H.T. - Rahmani Chokanlu, A. - Frederick, B.G. - Schwartz, T.J. **Reaction Kinetics Analysis of Ethanol Dehydrogenation Catalyzed by MgO-SiO2** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 11, [online]. ISSN (online) 2155-5435. - SCO, s. 6318 - 6331

2020 [01/12] / **NLD** - Li, H. - Pang, J. - Jaegers, N.R. - Kovarik, L. - Engelhard, M. - Savoy, A.W. - Hu, J. - Sun, J. - Wang, Y. **Conversion of ethanol to 1,3-butadiene over Ag-ZrO2/SiO2 catalysts: The role of surface interfaces** In: **Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 54, [tlačená forma] [online]. ISSN 2095-4956. - SCO, s. 7 - 15

2019 [01/12] / **NLD** - Durgalakshmi, D. - Ajay Rakkesh, R. - Kamil, S. - Karthikeyan, S. - Balakumar, S. **In: Journal of Inorganic and Organometallic Polymers and Materials**. Amsterdam: Springer Nature, 2019, Roč. 29, č. 4, [tlačená forma] [online]. ISSN 1574-1443. ISSN (online) 1574-1451. - SCIE ; WOS CC, s. 1390 - 1399

2019 [01/12] / **USA** - Grim, R.G. - To, A.T. - Farberow, C.A. - Hensley, J.E. - Ruddy, D.A. - Schaidle, J.A. **In: ACS Catalysis**. Washington: American Chemical Society, 2019, Roč. 9, č. 5, [online]. ISSN (online) 2155-5435. - SCIE ; WOS CC, s. 4145 - 4172

2019 [01/12] / **GBR** - Chen, D. - Wang, W.J. - Liu, C.L. **In: International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2019, Roč. 44, č. 13, [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCIE ; WOS CC, s. 6560 - 6572

2019 [01/12] / Yan, B. - Wang, L.Y. - Wang, B.L. - Alam, F. - Xiao, Z.Z. - Li, J. - Jiang, T. **In: Applied Catalysis A-General**, 2019, Roč. 572. - SCIE ; WOS CC, s. 71 - 79

2019 [01/12] / Rosset, M. - Perez-Lopez, O.W. **In: Reaction Kinetics Mechanisms and Catalysis**, 2019, Roč. 126, č. 1. - SCIE ; WOS CC, s. 497 - 511

2019 [01/12] / Gonzalez, G.M.C. - Murciano, R. - Perales, A.L.V. - Martinez, A. - Vidal-Barrero, F. - Campoy, M. **In: Applied Catalysis A-General**, 2019, Roč. 570. - SCIE ; WOS CC, s. 96 - 106

2019 [01/12] / **USA** - Yan, H. - Zhao, S.M. - Yao, S. - Liang, W. - Feng, X. - Jin, X. - Chen, X.B. - Liu, Y.B. - Yang, C.H. **In: Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2019, Roč. 58, č. 44, [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCIE ; WOS CC, s. 20259 - 20269

2019 [01/20] / **GBR** - Liu, Jiwei - Jiang, Jianguo - Aihemaiti, Aikelaimu - Meng, Yuan - Yang, Meng - Xu, Yiwen - Gao, Yuchen - Zou, Quan - Chen, Xuejing. **Removal of phosphate from aqueous solution using MgO-modified magnetic biochar derived from anaerobic digestion residue** [elektronický dokument]. DOI 10.1016/j.jenvman.2019.109438 In: **Journal of Environmental Management**. Londýn: Elsevier. Academic Press, 2019, Roč. 250, art. no. 109438 [tlačená forma] [online]. ISSN 0301-4797. ISSN (online) 1095-8630. - SCO, s. art. no. 109438

2019 [01/20] / **USA** - Yan, Hao - Zhao, Siming - Yao, Shuang - Liang, Wei - Feng, Xiang - Jin, Xin - Chen, Xiaobo - Liu, Yibin - Yang, Chaohe. **Influence of Lewis Acid on the Activity and Selectivity of Pt/MCM-41 (Al) Catalysts for Oxidation of C<inf>3</inf> Polyols in Base-Free Medium** [elektronický dokument]. DOI 10.1021/acs.iecr.9b04478 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2019, Roč. 58, č. 44, s. 20259-20269 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO, s. 20259 - 20269

2019 [01/20] / **NLD** - Durgalakshmi, D. - Ajay Rakkesh, R. - Kamil, Syed - Karthikeyan, S. - Balakumar, S. **Rapid Dilapidation of Alcohol Using Magnesium Oxide and Magnesium Aspartate based Nanostructures: A Raman Spectroscopic and Molecular Simulation Approach** [elektronický dokument]. DOI 10.1007/s10904-019-01105-3 In: **Journal of Inorganic and Organometallic Polymers and Materials**. Amsterdam: Springer Nature, 2019, Roč. 29, č. 4, s. 1390-1399 [tlačená forma] [online]. ISSN 1574-1443. ISSN (online) 1574-1451. - SCO, s. 1390 - 1399

2019 [01/20] / **USA** - Grim, R. Gary - To, Anh T. - Farberow, Carrie A. - Hensley, Jesse E. - Ruddy, Daniel A. - Schaidle, Joshua A. **Growing the Bioeconomy through Catalysis: A Review of Recent Advancements in the Production of Fuels and Chemicals from Syngas-Derived Oxygenates** [elektronický dokument]. DOI 10.1021/acscatal.8b03945 In: **ACS Catalysis**. Washington: American Chemical Society, 2019, Roč. 9, č. 5, s. 4145-4172 [online]. ISSN (online) 2155-5435. - SCO, s. 4145 - 4172

2019 [01/20] / **USA** - Zhao, Guo Ming - Sun, Wang Jie - Zhang, Hai Long - Li, Da Lei - Yang, Xue. **DFT study on selective autocatalyzed A-alkylation of ketones with alcohols** [elektronický dokument]. DOI 10.1016/j.jcat.2019.03.033 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2019, Roč. 373, s. 126-138 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 126 - 138

2019 [01/20] / **GBR** - Chen, Dong - Wang, Wenju - Liu, Chenlong. **Ni-encapsulated graphene chainmail catalyst for ethanol steam reforming** [elektronický dokument]. DOI 10.1016/j.ijhydene.2019.01.204 In: **International Journal of Hydrogen Energy**: Official Journal of the International Association for Hydrogen Energy. Amsterdam: Elsevier, 2019, Roč. 44, č. 13, s. 6560-6572 [tlačená forma] [online]. ISSN 0360-3199. ISSN (online) 1879-3487. - SCO, s. 6560 - 6572

2019 [01/20] / **GBR** - Pang, Jifeng - Zheng, Mingyuan - Zhang, Tao. **Synthesis of ethanol and its catalytic conversion**. DOI 10.1016/bs.acat.2019.08.001 In: **Advances in Catalysis**. Londýn: Elsevier. Academic Press, 2019, s. 89-191. ISBN 978-0-12-817099-1. ISSN 0360-0564. - SCO, s. 89 - 191

2019 [01/20] / **NLD** - Yan, Bing - Wang, Luyi - Wang, Bolong - Alam, Fakhre - Xiao, Zaozao - Li, Jian - Jiang, Tao. **Constructing a high-efficiency iron-based catalyst for carbon dioxide oxidative dehydrogenation of 1-butene: The role of oxygen mobility and proposed reaction mechanism**. DOI 10.1016/j.apcata.2018.12.025 In: **Applied catalysis A, General**: An International Journal Devoted to Catalytic Science and its Applications. Amsterdam: Elsevier, 2019, Roč. 572, s. 71-79 [tlačená forma]. ISSN 0926-860X. - SCO, s. 71 - 79

2019 [01/20] / **NLD** - Rosset, Morgana - Perez-Lopez, Oscar W. **Cu–Ca–Al catalysts derived from hydrocalumite and their application to ethanol dehydrogenation** [elektronický dokument]. DOI 10.1007/s11144-018-1513-y In: **Reaction Kinetics, Mechanisms and Catalysis**. Dordrecht: Springer Nature. Springer, 2019, Roč. 126, č. 1, s. 497-511 [tlačená forma]. ISSN 1878-5190. ISSN (online) 1878-5204. - SCO, s. 497 - 511

2019 [01/20] / **USA** - Yan, Hao - Qin, Hansong - Feng, Xiang - Jin, Xin - Liang, Wei - Sheng, Nan - Zhu, Chao - Wang, Hongmei - Yin, Bin - Liu, Yibin - Chen, Xiaobo - Yang, Chaohe. **Synergistic Pt/MgO/SBA-15 nanocatalysts for glycerol oxidation in base-free medium: Catalyst design and mechanistic study** [elektronický dokument]. DOI 10.1016/j.jcat.2019.01.015 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2019, Roč. 370, s. 434-446 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 434 - 446

2019 [01/20] / **NLD** - Cabello González, G. M. - Murciano, R. - Villanueva Perales, A. L. - Martínez, A. - Vidal-Barrero, F. - Campoy, M. **Ethanol conversion into 1,3-butadiene over a mixed Hf-Zn catalyst: A study of the reaction pathway and catalyst deactivation**. DOI 10.1016/j.apcata.2018.11.010 In: **Applied catalysis A, General**: An International Journal Devoted to Catalytic Science and its Applications. Amsterdam: Elsevier, 2019, Roč. 570, s. 96-106 [tlačená forma]. ISSN 0926-860X. - SCO, s. 96 - 106

2019 [01/20] / **DEU** - Deepankeaw, Nutsara - Maihom, Thana - Probst, Michael - Prasertsab, Anittha - Homlamai, Kan - Sittiwong, Jarinya - Limtrakul, Jumras. **Phenol Tautomerization Catalyzed by Acid-Base Pairs in Lewis Acidic Beta**

Zeolites: A Computational Study [elektronický dokument]. DOI 10.1002/cphc.201900377 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2019, Roč. 20, č. 16, s. 2122-2126 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO, s. 2122 - 2126

2018 [01/20] / **USA** - Xia, Wei - Wang, Fangfang - Wang, Longxiang - Wang, Junguo - Mu, Xichuan - Chen, Kun. **High Performance SiO2–ZrO2 Binary Oxide for Ethanol Conversion to Ethylene** [elektronický dokument]. DOI 10.1007/s10562-018-2500-7 In: **Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2018, Roč. 148, č. 10, s. 3024-3034 [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCO, s. 3024 - 3034

2018 [01/20] / **DEU** - Farrar-Tobar, Ronald A. - Wei, Zhihong - Jiao, Haijun - Hinze, Sandra - de Vries, Johannes G. **Selective Base-free Transfer Hydrogenation of α,β-Unsaturated Carbonyl Compounds using iPrOH or EtOH as Hydrogen Source** [elektronický dokument]. DOI 10.1002/chem.201705423 In: **Chemistry - A European Journal**. Weinheim: John Wiley & Sons. Wiley-VCH, 2018, Roč. 24, č. 11, s. 2725-2734 [tlačená forma] [online]. ISSN 0947-6539. ISSN (online) 1521-3765. - SCO, s. 2725 - 2734

2018 [01/20] / **NLD** - Zhang, Minhua - Zhuang, Jianyu - Yu, Yingzhe. **A DFT study on ZrO 2 surface in the process of ethanol to 1,3-butadiene: A comprehensive mechanism elucidation** [elektronický dokument]. DOI 10.1016/j.apsusc.2018.07.115 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 458, s. 1026-1034 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. 1026 - 1034

2018 [01/20] / **NLD** - Wang, Fangfang - Xia, Wei - Mu, Xichuan - Chen, Kun - Si, Huimin - Li, Zhihao. **A combined experimental and theoretical study on ethanol conversion to propylene over Y/ZrO <inf>2</inf> catalyst** [elektronický dokument]. DOI 10.1016/j.apsusc.2017.12.253 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2018, Roč. 439, s. 405-412 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO, s. 405 - 412

2018 [01/20] / **USA** - Bing, Weihan - Zheng, Lei - He, Shan - Rao, Deming - Xu, Ming - Zheng, Lirong - Wang, Bin - Wang, Yangdong - Wei, Min. **Insights on Active Sites of CaAl-Hydrotalcite as a High-Performance Solid Base Catalyst toward Aldol Condensation** [elektronický dokument]. DOI 10.1021/acscatal.7b03022 In: **ACS Catalysis**. Washington: American Chemical Society, 2018, Roč. 8, č. 1, s. 656-664 [online]. ISSN (online) 2155-5435. - SCO, s. 656 - 664

2017 [01/20] / **GBR** - Fan, Dan - Dong, Xiuqin - Yu, Yingzhe - Zhang, Minhua. **A DFT study on the aldol condensation reaction on MgO in the process of ethanol to 1,3-butadiene: Understanding the structure-activity relationship** [elektronický dokument]. DOI 10.1039/c7cp04502f In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2017, Roč. 19, č. 37, s. 25671-25682 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 25671 - 25682

ADC_053: / Bučko, Tomáš (Autor) [UKOPRCFZ] (90%) - Chibani, Siwar (Autor) (1%) - Paul, Jean-Francois (Autor) (1%) - Cantrel, Laurent (Autor) (1%) - Badawi, Michael (Autor) (7%): **Dissociative iodomethane adsorption on Ag-MOR and the formation of AgI clusters: an ab initio molecular dynamics study**. – text, obr. – [recenzované]. – DOI 10.1039/c7cp05562e. – CCC ; SCO ; SCIE ; OA ; WOS CC.
In: *Physical Chemistry Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Londýn (Veľká Británia) : The Royal Society of Chemistry, Cambridge (Veľká Británia) : The Royal Society of Chemistry. – ISSN 1463-9076. – ISSN (online) 1463-9084. – Roč. 19, č. 40 (2017), s. 27530-27543 [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]

Lit.: 64
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 3,906 - 2017
SNIP: 1,072 - 2017
SJR: 1,686 - 2017
CiteScore: 7,0 - 2017
Kvartil Q:
2017, JIF - Physics, atomic, molecular & chemical - Q1; **2017, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (22):

2025 [01/20] / **USA** - Plessow, Philipp N. **Anharmonic Adsorption Free Energies and Apparent Activation Barriers for Mobile Reactants Based on Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jctc.5c01100 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 17, s. 8518-8532 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 8518 - 8532

2025 [01/20] / **GBR** - De, Arup K. - Srivastava, Ravishankar - Das, Nirupam - Pattader, Partho Sarathi Gooh - Kar, Rajiv K. **Mechanistic insights on sulfur functionalization of Ag nanoflowers** [elektronický dokument]. DOI 10.1039/d5cp00645g In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2025, Roč. 27, č. 24, s. 13157-13166 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 13157 - 13166

2024 [01/20] / **CHE** - Elmekawy, Ahmed - Quach, Qui - Abdel-Fattah, Tarek M. **Synthesis and Characterization of Silver-Modified Nanoporous Silica Materials for Enhanced Iodine Removal** [elektronický dokument]. DOI 10.3390/nano14131143 In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 14, č. 13, art. no. 1143 [online]. ISSN (online) 2079-4991. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Li, Qian - Ding, Yan - Cong, Erli - Xu, Shijia - Li, Lanxin - Ma, Xinchi - Xiao, Songtao - Gao, Chenyu - Yang, Libin. **Regulation pore size distribution of FAU deposited by Ag-oxide nanoparticles with F anions corrosion for the adsorption of CH3I** [elektronický dokument]. DOI 10.1007/s10853-024-09738-7 In: **Journal of Materials Science**. Norwell: Springer Nature. Springer International Publishing AG, 2024, Roč. 59, č. 21, s. 9276-9290 [tlačená forma] [online]. ISSN 0022-2461. ISSN (online) 1573-4803. - SCO ; CCC ; WOS CC, s. 9276 - 9290

2024 [01/20] / **DEU** - Tian, Zhenjiang - Hao, Yuxun - Chee, Tien Shee - Cai, He - Zhu, Lin - Duan, Tao - Xiao, Chengliang. **Hollow Core–Shell Bismuth Based Al-Doped Silica Materials for Powerful Co-Sequestration of Radioactive I2 and CH3I** [elektronický dokument]. DOI 10.1002/smll.202308451 In: **Small**. Weinheim: John Wiley & Sons, 2024, Roč. 20, č. 18, art. no. 2308451 [tlačená forma] [online]. ISSN 1613-6810. ISSN (online) 1613-6829. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - He, Qing - Zhang, Lei - Han, Peize - Fu, Man - Zhu, Guorui. **Experimental and modeling study of adsorption behavior of CH3I over microchannel reactors** [elektronický dokument]. DOI 10.1016/j.psep.2024.02.019 In: **Process Safety and Environmental Protection**: Official Journal of the European Federation of Chemical Engineering: Part B. London: Institution of Chemical Engineers, 2024, Roč. 184, s. 391-399 [tlačená forma] [online]. ISSN 0957-5820. ISSN (online) 1744-3598. - SCO ; CCC ; WOS CC, s. 391 - 399

2023 [01/20] / **CHE** - Tao, Qi - Zhang, Xiao - Jing, Liping - Sun, Lu - Dang, Peipei. **Construction of Ketoenamine-Based Covalent Organic Frameworks with Electron-Rich Sites for Efficient and Rapid Removal of Iodine from Solution** [elektronický dokument]. DOI 10.3390/molecules28248151 In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 28, č. 24, art. no. 8151 [online]. ISSN (online) 1420-3049. - SCO ; CCC ; WOS CC, s. art. no. 8151

2023 [01/20] / **DEU** - Ahad, Jawaria - Ahmad, Masroor - Farooq, Amjad - Waheed, Khalid - Irfan, Naseem. **Removal of iodine by dry adsorbents in filtered containment venting system after 10 years of Fukushima accident** [elektronický

dokument]. DOI 10.1007/s11356-023-27485-1 In: **Environmental science and pollution research**. Heidelberg: Springer Nature. Springer International Publishing AG, 2023, Roč. 30, č. 30, s. 74628-74670 [tlačená forma] [online]. ISSN 0944-1344. ISSN (online) 1614-7499. - SCO ; CCC ; WOS CC, s. 74628 - 74670

2023 [01/20] / **GBR** - Van Speybroeck, Veronique. **Challenges in modelling dynamic processes in realistic nanostructured materials at operating conditions** [elektronický dokument]. DOI 10.1098/rsta.2022.0239 In: **Philosophical Transactions of the Royal Society A**: Mathematical, Physical & Engineering Sciences. Londýn: Royal Society, 2023, Roč. 381, č. 2250, art. no. 20220239 [tlačená forma] [online]. ISSN 1364-503X. ISSN (online) 1471-2962. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Bocus, Massimo - Goeminne, Ruben - Lamaire, Aran - Cools-Ceuppens, Maarten - Verstraelen, Toon - Van Speybroeck, Veronique. **Nuclear quantum effects on zeolite proton hopping kinetics explored with machine learning potentials and path integral molecular dynamics** [elektronický dokument]. DOI 10.1038/s41467-023-36666-y In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2023, Roč. 14, č. 1, art. no. 1008 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Cnudde, Pieter - Waroquier, Michel - Van Speybroeck, Veronique. **Universal descriptors for zeolite topology and acidity to predict the stability of butene cracking intermediates** [elektronický dokument]. DOI 10.1039/d3cy00642e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 16, s. 4857-4872 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4857 - 4872

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2022 [01/20] / **USA** - Devergne, T. - Magrino, T. - Pietrucci, F. - Saitta, A.M. **Combining Machine Learning Approaches and Accurate Ab Initio Enhanced Sampling Methods for Prebiotic Chemical Reactions in Solution** [elektronický dokument] In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 9, [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 5410 - 5421

2022 [01/20] / **USA** - Dietschreit, J.C.B. - Diestler, D.J. - Hulm, A. - Ochsenfeld, C. - Gomez-Bombarelli, R. **From free-energy profiles to activation free energies** [elektronický dokument] In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2022, Roč. 157, č. 8, [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO, s. Art. No. 084113

2021 [01/20] / **CHN** - Yu, J. - Xv, X. - Ye, S. **Research Progress on the Applications of Silver-loaded Zeolites** In: **Cailiao Yanjiu Xuebao/Chinese Journal of Materials Research**, 2021, Roč. 35, č. 11. - SCO, s. 801 - 810

2021 [01/20] / **GBR** - Wang, J. - Fan, D. - Jiang, C. - Lu, L. **Host-guest interaction-mediated nanointerface engineering for radioiodine capture** [elektronický dokument] In: **Nano today**. Londýn: Elsevier. Elsevier Science, 2021, Roč. 36, [tlačená forma] [online]. ISSN 1748-0132. ISSN (online) 1878-044X. - SCO, s. Art. No. 101034

2020 [01/12] / **CHE** - An, H. - Kweon, S. - Park, S. - Lee, J. - Min, H.-K. - Park, M.B. **Immobilization of radioiodine via an interzeolite transformation to iodosodalite** [elektronický dokument] In: **Nanomaterials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2020, Roč. 10, č. 11, [online]. ISSN (online) 2079-4991. - SCO, s. Art. No. 2157

2020 [01/12] / **USA** - Nastase, S.A.F. - Cnudde, P. - Vanduyfhuys, L. - De Wispelaere, K. - Van Speybroeck, V. - Catlow, C.R.A. - Logsdail, A.J. **Mechanistic Insight into the Framework Methylation of H-ZSM-5 for Varying Methanol Loadings and Si/Al Ratios Using First-Principles Molecular Dynamics Simulations** [elektronický dokument] In: **ACS**

Catalysis. Washington: American Chemical Society, 2020, Roč. 10, č. 15, [online]. ISSN (online) 2155-5435. - SCO, s. 8904 - 8915

2020 [01/12] / **GBR** - Plessow, P.N. **The transformation of cuboctahedral to icosahedral nanoparticles: Atomic structure and dynamics** [elektronický dokument] In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2020, Roč. 22, č. 23, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 12939 - 12945

2020 [01/12] / **NLD** - Park, S. - An, H. - Park, M.B. - Lee, J. **Adsorption behavior of methyl iodide on a silver ion-exchanged ZSM-5** [elektronický dokument] In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2020, Roč. 294, [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO, s. Art. No. 109842

2019 [01/12] / **USA** - Bailleul, S. - Rogge, S.M.J. - Vanduyfhuys, L. - Van Speybroeck, V. **In: ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2019, Roč. 11, č. 16, [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCIE ; WOS CC, s. 3993 - 4010

2018 [01/12] / **GBR** - Huve, J. - Ryzhikov, A. - Nouali, H. - Lalia, V. - Auge, G. - Daou, T.J. **In: RSC advances**. Cambridge: The Royal Society of Chemistry, 2018, Roč. 8, č. 51, [online]. ISSN (online) 2046-2069. - SCIE ; WOS CC, s. 29248 - 29273

ADC_054: / Broclawik, E. (Autor) (25%) - Góra-Marek, K. (Autor) (20%) - Radon, M. (Autor) (20%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (10%) - Stepniewski, A. (Autor) (25%): **The dependence on ammonia pretreatment of N-O activation by Co(II) sites in zeolites: a DFT and ab initio molecular dynamics study**. – text, tab., obr. – [recenzované]. – DOI 10.1007/s00894-017-3322-z. – CCC ; SCO ; OA ; WOS CC.
In: *Journal of Molecular Modeling* [textový dokument (print)] [elektronický dokument] : Computational Chemistry : Life Science : Advanced Materials : New Methods. – New York (USA) : Springer Nature. Springer-VDI-Verlag. – ISSN 1610-2940. – ISSN (online) 0948-5023. – Roč. 23, č. 5 (2017), 160 , s. [1-13] [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 40
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 1,507 - 2017
SNIP: 0,534 - 2017
SJR: 0,36 - 2017
CiteScore: 2,3 - 2017

Ohlasy (2):
2020 [01/12] / Hu, P. - Nakamura, K. - Matsubara, H. - Iyoki, K. - Yanaba, Y. - Okumura, K. - Okubo, T. - Katada, N. - Wakihara, T. **Comparative study of direct methylation of benzene with methane on cobalt-exchanged ZSM-5 and ZSM-11 zeolites** In: **Applied Catalysis A: General**, 2020, Roč. 601. - SCO, s. Art. No. 117661

2020 [01/12] / **USA** - Collinge, G. - Yuk, S.F. - Nguyen, M.-T. - Lee, M.-S. - Glezakou, V.-A. - Rousseau, R. **Effect of Collective Dynamics and Anharmonicity on Entropy in Heterogenous Catalysis: Building the Case for Advanced Molecular Simulations** [elektronický dokument] In: **ACS Catalysis**. Washington: American Chemical Society, 2020, Roč. 10, č. 16, [online]. ISSN (online) 2155-5435. - SCO, s. 9236 - 9260

2018 - spolu : 5

ADC_055: / Koettgen, Julius (Autor) (40%) - Schmidt, Peter C. (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%) - Martin, Manfred (Autor) (10%): **Ab initio calculation of the migration free energy of oxygen diffusion in pure and samarium-doped ceria**. – text, graf., obr. – DOI 10.1103/PhysRevB.97.024305. – CCC ; WOS CC ; SCO.
In: *Physical Review B* [textový dokument (print)] [elektronický dokument] . – College Park (USA) : American Institute of Physics. American Physical Society. – ISSN 2469-9950. – ISSN 1538-4489. – ISSN (online) 2469-9969. – Roč. 97, č. 2 (2018), Art. No. 024305, s. [1-11] [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 3,736 - 2018
SNIP: 1,097 - 2018
SJR: 1,502 - 2018
CiteScore: 6,6 - 2018
Kvartil Q:
2018, JIF - Materials science, multidisciplinary - Q2; **2018, JIF** - Physics, applied - Q1; **2018, JIF** - Physics, condensed matter - Q2; **2018, Scimago** - Condensed matter physics - Q1; **2018, Scimago** - Electronic, optical and magnetic materials - Q1

Ohlasy (17):
2024 [01/20] / **GBR** - Yan, Wei Xin - Ji, Zhi Lin - Gui, Dong Yun - Luo, Fa - Zhu, Dong Mei - Wang, Chun Hai. **Zr and Gd co-doped ceria oxide conductor with low electronic conductivity in reducing atmosphere** [elektronický dokument]. DOI 10.1016/j.ceramint.2024.07.061 In: **Ceramics International**. Oxon: Elsevier, 2024, Roč. 50, č. 19, s. 36758-36764 [tlačená forma] [online]. ISSN 0272-8842. ISSN (online) 1873-3956. - SCO ; CCC ; WOS CC, s. 36758 - 36764

2023 [01/20] / **DEU** - Körfer, Sylvia - Bonkowski, Alexander - Kler, Joe - Hatton, Peter - Uberuaga, Blas Pedro - De Souza, Roger A. **The Sluggish Diffusion of Cations in CeO2 Probed through Molecular Dynamics and Metadynamics Simulations** [elektronický dokument]. DOI 10.1002/adem.202201788 In: **Advanced Engineering Materials**. Weinheim: John Wiley & Sons. Wiley Blackwell, 2023, Roč. 25, č. 18, art. no. 2201788 [tlačená forma] [online]. ISSN 1438-1656. ISSN (online) 1527-2648. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Madhual, Sudeshna - Kumar, P. Padma. **Insights on oxide ion transport in yttria-doped ceria from molecular dynamics simulations** [elektronický dokument]. DOI 10.1007/s10853-023-08275-z In: **Journal of Materials Science**. Norwell: Springer Nature. Springer International Publishing AG, 2023, Roč. 58, č. 10, s. 4499-4512 [tlačená forma] [online]. ISSN 0022-2461. ISSN (online) 1573-4803. - SCO ; CCC ; WOS CC, s. 4499 - 4512

2022 [01/20] / **USA** - Zhao, Qinfu - Guo, Jianpeng - Su, Mengyu - Suo, Bingbing - Zhu, Haiyan - Zhou, Bo - Zhang, Zhiyong - Song, Qi. **Design Principles for Rotational Cluster Anion [BH<inf>4</inf>]⁻Promote Superionic Conductivity in Sodium-Rich Antiperovskite Na<inf>3</inf>OBH<inf>4</inf>** [elektronický dokument]. DOI 10.1021/acs.jpcc.2c05262 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2022, Roč. 126, č. 38, s. 16546-16555 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO, s. 16546 - 16555

2022 [01/20] / **NLD** - Lam, Le Thu. **Effects of temperature on the electrical properties of samaria-doped ceria predicted with the statistical moment method** [elektronický dokument]. DOI 10.1016/j.jpcs.2022.110907 In: **Journal of Physics and Chemistry of Solids**: an International Journal. Amsterdam: Elsevier, 2022, Roč. 170, art. no. 110907 [tlačená forma]. ISSN (online) 0022-3697. - SCO, s. art. no. 110907

2022 [01/20] / **USA** - Dholabhai, Pratik P. **Oxygen Vacancy Formation and Interface Charge Transfer at Misfit Dislocations in Gd-Doped CeO2/MgO Heterostructures** [elektronický dokument]. DOI 10.1021/acs.jpcc.2c02009 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2022, Roč. 126, č. 28, s. 11735-11750 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO, s. 11735 - 11750

2022 [01/20] / **GBR** - Yang, Hualong - Ma, Siqi - Duan, Wenjiu - Zhao, Shengjian - Wang, Qikun - Liu, Xuehui - Jiang, Yuqi - He, Peigang - Duan, Xiaoming - Jia, Dechang - Zhou, Yu. **Atomistic insight into the structure and diffusion properties of pollucite glass-ceramics** [elektronický dokument]. DOI 10.1016/j.ceramint.2021.12.333 In: **Ceramics International**. Oxon: Elsevier, 2022, Roč. 48, č. 8, s. 11134-11144 [tlačená forma] [online]. ISSN 0272-8842. ISSN (online) 1873-3956. - SCO, s. 11134 - 11144

2022 [01/20] / **GBR** - Robens, Elisabeth - Rauschen, Robert - Kaub, Johannes - Parras, Jana P. - Kemp, Dennis - Freeman, Colin L. - De Souza, Roger A. **Perovskite crystal symmetry and oxygen-ion transport: A molecular-dynamics study of perovskite** [elektronický dokument]. DOI 10.1039/d1ta06293j In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2022, Roč. 10, č. 5, s. 2388-2397 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO, s. 2388 - 2397

2021 [01/20] / **NLD** - Han, Xiaoping - Amrane, Noureddine - Qamhieh, Naser - Benkraouda, Maamar. **Enhanced optoelectronic functionality of N + H codoped monoclinic WO3: A hybrid functional study** [elektronický dokument]. DOI 10.1016/j.chemphys.2021.111283 In: **Chemical Physics**: a Frontier Research on Physical Phenomena in Chemistry, Biology and Materials Science. Amsterdam: Elsevier, 2021, Roč. 549, art. no. 111283 [tlačená forma] [online]. ISSN 0301-0104. ISSN (online) 1873-4421. - SCO, s.

2021 [01/20] / **NLD** - Acharya, Smita - Shirbhate, Shraddha - Yadav, Ashok. **Spectroscopic tools to probe multiple dopant induced elastic strain effect in doped ceria matrix: As electrolyte for ITSOFCs** [elektronický dokument]. DOI 10.1016/j.molstruc.2021.130258 In: **Journal of Molecular Structure**. Amsterdam: Elsevier, 2021, Roč. 1235, art. no. 130258 [tlačená forma] [online]. ISSN 0022-2860. ISSN (online) 1872-8014. - SCO, s.

2021 [01/20] / **USA** - Chen, Ronghan - Xu, Zhenming - Lin, Yuechuan - Lv, Buyao - Bo, Shou Hang - Zhu, Hong. **Influence of Structural Distortion and Lattice Dynamics on Li-Ion Diffusion in Li3OCl1- xBr xSuperionic Conductors** [elektronický dokument]. DOI 10.1021/acsaem.0c02519 In: **ACS Applied Energy Materials**. Washington: American Chemical Society. ACS Publications, 2021, Roč. 4, č. 3, s. 2107-2114. ISSN (online) 2574-0962. - SCO ; CCC ; WOS CC, s. 2107 - 2114

2021 [01/20] / **USA** - Heelweg, Henrik J. - De Souza, Roger A. **Metadynamics simulations of strontium-vacancy diffusion in SrTiO3** [elektronický dokument]. DOI 10.1103/PhysRevMaterials.5.013804 In: **Physical Review Materials**. College Park: American Institute of Physics. American Physical Society, 2021, Roč. 5, č. 1, art. no. 3804 [online] [CD-ROM]. ISSN (online) 2475-9953. ISSN (online) 2476-0455. - SCO ; CCC ; WOS CC, s.

2020 [01/20] / **GBR** - Ding, Yong - Choi, Yong Man - Chen, Yu - Pradel, Ken C. - Liu, Meilin - Wang, Zhong Lin. **Quantitative nanoscale tracking of oxygen vacancy diffusion inside single ceria grains by in situ transmission electron microscopy** [elektronický dokument]. DOI 10.1016/j.mattod.2020.04.006 In: **Materials today**: science, technology, policy. Kidlington: Elsevier. Elsevier Science, 2020, Roč. 38, s. 24-34 [tlačená forma] [online]. ISSN 1369-7021. ISSN (online) 1873-4103. ISSN (chybné) 1396-7021. - SCO ; CCC ; WOS CC ; SCIE, s. 24 - 34

2020 [01/20] / **USA** - Maier, Russell A. - Cockayne, Eric - Donohue, Matthew - Cibin, Giannantonio - Levin, Igor. **Substitutional Mechanisms and Structural Relaxations for Manganese in SrTiO3: Bridging the Concentration Gap for Point-Defect Metrology** [elektronický dokument]. DOI 10.1021/acs.chemmater.0c01082 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2020, Roč. 32, č. 11, s. 4651-4662

[tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC ; SCIE, s. 4651 - 4662

2019 [01/20] / **DEU** - Gilbile, T. L. - Pawar, R. S. - Kapatkar, V. N. - Kamble, R. C. - Pawar, S. S. **Synthesis and Performance Tuning of Sm 0.2 Ce 0.8 O 2−δ Electrolyte for Low Temperature Solid Oxide Fuel Cell Application** [elektronický dokument]. DOI 10.1007/s11664-019-07184-9 In: **Journal of Electronic Materials**. Berlín: Springer Nature. Springer International Publishing AG, 2019, Roč. 48, č. 6, s. 4117-4124 [tlačená forma] [online]. ISSN 0361-5235. ISSN (online) 1543-186X. - SCO, s. 4117 - 4124

2019 [01/20] / **GBR** - Dholabhai, Pratik P. **Atomic-scale structure of misfit dislocations in CeO2/MgO heterostructures and thermodynamic stability of dopant-defect complexes at the heterointerface** [elektronický dokument]. DOI 10.1039/c9cp03727f In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2019, Roč. 21, č. 37, s. 20878-20891 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 20878 - 20891

2018 [01/20] / **GBR** - Grieshammer, Steffen. **Influence of the lattice constant on defects in cerium oxide** [elektronický dokument]. DOI 10.1039/c8cp03677b In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2018, Roč. 20, č. 30, s. 19792-19799 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC ; SCIE, s. 19792 - 19799

ADC_056: / Kubota, Yoshiyuki (Autor) (70%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (30%): **Carbon dioxide capture in 2,2′-iminodiethanol aqueous solution from ab initio molecular dynamics simulations**. – text, tab., obr. – DOI 10.1063/1.5025016. – SCO ; CCC ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 149, č. 22 (2018), Art. No. 224103, s. [1-9] [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
Lit.: 63
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 2.997 - 2018
SNIP: 0,975 - 2018
SJR: 1.159 - 2018
CiteScore: 5,3 - 2018
Nordic List: 1 - 2018
Kvartil Q:
2018, JIF - Chemistry, physical - Q2; **2018, JIF** - Physics, atomic, molecular & chemical - Q2; **2018, Scimago** - Medicine (miscellaneous) - Q1; **2018, Scimago** - Physical and theoretical chemistry - Q1; **2018, Scimago** - Physics and astronomy (miscellaneous) - Q1

Ohlasy (5):
2024 [01/20] / **CHE** - Hafizi Yazdabadi, Sahar - Mihrin, Dmytro - Feilberg, Karen Louise - Wugt Larsen, René. **Spectroscopic and Quantum Chemical Evidence of Amine–CO2 and Alcohol–CO2 Interactions: Confirming an Intriguing Affinity of CO2 to Monoethanolamine (MEA)** [elektronický dokument]. DOI 10.3390/molecules29235521 In: **Molecules**. Bazilej: Multidisciplinary Digital Publishing Institute, 2024, Roč. 29, č. 23, art. no. 5521 [online]. ISSN (online) 1420-3049. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Chen, Meisi - Li, Mengjia - Liang, Yinchun - Meng, Weimin - Zhang, Zhibing - Wu, Youting - Li,

Xinyao - Zhang, Feng. **Improvement in CO2 Capture of Polyamine with Micro-Interfacial System** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c02053 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 40, s. 14451-14458 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 14451 - 14458

2023 [01/20] / **DEU** - Xie, Fan - Sun, Wenhao - Pinacho, Pablo - Schnell, Melanie. **CO2 Aggregation on Monoethanolamine: Observations from Rotational Spectroscopy** [elektronický dokument]. DOI 10.1002/anie.202218539 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2023, Roč. 62, č. 14, art. no. e202218539 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Ma, Xinyou - Bryantsev, Vyacheslav S. - Roy, Santanu. **An ab initio free energy study of the reaction mechanism and rate-limiting steps of CO2 capture by aqueous glycine** [elektronický dokument]. DOI 10.1016/j.xcrp.2023.101642 In: **Cell Reports Physical Science**. Cambridge: Elsevier. Cell Press, 2023, Roč. 4, č. 11, art. no. 101642 [tlačená forma] [online]. ISSN (online) 2666-3864. - SCO ; CCC ; WOS CC, s. art. no. 101642

2022 [01/20] / **USA** - Luo, Qinlan - Zhou, Qulan - Feng, Bin - Li, Na - Liu, Shicheng. **A Combined Experimental and Computational Study on the Shuttle Mechanism of Piperazine for the Enhanced CO<inf>2</inf>Absorption in Aqueous Piperazine Blends** [elektronický dokument]. DOI 10.1021/acs.iecr.1c04123 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2022, Roč. 61, č. 3, s. 1301-1312 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO, s. 1301 - 1312

ADC_057: / Bučko, Tomáš (Autor) [UKOPRCFZ] (95%) - Šimko, František (Autor) (5%): **Effect of alkaline metal cations on the ionic structure of cryolite melts: Ab-initio NpT MD study**. – text, tab., obr. – DOI 10.1063/1.5017106. – SCO ; CCC ; WOS CC.
In: *Journal of Chemical Physics* [textový dokument (print)] [elektronický dokument] . – Melville (USA) : American Institute of Physics. AIP Publishing. – ISSN 0021-9606. – ISSN (online) 1089-7690. – Roč. 148, č. 6 (2018), Art. No. 064501, s. [1-9] [tlačená forma] [online]
Počet všetkých autorov: 2
[článok]
Lit.: 63
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 2.997 - 2018
SNIP: 0,975 - 2018
SJR: 1.159 - 2018
CiteScore: 5,3 - 2018
Nordic List: 1 - 2018
Kvartil Q:
2018, JIF - Chemistry, physical - Q2; **2018, JIF** - Physics, atomic, molecular & chemical - Q2; **2018, Scimago** - Medicine (miscellaneous) - Q1; **2018, Scimago** - Physical and theoretical chemistry - Q1; **2018, Scimago** - Physics and astronomy (miscellaneous) - Q1

Ohlasy (14):
2025 [01/20] / **USA** - Betsis, Konstantinos - Karalis, Konstantinos - Xenidis, Anthimos. **Ab Initio Molecular Dynamics Simulation Study on the Molten Structure of Cryolite to the Cryolitic Bath, Na3AlF6–AlF3–Al2O3–CaF2** [elektronický dokument]. DOI 10.1021/acsomega.5c05781 In: **ACS Omega**. Washington: American Chemical Society, 2025, Roč. 10, č. 36, s. 41820-41827 [online]. ISSN (online) 2470-1343. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 41820 -

41827

2025 [01/20] / **GBR** - Zhang, Wendi - Hu, Xianwei - Diop, Mouhamadou Aziz - Kang, Hongguang - Yu, Jiangyu - Liu, Aimin - Shi, Zhongning - Wang, Zhaowen. **Analysis of the microscopic properties and Raman spectra of molten NaF-AlF3-CaF2-Al2O3 using first-principles molecular dynamics** [elektronický dokument]. DOI 10.1088/1402-4896/add3a0 In: **Physica Scripta**: an international journal for experimental and theoretical physics. Bristol: Institute of Physics. IOP Publishing, 2025, Roč. 100, č. 6, art. no. 065946 [tlačená forma] [online]. ISSN 0031-8949. ISSN (online) 1402-4896. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 065946

2025 [01/20] / **USA** - Zhang, Wendi - Hu, Xianwei - Kang, Hongguang - Guo, Ruidong - Yu, Jiangyu - Wang, Zhaowen. **First-Principles Molecular Dynamics Study of M3AlF6 (M= Li/Na/K) Molten Salts** [elektronický dokument]. DOI 10.1021/acs.jpcb.4c07043 In: **Journal of Physical Chemistry B**: Biophysical Chemistry, Biomaterials, Liquids, and Soft Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 8, s. 2246-2258 [tlačená forma] [online]. ISSN 1520-6106. ISSN (online) 1520-5207. ISSN (zrušené) 1089-5647. - SCO ; CCC ; WOS CC ; SCIE, s. 2246 - 2258

2024 [01/20] / **NLD** - Li, Xuejiao - Cui, Rongrong - Song, Yulong - Gong, Yu. **Insights on the microstructural correlations of density and specific heat capacity for halophilic fission products and NaF-BeF2 molten mixtures** [elektronický dokument]. DOI 10.1016/j.jnucmat.2024.155201 In: **Journal of Nuclear Materials**. Amsterdam: Elsevier, 2024, Roč. 599, art. no. 155201 [tlačená forma] [online]. ISSN 0022-3115. ISSN (online) 1873-4820. - SCO ; CCC ; WOS CC, s. art. no. 155201

2023 [01/20] / **DEU** - Chen, Liyu - Wang, Zhaowen - Yang, Youjian - Tao, Wenju - Shi, Zhongning - Hu, Xianwei. **Separation of Al3Zr Intermetallic Compound from Al–Zr Master Alloy Prepared by Molten Salt Electrolysis** [elektronický dokument]. DOI 10.1134/S0036024423100151 In: **Russian Journal of Physical Chemistry A**. Cham: Springer Nature, 2023, Roč. 97, č. 10, s. 2314-2320 [tlačená forma] [online]. ISSN 0036-0244. ISSN (online) 1531-863X. - SCO ; CCC ; WOS CC, s. 2314 - 2320

2023 [01/20] / **DEU** - Zhang, Yifan - Hu, Xianwei - Zhang, Wendi - Yang, Jiaxin - Chen, Liyu - Tang, Shuai - Liu, Aimin - Shi, Zhongning - Wang, Zhaowen. **Study on Decomposition Mechanism of K3AlF6 by Quantum Chemical Calculations** [elektronický dokument]. DOI 10.1134/S0036024423050308 In: **Russian Journal of Physical Chemistry A**. Cham: Springer Nature, 2023, Roč. 97, č. 5, s. 997-1006 [tlačená forma] [online]. ISSN 0036-0244. ISSN (online) 1531-863X. - SCO ; CCC ; WOS CC, s. 997 - 1006

2022 [01/20] / **NLD** - Sema Özen, Alimet - Akdeniz, Zehra. **Structure and bonding in cryolitic melts a combined study by density functional theory and ionic model calculations** [elektronický dokument]. DOI 10.1016/j.molliq.2022.120771 In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2022, Roč. 368, art. no. 120771 [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. art. no. 120771

2022 [01/20] / **DEU** - Zhang, Yifan - Hu, Xianwei - Lin, Ming - Liu, Aimin - Shi, Zhongning - Wang, Zhaowen. **Quantum Chemical Calculation on the Decomposition Mechanism of Na<inf>3</inf>AlF<inf>6</inf>** [elektronický dokument]. DOI 10.1134/S0036024422050302 In: **Russian Journal of Physical Chemistry A**. Cham: Springer Nature, 2022, Roč. 96, č. 5, s. 1035-1043 [tlačená forma] [online]. ISSN 0036-0244. ISSN (online) 1531-863X. - SCO, s. 1035 - 1043

2022 [01/20] / **NLD** - Xu, Tingrui - Li, Xuejiao - Li, Na - Liu, Mengmeng - Wang, Feng - Tang, Zhongfeng. **In-depth explorations on the microstructural, thermodynamic and kinetic characteristics of MgCl2-KCl eutectic salt** [elektronický dokument]. DOI 10.1016/j.molliq.2021.118275 In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2022, Roč. 347, art. no. 118275 [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. art. no. 118275

2022 [01/20] / **NLD** - Liu, Mengmeng - Li, Xuejiao - Wang, Yang - Xu, Tingrui - Yan, Liuming - Tang, Zhongfeng. **Elaborating the high thermal storage and conductivity of molten NaCl-KCl-NaF eutectic from microstructures by**

FPMD simulations [elektronický dokument]. DOI 10.1016/j.molliq.2021.117054 In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2022, Roč. 346, art. no. 117054 [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO, s. art. no. 117054

2022 [01/20] / **TUR** - Özen, Alimet Sema - Akdenız, Zehra. **Dissolution of alumina in cryolite melts: a conceptual DFT study** [elektronický dokument]. DOI 10.55730/1300-0101.2729 In: **Turkish Journal of Physics**. Ankara: The Scientific and Technological Research Council of Türkiye, 2022, Roč. 46, č. 6, s. 228-238 [tlačená forma] [online]. ISSN 1300-0101. ISSN (online) 1303-6122. - SCO, s. 228 - 238

2020 [01/20] / **NLD** - Liang, Wenshuo - Lu, Guimin - Yu, Jianguo. **Composition-dependent microstructure evolution in liquid MgCl2-KCl: A first-principles molecular dynamics study** [elektronický dokument]. DOI 10.1016/j.molliq.2020.113131 In: **Journal of Molecular Liquids**. Amsterdam: Elsevier, 2020, Roč. 309, art. no. 113131 [tlačená forma] [online]. ISSN 0167-7322. ISSN (online) 1873-3166. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 113131

2020 [01/20] / **NLD** - Lin, Ming - Hu, Xianwei - Shi, Zhongning - Gao, Bingliang - Yu, Jiangyu - Wang, Zhaowen. **Existence of Al2F7− in molten MF–AlF3 (M = K, Cs) systems as determined by Raman spectroscopy and structural simulation**. DOI 10.1016/j.jechem.2019.09.009 In: **Journal of Energy Chemistry**. Amsterdam: Elsevier. Elsevier Science, 2020, Roč. 44, s. 19-23 [tlačená forma] [online]. ISSN 2095-4956. - SCO ; WOS CC ; SCIE, s. 19 - 23

2019 [01/20] / **CHE** - Rakhmatullin, Aydar - Machado, Kelly - Zanghi, Didier - Polovov, Ilya B. - Bakirov, Rinat - Maksimtsev, Konstantin V. - Bessada, Catherine. **Study of the NaF-ScF3 system as a molten bath for production of Sc alloys: A combination of NMR and molecular dynamics simulations** [elektronický dokument]. DOI 10.1016/j.jallcom.2019.02.057 In: **Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2019, Roč. 786, s. 953-959 [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCO ; CCC ; WOS CC ; SCIE, s. 953 - 959

ADC_058: / Bučko, Tomáš (Autor) [UKOPRCFZ] (70%) - Novotný, Michal (Autor) [Interný doktorand] [UKOPRCFZ] (20%) - Černušák, Ivan (Autor) [UKOPRCFZ] (10%): **On the work function of the surface Mo(001) and its temperature dependence: an ab initio molecular dynamics study**. – text, tab., obr. – DOI 10.1088/1361-648X/aaeb76. – CCC ; WOS CC ; SCO.
In: *Journal of Physics* [textový dokument (print)] [elektronický dokument] : Condensed Matter. – Bristol (Veľká Británia) : Institute of Physics. IOP Publishing. – ISSN 0953-8984. – ISSN (online) 1361-648X. – Roč. 30, č. 50 (2018), Art. No. 5001, s. [1-8] [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 39
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 2.711 - 2018
SNIP: 1 - 2018
SJR: 0,943 - 2018
CiteScore: 4,7 - 2018
Kvartil Q:
2018, JIF - Physics, condensed matter - Q2; **2018, Scimago** - Condensed matter physics - Q1; **2018, Scimago** - Materials science (miscellaneous) - Q1

Ohlasy (3):
2025 [01/20] / **NLD** - Ma, Yubo - Li, Wei - Hu, Jun - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Geng, Shaofei - Liu,

Haifeng - Wang, Xianqu - Huang, Jie - Liu, Hai - Cheng, Jun - Tang, Changjian. **Investigating the stability and work function effects of Ba atoms adsorption on the Mo (110) surface** [elektronický dokument]. DOI 10.1016/j.nme.2025.101984 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2025, Roč. 45, art. no. 101984 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101984

2025 [01/20] / **CHE** - Yu, Di - Shi, Gui Mei - Gao, Qiang - Shi, Fa Nian - Liu, Feng - Qu, Xing Hao. **A novel heterogeneous Mo/Mo2C embedded N, P co-doped carbon nanofiber for C-band broadband and strong microwave absorption** [elektronický dokument]. DOI 10.1016/j.cej.2025.170001 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2025, Roč. 525, art. no. 170001 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 170001

2023 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Tsumori, Katsuyoshi - Nakano, Haruhisa - Osakabe, Masaki - Isobe, Mitsutaka - Okamura, Shoichi - Shimizu, Akihiro - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Zheng, Huaqing - Liu, Xiaoqiao - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **Effect of H atoms and O impurities on the adsorption stability and work function of the cesiated Mo(0 0 1) surface: A study about negative hydrogen ion sources for neutral beam injection systems** [elektronický dokument]. DOI 10.1016/j.nme.2023.101550 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2023, Roč. 37, art. no. 101550 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC, s. art. no. 101550

ADC_059: / Bučko, Tomáš (Autor) [UKOPRCFZ] (100%): **Transition state optimization of periodic systems using delocalized internal coordinates**. – text, tab., obr. – DOI 10.1007/s00214-018-2367-0. – CCC ; SCO ; WOS CC.
In: *Theoretical Chemistry Accounts* [textový dokument (print)] [elektronický dokument] : Theory, Computation, and Modeling. – Berlín (Nemecko) : Springer Nature. Springer International Publishing AG. – ISSN 1432-881X. – ISSN (online) 1432-2234. – Roč. 137, č. 12 (2018), Art. No. 164, s. [1-11] [tlačená forma] [online]
Počet všetkých autorov: 1
[článok]
Lit.: 40
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 1,598 - 2018
SNIP: 0,504 - 2018
SJR: 0,462 - 2018
CiteScore: 2,7 - 2018
Kvartil Q:
2018, JIF - Chemistry, physical - Q4; **2018, Scimago** - Physical and theoretical chemistry - Q3

Ohlasy (4):
2023 [01/20] / **NLD** - Bac, Selin - Lan, Zhenzhuo - Mallikarjun Sharada, Shaama. **Transition Structures, Reaction Paths, and Kinetics: Methods and Applications in Catalysis** [elektronický dokument]. DOI 10.1016/B978-0-12-821978-2.00006-4 In: **Comprehensive Computational Chemistry**. Amsterdam: Elsevier, 2023, s. 496-518 [tlačená forma]. ISBN 978-0-12-821978-2. ISBN (online) 978-0-12-823256-9. ISBN (chybné) 978-0-12-823256-9. - SCO, s. 496 - 518

2023 [01/20] / **USA** - Kendrick, John - Burnett, Andrew David. **Exploring the Stability and Disorder in the Polymorphs of L-Cysteine through Density Functional Theory and Vibrational Spectroscopy** [elektronický dokument]. DOI 10.1021/acs.cgd.3c00375 In: **Crystal Growth & Design**. Washington, DC: American Chemical Society. ACS Publications, 2023, Roč. 23, č. 8, s. 5734-5747 [tlačená forma] [online]. ISSN 1528-7483. ISSN (online) 1528-7505. - SCO ; CCC ; WOS CC, s. 5734 - 5747

2023 [01/20] / **USA** - Pracht, Philipp - Morgan, John W.R. - Wales, David J. **Exploring energy landscapes for solid-state systems with variable cells at the extended tight-binding level** [elektronický dokument]. DOI 10.1063/5.0159367 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 6, art. no. 064801 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s.

2021 [01/20] / **GBR** - Xu, Jiayan - Cao, Xiao Ming - Hu, P. **Perspective on computational reaction prediction using machine learning methods in heterogeneous catalysis** [elektronický dokument]. DOI 10.1039/d1cp01349a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2021, Roč. 23, č. 19, s. 11155-11179 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO ; CCC ; WOS CC, s. 11155 - 11179

2019 - spolu : **4**

ADC_060: / Rocca, Dario (Autor) (30%) - Dixit, Anant (Autor) (5%) - Badawi, Michael (Autor) (10%) - Lebegue, Sebastien (Autor) (5%) - Gould, Tim (Autor) (20%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (30%): **Bridging molecular dynamics and correlated wave-function methods for accurate finite-temperature properties**. – text, tab., obr. – SCO ; CCC ; WOS CC.
In: *Physical Review Materials* [elektronický dokument] . – College Park (USA) : American Institute of Physics. American Physical Society. – ISSN (online) 2475-9953. – ISSN (online) 2476-0455. – Roč. 3, č. 4 (2019), Art. No. 040801, s. [1-6] [online] [CD-ROM]
Počet všetkých autorov: 6
[článok]
Lit.: 64
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 3.337 - 2019
SNIP: 1,139 - 2019
SJR: 1,365 - 2019
CiteScore: 3,2 - 2019
Kvartil Q:
2019, JIF - Materials science, multidisciplinary - Q2; **2019, Scimago** - Materials science (miscellaneous) - Q1; **2019, Scimago** - Physics and astronomy (miscellaneous) - Q1

Ohlasy (4):
2025 [01/20] / **GBR** - Cascella, Michele - Bore, Sigbjørn Løland - Eisenstein, Odile. **The fellowship of the Grignard: 21st century computational tools for hundred-year-old chemistry** [elektronický dokument]. DOI 10.1039/d5sc01078k In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 19, s. 8196-8216 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 8196 - 8216

2023 [01/20] / **USA** - Berger, Fabian - Rybicki, Marcin - Sauer, Joachim. **Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites** [elektronický dokument]. DOI 10.1021/acscatal.2c05493 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 3, s. 2011-2024 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 2011 - 2024

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2022 [01/20] / **USA** - De Wispelaere, Kristof - Plessow, Philipp N. - Studt, Felix. **Toward Computing Accurate Free Energies in Heterogeneous Catalysis: a Case Study for Adsorbed Isobutene in H-ZSM-5** [elektronický dokument]. DOI 10.1021/acsphyschemau.2c00020 In: **ACS Physical Chemistry Au**. Washington: American Chemical Society, 2022, Roč. 2, č. 5, s. 399-406 [online]. ISSN (online) 2694-2445. - SCO, s. 399 - 406

ADC_061: / Rey, Jerome (Autor) (40%) - Raybaud, Pascal (Autor) (5%) - Chizallet, Celine (Autor) (15%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%): **Competition of Secondary versus Tertiary Carbenium Routes for the Type B Isomerization of Alkenes over Acid Zeolites Quantified by Ab Initio Molecular Dynamics Simulations**. – text, tab., obr. – SCO ; CCC ; WOS CC.
In: *ACS Catalysis* [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN (online) 2155-5435. – Nordic list level 2 - 2021 koeficient 6. – Nordic list level 1 - 2022 koeficient 4. – Roč. 9, č. 11 (2019), s. 9813-9828 [online]
Počet všetkých autorov: 4
[článok]
Lit.: 79
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 12,35 - 2019
SNIP: 2,178 - 2019
SJR: 4,633 - 2019
CiteScore: 19,6 - 2019
Kvartil Q:
2019, JIF - Chemistry, physical - Q1; **2019, Scimago** - Catalysis - Q1; **2019, Scimago** - Chemistry (miscellaneous) - Q1

Ohlasy (22):
2025 [01/20] / **GBR** - Kolganov, Alexander A. - Pidko, Evgeny A. **Computational Chemistry in Zeolite Catalysis**. DOI 10.1039/9781837676859-00312 In: **Zeolites from Fundamentals to Emerging Applications**. London: The Royal Society of Chemistry, 2025, s. 312-369 [tlačená forma] [online]. ISBN [9781837675456, 9781837676859]. - SCO, s. 312 - 369

2025 [01/20] / **GBR** - Ureel, Yannick - Tomme, Lowie - Sabbe, Maarten K. - Van Geem, Kevin M. **Genesys-Cat: automatic microkinetic model generation for heterogeneous catalysis with improved Bayesian optimization** [elektronický dokument]. DOI 10.1039/d4cy01344a In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 15, č. 3, s. 750-764 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 750 - 764

2025 [01/20] / **GBR** - Guo, Zhichao - Chen, Qingteng - Liu, Jian - Yang, Bo. **Discovery of ketene/acetyl as a potential receptor for hydrogen-transfer reactions in zeolites** [elektronický dokument]. DOI 10.1038/s41467-024-55514-1 In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 16, č. 1, art. no. 1152 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 1152

2025 [01/20] / **USA** - Ureel, Yannick - Abdulrahman, Anas Jamil - Akin, Oğuzhan - Sabbe, Maarten K. - Van Geem, Kevin M. **Microkinetic Modeling of Plastic Waste Catalytic Cracking with Phosphorus-Modified Mesoporous HZSM-5: An Iso-Octane Model Compound Study** [elektronický dokument]. DOI 10.1021/acs.iecr.5c01928 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2025, Roč. 64, č. 34, s. 16563-16573 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 16563 - 16573

2024 [01/20] / **GBR** - Potter, Matthew E. - Spiske, Lucas - Plessow, Philipp N. - McShane, Evangeline B. - Carravetta, Marina - Oakley, Alice E. - Bere, Takudzwa - Carter, James H. - Vandegehuchte, Bart D. - Kaźmierczak, Kamila M. - Studt, Felix - Raja, Robert. **Combining computational and experimental studies to gain mechanistic insights for n-butane**

isomerisation with a model microporous catalyst [elektronický dokument]. DOI 10.1039/d4cy01035c In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 24, s. 7140-7151 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 7140 - 7151

2024 [01/20] / **GBR** - Gao, Zhiwen - Wang, Yu - Yuan, Lei - Shi, Xinrui - Shang, Yihao - Jiang, Jingang - Zhang, Min - Fang, Shuhui - Zhang, Wei - Liu, Yue. **Room-temperature co-upcycling of polyvinyl chloride and polypropylene** [elektronický dokument]. DOI 10.1038/s41893-024-01468-7 In: **Nature sustainability**. London: Springer Nature. Macmillan Publishers, 2024, Roč. 7, č. 12, s. 1691-1698 [online]. ISSN (online) 2398-9629. - SCO ; CCC ; WOS CC, s. 1691 - 1698

2024 [01/20] / **CHE** - Goshayeshi, Bahman - Alexandros Theofanidis, Stavros - Abbas-Abadi, Mehrdad Seifali - Mahmoudi, Ehsan - Akin, Oguzhan - John Varghese, Robin - Lemonidou, Angeliki - Van Geem, Kevin M. **Selective catalytic conversion of model olefin and diolefin compounds of waste plastic pyrolysis oil: Insights for light olefin production and coke minimization** [elektronický dokument]. DOI 10.1016/j.cej.2024.156987 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2024, Roč. 500, art. no. 156987 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 156987

2024 [01/20] / **USA** - Mancuso, Jenna L. - Van Speybroeck, Veronique. **The nature of extraframework aluminum species and Brønsted acid site interactions under catalytic operating conditions** [elektronický dokument]. DOI 10.1016/j.jcat.2023.115211 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 429, art. no. 115211 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. art. no. 115211

2023 [01/20] / **USA** - Dai, Xiaojun - Cheng, Yan - Liu, Tingting - Mao, Lingjuan - Wei, Qiang - Zhou, Yasong. **Deep Hydroisomerization of n-Hexadecane over NiWS/SAPO-11 Catalyst: Size Effect of the Support and Revelation of the Reaction Network** [elektronický dokument]. DOI 10.1021/acs.energyfuels.3c02920 In: **Energy & Fuels**: an American Chemical Society journal. Washington: American Chemical Society, 2023, Roč. 37, č. 20, s. 15995-16010 [tlačená forma] [online]. ISSN 0887-0624. ISSN (online) 1520-5029. - SCO ; CCC ; WOS CC, s. 15995 - 16010

2023 [01/20] / **NLD** - Bocus, Massimo - Neale, Samuel E. - Cnudde, Pieter - Van Speybroeck, Véronique. **Dynamic evolution of catalytic active sites within zeolite catalysis**. DOI 10.1016/B978-0-12-823144-9.00012-1 In: **Comprehensive Inorganic Chemistry III, Third Edition**. Amsterdam: Elsevier. Elsevier Science, 2023, s. 165-200. ISBN 9780128231531. - SCO, s. 165 - 200

2023 [01/20] / **CHN** - Gao, Shanbin - Li, Mengchen - Yu, Hongyue - Shen, Yuge - Qiao, Liang - Chi, Kebin - Shi, Dejun. **In-situ acid regulation and hydroisomerization performance of Pt/ZSM-22 catalyst**. DOI 10.11949/0438-1157.20230362 In: **Chemical industry and engineering**. Beijing: China Association for Science and Technology, 2023, Roč. 74, č. 10, s. 4164-4172 [tlačená forma]. ISSN 0438-1157. - SCO, s. 4164 - 4172

2023 [01/20] / **USA** - Chen, Wei - Huang, Mengdi - Yi, Xianfeng - Hui, Yu - Gao, Pan - Hou, Guangjin - Stepanov, Alexander G. - Qin, Yucai - Song, Lijuan - Liu, Shang Bin - Chen, Zhongfang - Zheng, Anmin. **Protonated methylcyclopropane is an intermediate providing complete 13C-label scrambling at C4 olefin isomerization in zeolite** [elektronický dokument]. DOI 10.1016/j.checat.2022.100503 In: **Chem Catalysis**. Philadelphia: Elsevier, 2023, Roč. 3, č. 2, art. no. 100503 [tlačená forma] [online]. ISSN 2667-1107. ISSN (online) 2667-1093. - SCO ; WOS CC, s.

2023 [01/20] / **GBR** - Cnudde, Pieter - Waroquier, Michel - Van Speybroeck, Veronique. **Universal descriptors for zeolite topology and acidity to predict the stability of butene cracking intermediates** [elektronický dokument]. DOI 10.1039/d3cy00642e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 16, s. 4857-4872 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4857 - 4872

2023 [01/20] / **USA** - Moreira, V. M. **Carbocations** [elektronický dokument]. DOI 10.1002/9781119608288.ch6 In:

Organic Reaction Mechanisms 2019: An annual survey covering the literature dated January to December 2019. Hoboken: John Wiley & Sons, 2023, s. 257-285 [tlačená forma] [online]. ISBN 9781119608271. ISBN (online) 9781119608288. - SCO, s. 257 - 285

2022 [01/20] / **NLD** - Kollias, Loukas - Collinge, Gregory - Zhang, Difan - Allec, Sarah I. - Gurunathan, Pradeep Kumar - Piccini, Giovanni Maria - Yuk, Simuck F. - Nguyen, Manh Thuong - Lee, Mal Soon - Glezakou, Vassiliki Alexandra - Rousseau, Roger. **Assessing entropy for catalytic processes at complex reactive interfaces** [elektronický dokument]. DOI 10.1016/bs.arcc.2022.09.004 In: **Annual Reports in Computational Chemistry**. Amsterdam: Elsevier, 2022, s. 3-51 [tlačená forma] [online]. ISBN 978-0-323-99092-9. ISBN (online) 978-0-323-99093-6. ISSN 1574-1400. ISSN (online) 1875-5232. - SCO, s. 3 - 51

2022 [01/20] / **GBR** - Liu, Peng - Liu, Qian - Liu, Wei - Peng, Shaozhong - Mei, Donghai. **Mechanistic insights into positional and skeletal isomerization of cyclohexene in the H-BEA zeolite** [elektronický dokument]. DOI 10.1039/d2cp02310e In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s.

2022 [01/20] / **GBR** - Wei, Chenhao - Zhang, Guohao - Zhao, Liang - Gao, Jinsen - Xu, Chunming. **Effect of metal–acid balance and textual modifications on hydroisomerization catalysts for n-alkanes with different chain length: A mini-review** [elektronický dokument]. DOI 10.1016/j.fuel.2021.122809 In: **Fuel**: the science and technology of fuel and energy. Oxford: Elsevier, 2022, Roč. 315, art. no. 122809 [tlačená forma] [online]. ISSN 0016-2361. ISSN (online) 1873-7153. - SCO, s. art. no. 122809

2022 [01/20] / **USA** - Agarwal, Umang - Rigutto, Marcello S. - Zuidema, Erik - Jansen, A. P.J. - Poursaeidesfahani, Ali - Sharma, Shrinjay - Dubbeldam, David - Vlugt, Thijs J.H. **Kinetics of zeolite-catalyzed heptane hydroisomerization and hydrocracking with CBMC-modeled adsorption terms: Zeolite Beta as a large pore base case** [elektronický dokument]. DOI 10.1016/j.jcat.2022.09.026 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2022, Roč. 415, s. 37-50 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 37 - 50

2022 [01/20] / **USA** - Zhang, Mingwei - Liu, Linlin - Wang, Li - Zhang, Xiangwen - Li, Guozhu. **Four-Carbon Segmented Discrete Hydrocracking of Long-Chain Paraffins in MTT Channels Following a Pore-Mouth Mechanism** [elektronický dokument]. DOI 10.1021/acscatal.2c03090 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 16, s. 10313-10325 [online]. ISSN (online) 2155-5435. - SCO, s. 10313 - 10325

2022 [01/20] / **USA** - Rybicki, Marcin - Sillar, Kaido - Sauer, Joachim. **Dual-Site Model for Ab Initio Calculations of Gibbs Free Energies and Enthalpies of Adsorption: Methane in Zeolite Mobile Five (H-MFI)** [elektronický dokument]. DOI 10.1021/acs.jpclett.2c03302 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2022, Roč. 13, č. 50, s. 11595-11600 [online]. ISSN (online) 1948-7185. - SCO, s. 11595 - 11600

2022 [01/20] / **GBR** - Piccini, Giovannimaria - Lee, Mal Soon - Yuk, Simuck F. - Zhang, Difan - Collinge, Greg - Kollias, Loukas - Nguyen, Manh Thuong - Glezakou, Vassiliki Alexandra - Rousseau, Roger. **Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis** [elektronický dokument]. DOI 10.1039/d1cy01329g In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 12, č. 1, s. 12-37 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 12 - 37

2022 [01/20] / **GBR** - Chen, Wei - Yi, Xianfeng - Liu, Zhiqiang - Tang, Xiaomin - Zheng, Anmin. **Carbocation chemistry confined in zeolites: spectroscopic and theoretical characterizations** [elektronický dokument]. DOI 10.1039/d1cs00966d In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 51, č. 11, s. 4337-4385 [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO, s. 4337 - 4385

ADC_062: / Chehaibou, Bilal (Autor) (40%) - Badawi, Michael (Autor) (5%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (10%) - Bazhirov, Timur (Autor) (5%) - Rocca, Dario (Autor) (40%): **Computing RPA Adsorption Enthalpies by Machine Learning Thermodynamic Perturbation Theory**. – text, obr. – SCO ; CCC ; WOS CC.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 15, č. 11 (2019), s. 6333-6342 [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 76
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 5.011 - 2019
SNIP: 1,453 - 2019
SJR: 1,759 - 2019
CiteScore: 9,2 - 2019
Kvartil Q:
2019, JIF - Chemistry, physical - Q2; **2019, JIF** - Physics, atomic, molecular & chemical - Q1; **2019, Scimago** - Computer science applications - Q1; **2019, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (32):
2025 [01/20] / **USA** - Plessow, Philipp N. **Anharmonic Adsorption Free Energies and Apparent Activation Barriers for Mobile Reactants Based on Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jctc.5c01100 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 17, s. 8518-8532 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 8518 - 8532

2025 [01/20] / **USA** - Liang, Yu Hsuan - Zhang, Xing - Chan, Garnet Kin Lic - Berkelbach, Timothy C. - Ye, Hong Zhou. **Efficient Implementation of the Random Phase Approximation with Domain-Based Local Pair Natural Orbitals** [elektronický dokument]. DOI 10.1021/acs.jctc.4c01540 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 6, s. 2918-2927 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 2918 - 2927

2025 [01/20] / **DEU** - Huber, Philipp - Plessow, Philipp N. **Accurate and Efficient Description of Acidic Zeolites with Plane-Wave Density Functional Theory Using Range-Separated Hybrid Functionals** [elektronický dokument]. DOI 10.1002/cphc.202500147 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 15, art. no. e202500147 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **USA** - Zheng, Mingze - Orr, Lainey - Bukowski, Brandon C. **Opportunities for Connecting Computational and Experimental Approaches to Design Zeolite Catalysts for Ethanol-to-Olefin Reactions** [elektronický dokument]. DOI 10.1021/acscatal.5c04133 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, s. 17101-17121 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE, s. 17101 - 17121

2025 [01/20] / **GBR** - Yang, Jinyu - Cao, Nianen - Liu, Yuhan - Lu, Yuan. **CO2 capture with adsorption strategies: Achievements, challenges, and prospects** [elektronický dokument]. DOI 10.1016/j.jclepro.2025.145798 In: **Journal of Cleaner Production**. Oxon: Elsevier, 2025, Roč. 515, art. no. 145798 [tlačená forma] [online]. ISSN 0959-6526. ISSN (online) 1879-1786. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 145798

2025 [01/20] / **USA** - Wu, Mengfan - Zhang, Shiyi - Ren, Jie. **AI-empowered digital design of zeolites: Progress, challenges, and perspectives** [elektronický dokument]. DOI 10.1063/5.0253847 In: **APL materials**. Melville: ACA and

AIP Publishing, 2025, Roč. 13, č. 2, art. no. 020601 [online]. ISSN (online) 2166-532X. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 020601

2025 [01/20] / **GBR** - Vacek, Jaroslav - Vrška, Dávid - Manna, Debashree - Lo, Rabindranath - Hobza, Pavel. **Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches** [elektronický dokument]. DOI 10.1039/D5SC06336A In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 48, s. 23129-23138 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; WOS CC ; CCC ; SCIE ; Nature Index ; OA, s. 23129 - 23138

2024 [01/20] / **USA** - Zhao, Xiang - Xiao, Shujuan - Yao, Bingming - Chen, Yifu - Yu, Shouwu. **DFT-Based Mechanistic Exploration and Application in Photocatalytic Heterojunctions** [elektronický dokument]. DOI 10.1021/acs.jctc.4c01051 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2024, Roč. 20, č. 22, s. 9770-9786 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 9770 - 9786

2024 [01/20] / **GBR** - Dong, Xiaowan - Yu, Shixin - Yang, Wen - Cheng, Lihua - Tang, Yizhen - Chen, Dong. **Homogeneous oxidation of EE2 by ozone: Influencing factors, degradation pathway, and toxicity assessment** [elektronický dokument]. DOI 10.1016/j.jece.2024.112360 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2024, Roč. 12, č. 2, art. no. 112360 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO ; CCC ; WOS CC, s. art. no. 112360

2024 [01/20] / **NLD** - Al-Sakkari, Eslam G. - Ragab, Ahmed - Dagdougui, Hanane - Boffito, Daria C. - Amazouz, Mouloud. **Carbon capture, utilization and sequestration systems design and operation optimization: Assessment and perspectives of artificial intelligence opportunities** [elektronický dokument]. DOI 10.1016/j.scitotenv.2024.170085 In: **Science of the total environment**. Amsterdam: Elsevier, 2024, Roč. 917, art. no. 170085 [tlačená forma] [online]. ISSN 0048-9697. ISSN (online) 1879-1026. - SCO ; CCC ; WOS CC, s. art. no. 170085

2023 [01/20] / **CHN** - Zhu, Minjie - Wang, Peng - Ma, Lei - Lu, Haibo - Yu, Ying - Chen, Yiming - Gao, Ting - Lin, Qi - Chen, Jiamin. **Research on the Practical Application of RPA Robot for Automatic Intelligent Investment Statistics in PIS System**. DOI 10.1145/3660395.3660403 In: **AIBDF '23: Proceedings of the 2023 3rd Guangdong-Hong Kong-Macao Greater Bay Area Artificial Intelligence and Big Data Forum**. Guangzhou : ACM Digital Library, 2023, s. 37-42. ISBN 979-8-4007-1636-2. - SCO, s. 37 - 42

2023 [01/20] / **GBR** - Zhang, Chao - Cheng, Jun - Chen, Yiming - Chan, Maria K.Y. - Cai, Qiong - Carvalho, Rodrigo P. - Marchiori, Cleber F.N. - Brandell, Daniel - Araujo, C. Moyses - Chen, Ming - Ji, Xiangyu - Feng, Guang - Goloviznina, Kateryna - Serva, Alessandra - Salanne, Mathieu - Mandai, Toshihiko - Hosaka, Tomooki - Alhanash, Mirna - Johansson, Patrik - Qiu, Yun Ze - Xiao, Hai - Eikerling, Michael - Jinnouchi, Ryosuke - Melander, Marko M. - Kastlunger, Georg. **2023 Roadmap on molecular modelling of electrochemical energy materials** [elektronický dokument]. DOI 10.1088/2515-7655/acfe9b In: **JPhys Energy**. Londýn: Institute of Physics, 2023, Roč. 5, č. 4, art. no. 041501. ISSN (online) 2515-7655. - SCO ; CCC ; WOS CC, s. art. no. 041501

2023 [01/20] / **NLD** - Mondaca, F. - Calderón, F. A. - Conejeros, S. - Mtz-Enriquez, A. I. **First-principles calculations of phosphorus-doped SnO2 transparent conducting oxide: Structural, electronic, and electrical properties** [elektronický dokument]. DOI 10.1016/j.commatsci.2022.111877 In: **Computational Materials Science**. Amsterdam: Elsevier, 2023, Roč. 216, art. no. 111877 [tlačená forma] [online]. ISSN 0927-0256. ISSN (online) 1879-0801. - SCO ; CCC ; WOS CC, s. art. no. 111877

2023 [01/20] / **USA** - Berger, Fabian - Rybicki, Marcin - Sauer, Joachim. **Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites** [elektronický dokument]. DOI 10.1021/acscatal.2c05493 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 3, s. 2011-2024 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 2011 - 2024

2023 [01/20] / **GBR** - Van Speybroeck, Veronique. **Challenges in modelling dynamic processes in realistic nanostructured materials at operating conditions** [elektronický dokument]. DOI 10.1098/rsta.2022.0239 In: **Philosophical Transactions of the Royal Society A**: Mathematical, Physical & Engineering Sciences. Londýn: Royal Society, 2023, Roč. 381, č. 2250, art. no. 20220239 [tlačená forma] [online]. ISSN 1364-503X. ISSN (online) 1471-2962. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Wang, Mengen - Boscoboinik, Jorge Anibal - Lu, Deyu. **First-Principles Study of n-Butane Monomolecular Cracking and Dehydrogenation on Two-Dimensional-Zeolite Model Systems: Reaction Mechanisms and Effects of Spatial Confinement** [elektronický dokument]. DOI 10.1021/acs.jpcc.3c01403 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2023, Roč. 127, č. 28, s. 13593-13600 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 13593 - 13600

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **USA** - Rizzi, Andrea - Carloni, Paolo - Parrinello, M. **Free energies at QM accuracy from force fields via multimap targeted estimation** [elektronický dokument]. DOI 10.1073/pnas.2304308120 In: **Proceedings of the National Academy of Sciences of the United States of America**. Washington: National Academy of Sciences of the United States of America, 2023, Roč. 120, č. 46, art. no. 4308120 [tlačená forma] [online]. ISSN 0027-8424. ISSN (online) 1091-6490. - SCO ; CCC ; WOS CC, s.

2022 [01/20] / **USA** - Giese, Timothy J. - Zeng, Jinzhe - York, Darrin M. **Multireference Generalization of the Weighted Thermodynamic Perturbation Method** [elektronický dokument]. DOI 10.1021/acs.jpca.2c06201 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2022, Roč. 126, č. 45, s. 8519-8533 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO, s. 8519 - 8533

2022 [01/20] / **GBR** - Chen, Wei - Yi, Xianfeng - Liu, Zhiqiang - Tang, Xiaomin - Zheng, Anmin. **Carbocation chemistry confined in zeolites: spectroscopic and theoretical characterizations** [elektronický dokument]. DOI 10.1039/d1cs00966d In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 51, č. 11, s. 4337-4385 [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO, s. 4337 - 4385

2022 [01/20] / **USA** - Chizallet, Céline. **Achievements and Expectations in the Field of Computational Heterogeneous Catalysis in an Innovation Context** [elektronický dokument]. DOI 10.1007/s11244-021-01489-y In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, s. 69-81 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 69 - 81

2022 [01/20] / **USA** - Sundararaman, Ravishankar - Vigil-Fowler, Derek - Schwarz, Kathleen. **Improving the Accuracy of Atomistic Simulations of the Electrochemical Interface** [elektronický dokument]. DOI 10.1021/acs.chemrev.1c00800 In: **Chemical Reviews**. Washington: American Chemical Society, 2022, Roč. 122, č. 12, s. 10651-10674 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO, s. 10651 - 10674

2022 [01/20] / **USA** - Cao, Liang. **Recent advances in the application of machine-learning algorithms to predict**

adsorption energies [elektronický dokument]. DOI 10.1016/j.trechm.2022.01.012 In: **Trends in chemistry**. New York: Elsevier, 2022, Roč. 4, č. 4, s. 347-360 [tlačená forma] [online]. ISSN 2589-7209. ISSN (online) 2589-5974. - SCO, s. 347 - 360

2022 [01/20] / **USA** - Liu, Peitao - Verdi, Carla - Karsai, Ferenc - Kresse, Georg. **Phase transitions of zirconia: Machine-learned force fields beyond density functional theory** [elektronický dokument]. DOI 10.1103/PhysRevB.105.L060102 In: **Physical Review B**. College Park: American Institute of Physics. American Physical Society, 2022, Roč. 105, č. 6, art. no. L060102 [tlačená forma] [online]. ISSN 2469-9950. ISSN 1538-4489. ISSN (online) 2469-9969. - SCO, s. art. no. L060102

2022 [01/20] / **GBR** - Saini, Vaneet - Sharma, Aditya - Nivatia, Dhruv. **A machine learning approach for predicting the nucleophilicity of organic molecules** [elektronický dokument]. DOI 10.1039/d1cp05072a In: **Physical Chemistry Chemical Physics**. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 3, s. 1821-1829 [tlačená forma] [online]. ISSN 1463-9076. ISSN (online) 1463-9084. - SCO, s. 1821 - 1829

2021 [01/20] / **NLD** - Cui, Weiyong - Chen, Jianhua. **Insight into mineral flotation fundamentals through the DFT method**. DOI 10.1016/j.ijmst.2021.10.001 In: **International journal of mining science and technology**. [Amsterdam]: Elsevier, 2021, Roč. 31, č. 6, s. 983-994 [tlačená forma]. ISSN 2095-2686. - SCO ; CCC ; WOS CC, s. 983 - 994

2021 [01/20] / **USA** - Rizzi, Andrea - Carloni, Paolo - Parrinello, Michele. **Targeted Free Energy Perturbation Revisited: Accurate Free Energies from Mapped Reference Potentials** [elektronický dokument]. DOI 10.1021/acs.jpclett.1c02135 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2021, Roč. 12, č. 39, s. 9449-9454 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 9449 - 9454

2021 [01/20] / **USA** - Roberts, Josiah - Bursten, Julia R.S. - Risko, Chad. **Genetic Algorithms and Machine Learning for Predicting Surface Composition, Structure, and Chemistry: A Historical Perspective and Assessment** [elektronický dokument]. DOI 10.1021/acs.chemmater.1c00538 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2021, Roč. 33, č. 17, s. 6589-6615 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC, s. 6589 - 6615

2021 [01/20] / **USA** - Xu, Jiayan - Cao, Xiao Ming - Hu, P. **Accelerating metadynamics-based free-energy calculations with adaptive machine learning potentials** [elektronický dokument]. DOI 10.1021/acs.jctc.1c00261 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 7, art. no. 4476, s. 4465-4476 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 4465 - 4476

2021 [01/20] / **USA** - Rybkin, Vladimir V. **Formulation and Implementation of Density Functional Embedding Theory Using Products of Basis Functions** [elektronický dokument]. DOI 10.1021/acs.jctc.1c00175 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 7, s. 3995-4005 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 3995 - 4005

2021 [01/20] / **USA** - Piaggi, Pablo M. - Panagiotopoulos, Athanassios Z. - Debenedetti, Pablo G. - Car, Roberto. **Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional** [elektronický dokument]. DOI 10.1021/acs.jctc.1c00041 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 5, s. 3065-3077 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 3065 - 3077

ADC_063: / Rey, Jerome (Autor) (35%) - Gomez, Axel (Autor) (5%) - Raybaud, Pascal (Autor) (10%) - Chizallet, Celine (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%): **On the origin of the difference between type A and type B skeletal isomerization of alkenes catalyzed by zeolites: The crucial input of ab initio molecular dynamics**. – text, obr. –

DOI 10.1016/j.jcat.2019.04.014. – SCO ; CCC ; WOS CC ; SCIE.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – č. 373 (2019), s. 361-373 [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 87
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 7.888 - 2019
SNIP: 1,797 - 2019
SJR: 2,256 - 2019
CiteScore: 11,9 - 2019
Kvartil Q:
2019, JIF - Chemistry, physical - Q1; **2019, JIF** - Engineering, chemical - Q1; **2019, Scimago** - Catalysis - Q1; **2019, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (27):

2025 [01/20] / **USA** - Plessow, Philipp N. **Anharmonic Adsorption Free Energies and Apparent Activation Barriers for Mobile Reactants Based on Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jctc.5c01100 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 17, s. 8518-8532 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 8518 - 8532

2025 [01/20] / **GBR** - Kolganov, Alexander A. - Pidko, Evgeny A. **Computational Chemistry in Zeolite Catalysis**. DOI 10.1039/9781837676859-00312 In: **Zeolites from Fundamentals to Emerging Applications**. London: The Royal Society of Chemistry, 2025, s. 312-369 [tlačená forma] [online]. ISBN [9781837675456, 9781837676859]. - SCO, s. 312 - 369

2025 [01/20] / **GBR** - Ureel, Yannick - Tomme, Lowie - Sabbe, Maarten K. - Van Geem, Kevin M. **Genesys-Cat: automatic microkinetic model generation for heterogeneous catalysis with improved Bayesian optimization** [elektronický dokument]. DOI 10.1039/d4cy01344a In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 15, č. 3, s. 750-764 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 750 - 764

2025 [01/20] / **DEU** - Han, Wanying - Lin, Longfei - Cen, Ziyu - Ke, Yubin - Xu, Qian - Zhu, Junfa - Mei, Xuelei - Xia, Zhanghui - Zheng, Xinrui - Wang, Yaqin - Liu, Yani - He, Mingyuan - Wu, Haihong - Han, Buxing. **Production of Branched Alkanes by Upcycling of Waste Polyethylene over Controlled Acid Sites of SO4/ZrO2-Al2O3 Catalyst** [elektronický dokument]. DOI 10.1002/anie.202417923 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 64, č. 6, art. no. e202417923 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC ; SCIE, s.

2025 [01/20] / **USA** - Ureel, Yannick - Abdulrahman, Anas Jamil - Akin, Oğuzhan - Sabbe, Maarten K. - Van Geem, Kevin M. **Microkinetic Modeling of Plastic Waste Catalytic Cracking with Phosphorus-Modified Mesoporous HZSM-5: An Iso-Octane Model Compound Study** [elektronický dokument]. DOI 10.1021/acs.iecr.5c01928 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2025, Roč. 64, č. 34, s. 16563-16573 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 16563 - 16573

2025 [01/20] / **GBR** - Karamanis, Ioannis - Dell'Angelo, David - Monnier, Hubert - Badawi, Michael. **Computational screening analysis of iron zeolites for selectively capturing NOx and CO over H2O and CO2** [elektronický dokument]. DOI 10.1039/d5me00003c In: **Molecular Systems Design and Engineering**. [s.l.]: The Royal Society of Chemistry, 2025, Roč. 10, č. 10, s. 855-867 [online]. ISSN (online) 20589689. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 855 - 867

2025 [01/20] / **GBR** - Vacek, Jaroslav - Vrška, Dávid - Manna, Debashree - Lo, Rabindranath - Hobza, Pavel. **Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches** [elektronický dokument]. DOI 10.1039/D5SC06336A In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 48, s. 23129-23138 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; WOS CC ; CCC ; SCIE ; Nature Index ; OA, s. 23129 - 23138

2024 [01/20] / **GBR** - He, Guangyuan - Mei, Donghai. **The critical role of the active [GaH]2+ site in n-heptane dehydrocyclization over Ga/H-ZSM-5 zeolite** [elektronický dokument]. DOI 10.1039/d4cy00648h In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 18, s. 5450-5463 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 5450 - 5463

2024 [01/20] / **USA** - He, Guangyuan - Mei, Donghai. **Deciphering reaction mechanism network of n-heptane dehydrocyclization over H-ZSM-5 zeolite** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115623 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 436, art. no. 115623 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **DEU** - Cen, Ziyu - Han, Xue - Lin, Longfei - Yang, Sihai - Han, Wanying - Wen, Weilong - Yuan, Wenli - Dong, Minghua - Ma, Zhiye - Li, Fang - Ke, Yubin - Dong, Juncai - Zhang, Jin - Liu, Shuhu - Li, Jialiang - Li, Qian - Wu, Ningning - Xiang, Junfeng - Wu, Hao - Cai, Lile - Hou, Yanbo - Cheng, Yongqiang - Daemen, Luke L. - Ramirez-Cuesta, Anibal J. - Ferrer, Pilar. **Upcycling of polyethylene to gasoline through a self-supplied hydrogen strategy in a layered self-pillared zeolite** [elektronický dokument]. DOI 10.1038/s41557-024-01506-z In: **Nature Chemistry**. Berlín: Springer Nature. Springer. Nature Portfolio, 2024, Roč. 16, č. 6, s. 871-880. ISSN 17554330. ISSN (online) 17554349. - SCO ; WOS CC, s. 871 - 880

2024 [01/20] / **USA** - Nimisha, N. P. - Narendranath, Soumya B. - Ganesh, V. - Sakthivel, A. **Ru Loaded MCM-22: A Potential Catalyst for the Isomerization and Cracking of 1-Dodecene** [elektronický dokument]. DOI 10.1007/s10562-023-04407-x In: **Catalysis Letters**. New York: Springer Nature. Springer Science+Business Media, 2024, Roč. 154, č. 4, s. 1694-1714 [tlačená forma] [online]. ISSN 1011-372X. ISSN (online) 1572-879X. - SCO ; CCC ; WOS CC, s. 1694 - 1714

2024 [01/20] / **GBR** - Potter, Matthew E. - Spiske, Lucas - Plessow, Philipp N. - McShane, Evangeline B. - Carravetta, Marina - Oakley, Alice E. - Bere, Takudzwa - Carter, James H. - Vandegehuchte, Bart D. - Kaźmierczak, Kamila M. - Studt, Felix - Raja, Robert. **Combining computational and experimental studies to gain mechanistic insights for n-butane isomerisation with a model microporous catalyst** [elektronický dokument]. DOI 10.1039/d4cy01035c In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2024, Roč. 14, č. 24, s. 7140-7151 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 7140 - 7151

2023 [01/20] / **USA** - Zhang, Jintu - Zhang, Haotian - Qin, Zhixin - Kang, Yu - Hong, Xin - Hou, Tingjun. **Quasiclassical Trajectory Simulation as a Protocol to Build Locally Accurate Machine Learning Potentials** [elektronický dokument]. DOI 10.1021/acs.jcim.2c01497 In: **Journal of Chemical Information and Modeling**. Washington, D.C.: American Chemical Society, 2023, Roč. 63, č. 4, s. 1133-1142 [tlačená forma] [online]. ISSN 1549-9596. ISSN (online) 1549-960X. - SCO ; WOS CC, s. 1133 - 1142

2023 [01/20] / **USA** - Kondratiuk, Mykhailo - Gopinath, Dhyanesh - Elrrays, Asmaa - Gooßen, Lukas J. **Double-Bond Isomerization of Rapeseed Oil Methyl Esters in a Continuous Flow Reactor Efficiently Catalyzed by H-Mordenite** [elektronický dokument]. DOI 10.1002/ejlt.202200163 In: **European Journal of Lipid Science and Technology**. Hoboken: John Wiley & Sons, 2023, Roč. 125, č. 5, art. no. 2200163 [tlačená forma] [online]. ISSN 1438-7697. ISSN (online) 1438-9312. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Skorynina, Alina A. - Protsenko, Bogdan O. - Usoltsev, Oleg A. - Guda, Sergey A. - Bugaev, Aram L. **Quantitative Structural Description of Zeolites by Machine Learning Analysis of Infrared Spectra** [elektronický dokument]. DOI 10.1021/acs.inorgchem.2c04395 In: **Inorganic Chemistry**. Washington: American Chemical Society,

2023, Roč. 62, č. 17, s. 6608-6616 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO ; CCC ; WOS CC, s. 6608 - 6616

2023 [01/20] / **NLD** - Cheng, Gong - Wang, Xin Xin - Zhang, Shuai Hui - Zhu, Ka Ke - Sui, Zhi Jun - Zhou, Xing Gui - Chen, De - Zhu, Yi An. **On the product and transition-state shape selectivities in 2-heptene isomerization** [elektronický dokument]. DOI 10.1016/j.cplett.2022.140263 In: **Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2023, Roč. 812, art. no. 140263 [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Chen, Wei - Huang, Mengdi - Yi, Xianfeng - Hui, Yu - Gao, Pan - Hou, Guangjin - Stepanov, Alexander G. - Qin, Yucai - Song, Lijuan - Liu, Shang Bin - Chen, Zhongfang - Zheng, Anmin. **Protonated methylcyclopropane is an intermediate providing complete 13C-label scrambling at C4 olefin isomerization in zeolite** [elektronický dokument]. DOI 10.1016/j.checat.2022.100503 In: **Chem Catalysis**. Philadelphia: Elsevier, 2023, Roč. 3, č. 2, art. no. 100503 [tlačená forma] [online]. ISSN 2667-1107. ISSN (online) 2667-1093. - SCO ; WOS CC, s.

2023 [01/20] / **USA** - Ke, Jun - Hu, Wen De - Du, Yu Jue - Wang, Yang Dong - Wang, Chuan Ming - Xie, Zai Ku. **Microkinetic Simulations of Methanol-to-Olefin Conversion in H-SAPO-34: Dynamic Distribution and Evolution of the Hydrocarbon Pool and Implications for Catalytic Performance** [elektronický dokument]. DOI 10.1021/acscatal.3c02140 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 13, s. 8642-8661 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 8642 - 8661

2023 [01/20] / **GBR** - Van Speybroeck, Veronique. **Challenges in modelling dynamic processes in realistic nanostructured materials at operating conditions** [elektronický dokument]. DOI 10.1098/rsta.2022.0239 In: **Philosophical Transactions of the Royal Society A**: Mathematical, Physical & Engineering Sciences. Londýn: Royal Society, 2023, Roč. 381, č. 2250, art. no. 20220239 [tlačená forma] [online]. ISSN 1364-503X. ISSN (online) 1471-2962. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **GBR** - Cnudde, Pieter - Waroquier, Michel - Van Speybroeck, Veronique. **Universal descriptors for zeolite topology and acidity to predict the stability of butene cracking intermediates** [elektronický dokument]. DOI 10.1039/d3cy00642e In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 16, s. 4857-4872 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 4857 - 4872

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2022 [01/20] / **NLD** - Kollias, Loukas - Collinge, Gregory - Zhang, Difan - Allec, Sarah I. - Gurunathan, Pradeep Kumar - Piccini, Giovanni Maria - Yuk, Simuck F. - Nguyen, Manh Thuong - Lee, Mal Soon - Glezakou, Vassiliki Alexandra - Rousseau, Roger. **Assessing entropy for catalytic processes at complex reactive interfaces** [elektronický dokument]. DOI 10.1016/bs.arcc.2022.09.004 In: **Annual Reports in Computational Chemistry**. Amsterdam: Elsevier, 2022, s. 3-51 [tlačená forma] [online]. ISBN 978-0-323-99092-9. ISBN (online) 978-0-323-99093-6. ISSN 1574-1400. ISSN (online) 1875-5232. - SCO, s. 3 - 51

2022 [01/20] / **USA** - Agarwal, Umang - Rigutto, Marcello S. - Zuidema, Erik - Jansen, A. P.J. - Poursaeidesfahani, Ali - Sharma, Shrinjay - Dubbeldam, David - Vlugt, Thijs J.H. **Kinetics of zeolite-catalyzed heptane hydroisomerization and hydrocracking with CBMC-modeled adsorption terms: Zeolite Beta as a large pore base case** [elektronický dokument]. DOI 10.1016/j.jcat.2022.09.026 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2022, Roč. 415, s. 37-50 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 37 - 50

2022 [01/20] / **USA** - Zhang, Mingwei - Liu, Linlin - Wang, Li - Zhang, Xiangwen - Li, Guozhu. **Four-Carbon Segmented Discrete Hydrocracking of Long-Chain Paraffins in MTT Channels Following a Pore-Mouth Mechanism** [elektronický dokument]. DOI 10.1021/acscatal.2c03090 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 16, s. 10313-10325 [online]. ISSN (online) 2155-5435. - SCO, s. 10313 - 10325

2022 [01/20] / **USA** - Ma, Sicong - Liu, Zhi Pan. **The Role of Zeolite Framework in Zeolite Stability and Catalysis from Recent Atomic Simulation** [elektronický dokument]. DOI 10.1007/s11244-021-01473-6 In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, s. 59-68 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 59 - 68

2022 [01/20] / **GBR** - Piccini, Giovannimaria - Lee, Mal Soon - Yuk, Simuck F. - Zhang, Difan - Collinge, Greg - Kollias, Loukas - Nguyen, Manh Thuong - Glezakou, Vassiliki Alexandra - Rousseau, Roger. **Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis** [elektronický dokument]. DOI 10.1039/d1cy01329g In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 12, č. 1, s. 12-37 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 12 - 37

2022 [01/20] / **GBR** - Chen, Wei - Yi, Xianfeng - Liu, Zhiqiang - Tang, Xiaomin - Zheng, Anmin. **Carbocation chemistry confined in zeolites: spectroscopic and theoretical characterizations** [elektronický dokument]. DOI 10.1039/d1cs00966d In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 51, č. 11, s. 4337-4385 [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO, s. 4337 - 4385

2020 - spolu : **3**

ADC_064: / Bučko, Tomáš (Autor) [UKOPRCFZ] (50%) - Gešvandtnerová, Monika (Autor) [Interný doktorand] [UKOPRCFZ] (20%) - Rocca, Dario (Autor) (30%): **Ab Initio Calculations of Free Energy of Activation at Multiple Electronic Structure Levels Made Affordable: An Effective Combination of Perturbation Theory and Machine Learning**. – text, obr. – [recenzované]. – DOI 10.1021/acs.jctc.0c00486. – SCO ; CCC ; WOS CC.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 16, č. 10 (2020), s. 6049-6060 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 52
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 6,006 - 2020
SNIP: 1,548 - 2020
SJR: 2,001 - 2020
CiteScore: 9,3 - 2020
AIS: 1.764 - 2020
Kvartil Q:
2020, AIS - Chemistry, physical - Q1; **2020, AIS** - Physics, atomic, molecular & chemical - Q1; **2020, JIF** - Chemistry, physical - Q2; **2020, JIF** - Physics, atomic, molecular & chemical - Q1; **2020, Scimago** - Computer science applications - Q1; **2020, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (20):
2025 [01/20] / **DEU** - Bocus, Massimo - Vandenhaute, Sander - Van Speybroeck, Veronique. **The Operando Nature of Isobutene Adsorbed in Zeolite H−SSZ−13 Unraveled by Machine Learning Potentials Beyond DFT Accuracy**

[elektronický dokument]. DOI 10.1002/anie.202413637 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 64, č. 1, art. no. e202413637 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **USA** - Plessow, Philipp N. **Anharmonic Adsorption Free Energies and Apparent Activation Barriers for Mobile Reactants Based on Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acs.jctc.5c01100 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 17, s. 8518-8532 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC ; SCIE, s. 8518 - 8532

2025 [01/20] / **USA** - Zheng, Mingze - Orr, Lainey - Bukowski, Brandon C. **Opportunities for Connecting Computational and Experimental Approaches to Design Zeolite Catalysts for Ethanol-to-Olefin Reactions** [elektronický dokument]. DOI 10.1021/acscatal.5c04133 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, s. 17101-17121 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE, s. 17101 - 17121

2025 [01/20] / **USA** - Yang, Timothy T. - Saidi, Wissam A. **Machine Learning-Accelerated First-Principles Molecular Dynamics Reveals C–C Coupling Mechanisms toward Ethylene on Cu(100)** [elektronický dokument]. DOI 10.1021/acscatal.5c02726 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, č. 17, s. 15093-15101 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE, s. 15093 - 15101

2025 [01/20] / **NLD** - Ejeromedoghene, Onome - Kumi, Moses - Akor, Ephraim - Zhang, Zexin. **The application of machine learning in 3D/4D printed stimuli-responsive hydrogels** [elektronický dokument]. DOI 10.1016/j.cis.2024.103360 In: **Advances in colloid and interface science**. Amsterdam: Elsevier. Elsevier Science, 2025, č. 336, art. no. 103360 [tlačená forma] [online]. ISSN 0001-8686. ISSN (online) 1873-3727. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 103360

2025 [01/20] / **GBR** - Vacek, Jaroslav - Vrška, Dávid - Manna, Debashree - Lo, Rabindranath - Hobza, Pavel. **Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches** [elektronický dokument]. DOI 10.1039/D5SC06336A In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 48, s. 23129-23138 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; WOS CC ; CCC ; SCIE ; Nature Index ; OA, s. 23129 - 23138

2024 [01/20] / **DEU** - Wan, Kaiwei - He, Jianxin - Shi, Xinghua. **Construction of High Accuracy Machine Learning Interatomic Potential for Surface/Interface of Nanomaterials—A Review** [elektronický dokument]. DOI 10.1002/adma.202305758 In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2024, Roč. 36, č. 22, art. no. 2305758 [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **USA** - Tsuji, Yuta. **Molecular Understanding of the Distinction between Adhesive Failure and Cohesive Failure in Adhesive Bonds with Epoxy Resin Adhesives** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c04015 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2024, Roč. 40, č. 14, s. 7479-7491 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 7479 - 7491

2023 [01/20] / **USA** - Chen, Yuxinxin - Ou, Yanchi - Zheng, Peikun - Huang, Yaohuang - Ge, Fuchun - Dral, Pavlo O. **Benchmark of general-purpose machine learning-based quantum mechanical method AIQM1 on reaction barrier heights** [elektronický dokument]. DOI 10.1063/5.0137101 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 158, č. 7, art. no. 074103 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 074103

2023 [01/20] / **USA** - Berger, Fabian - Rybicki, Marcin - Sauer, Joachim. **Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites** [elektronický dokument]. DOI 10.1021/acscatal.2c05493 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 3, s. 2011-2024 [online]. ISSN (online) 2155-5435. - SCO ;

CCC ; WOS CC, s. 2011 - 2024

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **GBR** - Bocus, Massimo - Goeminne, Ruben - Lamaire, Aran - Cools-Ceuppens, Maarten - Verstraelen, Toon - Van Speybroeck, Veronique. **Nuclear quantum effects on zeolite proton hopping kinetics explored with machine learning potentials and path integral molecular dynamics** [elektronický dokument]. DOI 10.1038/s41467-023-36666-y In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2023, Roč. 14, č. 1, art. no. 1008 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC, s. art. no. 1008

2023 [01/20] / **USA** - Snyder, Ryan - Kim, Bryant - Pan, Xiaoliang - Shao, Yihan - Pu, Jingzhi. **Bridging semiempirical and ab initio QM/MM potentials by Gaussian process regression and its sparse variants for free energy simulation** [elektronický dokument]. DOI 10.1063/5.0156327 In: **Journal of Chemical Physics**. Melville: American Institute of Physics. AIP Publishing, 2023, Roč. 159, č. 5, art. no. 054107 [tlačená forma] [online]. ISSN 0021-9606. ISSN (online) 1089-7690. - SCO ; CCC ; WOS CC, s. art. no. 054107

2023 [01/20] / **USA** - Rizzi, Andrea - Carloni, Paolo - Parrinello, M. **Free energies at QM accuracy from force fields via multimap targeted estimation** [elektronický dokument]. DOI 10.1073/pnas.2304308120 In: **Proceedings of the National Academy of Sciences of the United States of America**. Washington: National Academy of Sciences of the United States of America, 2023, Roč. 120, č. 46, art. no. 4308120 [tlačená forma] [online]. ISSN 0027-8424. ISSN (online) 1091-6490. - SCO ; CCC ; WOS CC, s.

2022 [01/20] / **USA** - De Wispelaere, Kristof - Plessow, Philipp N. - Studt, Felix. **Toward Computing Accurate Free Energies in Heterogeneous Catalysis: a Case Study for Adsorbed Isobutene in H-ZSM-5** [elektronický dokument]. DOI 10.1021/acsphyschemau.2c00020 In: **ACS Physical Chemistry Au**. Washington: American Chemical Society, 2022, Roč. 2, č. 5, s. 399-406 [online]. ISSN (online) 2694-2445. - SCO, s. 399 - 406

2022 [01/20] / **USA** - Giese, Timothy J. - Zeng, Jinzhe - York, Darrin M. **Multireference Generalization of the Weighted Thermodynamic Perturbation Method** [elektronický dokument]. DOI 10.1021/acs.jpca.2c06201 In: **The Journal of Physical Chemistry A**: Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; Theory. Washington: American Chemical Society, 2022, Roč. 126, č. 45, s. 8519-8533 [tlačená forma] [online]. ISSN 1089-5639. ISSN (online) 1520-5215. - SCO, s. 8519 - 8533

2022 [01/20] / **USA** - Joshi, Hrishikesh - Wilde, Nicole - Asche, Thomas S. - Wolf, Dorit. **Developing Catalysts via Structure-Property Relations Discovered by Machine Learning: An Industrial Perspective** [elektronický dokument]. DOI 10.1002/cite.202200071 In: **Chemie Ingenieur Technik**: Verfahrenstechnik, technische Chemie, Apparatewesen, Biotechnologie, 2022, Roč. 94, č. 11, s. 1645-1654 [tlačená forma]. ISSN 0009-286X. ISSN (online) 1522-2640. - SCO, s. 1645 - 1654

2022 [01/20] / **USA** - Devergne, Timothée - Magrino, Théo - Pietrucci, Fabio - Saitta, A. Marco. **Combining Machine Learning Approaches and Accurate Ab Initio Enhanced Sampling Methods for Prebiotic Chemical Reactions in Solution** [elektronický dokument]. DOI 10.1021/acs.jctc.2c00400 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 9, s. 5410-5421 [tlačená forma] [online]. ISSN 1549-9618.

ISSN (online) 1549-9626. - SCO, s. 5410 - 5421

2021 [01/20] / **USA** - Rizzi, Andrea - Carloni, Paolo - Parrinello, Michele. **Targeted Free Energy Perturbation Revisited: Accurate Free Energies from Mapped Reference Potentials** [elektronický dokument]. DOI 10.1021/acs.jpclett.1c02135 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2021, Roč. 12, č. 39, s. 9449-9454 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 9449 - 9454

ADC_065: / Rey, Jerome (Autor) (20%) - Bignaud, Charles (Autor) (20%) - Raybaud, Pascal (Autor) (20%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (20%) - Chizallet, Celine (Autor) (20%): **Dynamic Features of Transition States for beta-Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations**. – text. – [recenzované]. – SCO ; CCC ; WOS CC.
In: *Angewandte Chemie* [textový dokument (print)] [elektronický dokument] : International Edition. – Weinheim (Nemecko) : John Wiley & Sons. Wiley-VCH. – ISSN 1433-7851. – ISSN (online) 1521-3773. – Roč. 59, č. 43 (2020), s. 18938-18942 [tlačená forma] [online]
Počet všetkých autorov: 5
[článok]
Lit.: 42
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 15,336 - 2020
SNIP: 2,253 - 2020
SJR: 5,831 - 2020
CiteScore: 21,7 - 2020
AIS: 3.422 - 2020
Kvartil Q:
2020, AIS - Chemistry, multidisciplinary - Q1; **2020, JIF** - Chemistry, multidisciplinary - Q1; **2020, Scimago** - Catalysis - Q1; **2020, Scimago** - Chemistry (miscellaneous) - Q1

Ohlasy (28):
2025 [01/20] / **NLD** - Dai, Leilei - Lata, Suman - Chen, Junhui - Cobb, Kirk - Lei, Hanwu - Chen, Paul - Ruan, Roger. **Pyrolysis of municipal solid waste for bio-oil production**. DOI 10.1016/B978-0-443-29291-0.00003-X In: **Thermochemical Conversion of Biomass Feedstock and Solid Waste into Biofuels Production and Pollutant Control**. Amsterdam: Elsevier. Elsevier Science, 2025, s. 43-61 [tlačená forma] [online]. ISBN [9780443292927, 9780443292910]. - SCO, s. 43 - 61

2025 [01/20] / **DEU** - Göltl, Florian. **Exploring Quality Criteria for the Computational Modeling of Heterogeneous Catalysts** [elektronický dokument]. DOI 10.1002/cphc.202401123 In: **ChemPhysChem**: a European Journal of Chemical Physics and Physical Chemistry: a European Journal of Chemical Physics & Physical Chemistry. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 26, č. 11, art. no. e202401123 [tlačená forma] [online]. ISSN 1439-4235. ISSN (online) 1439-7641. - SCO ; CCC ; WOS CC, s.

2025 [01/20] / **GBR** - Kolganov, Alexander A. - Pidko, Evgeny A. **Computational Chemistry in Zeolite Catalysis**. DOI 10.1039/9781837676859-00312 In: **Zeolites from Fundamentals to Emerging Applications**. London: The Royal Society of Chemistry, 2025, s. 312-369 [tlačená forma] [online]. ISBN [9781837675456, 9781837676859]. - SCO, s. 312 - 369

2025 [01/20] / **USA** - Ureel, Yannick - Abdulrahman, Anas Jamil - Akin, Oğuzhan - Sabbe, Maarten K. - Van Geem, Kevin M. **Microkinetic Modeling of Plastic Waste Catalytic Cracking with Phosphorus-Modified Mesoporous HZSM-5: An Iso-Octane Model Compound Study** [elektronický dokument]. DOI 10.1021/acs.iecr.5c01928 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2025, Roč. 64, č. 34, s. 16563-16573 [tlačená

forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 16563 - 16573

2025 [01/20] / **GBR** - Zhang, Wenjun - Zhang, Mingwei - Liu, Linlin - Tang, Songzu - Wang, Li - Zhang, Xiangwen - Li, Guozhu. **Doping trace cerium in ZSM-48 in situ during hydrothermal synthesis for efficient hydroisomerization of a long-chain n-alkane** [elektronický dokument]. DOI 10.1039/d4cy01436g In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 15, č. 6, s. 1937-1947 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC ; SCIE, s. 1937 - 1947

2025 [01/20] / **USA** - Li, Lulu - Xu, Xiaofang - Ye, Mao - Liu, Zhongmin. **Toward Realistic Simulations of Zeolite Catalytic Processes: A Mini Review** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c07342 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 1, s. 24-36 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 24 - 36

2025 [01/20] / **USA** - Liu, Fengqing - Yi, Xianfeng - Liu, Tangkang - Chen, Wei - Yang, Jiabao - Xiao, Yao - Qin, Yucai - Song, Lijuan - Zheng, Anmin. **Microenvironment perturbations driving methanol low-temperature conversion over zeolite** [elektronický dokument]. DOI 10.1126/sciadv.ads4018 In: **Science advances**. Washington: American Association for the Advancement of Science, 2025, Roč. 11, č. 8, art. no. eads4018 [online]. ISSN (online) 2375-2548. - SCO ; CCC ; SCIE ; OA, s. art. no. eads4018

2025 [01/20] / **USA** - Zuo, Yanfen - Ye, Lei - Yang, Wenjie - Peng, Bo - Zhang, Jing - Shu, Xingtian - Xu, Youhao - Liu, Jichang. **Optimizing Ethylene Production through Enhanced Monomolecular β-Scission in Confined Catalytic Cracking of Olefin** [elektronický dokument]. DOI 10.1021/acscatal.4c05323 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, č. 3, s. 1576-1585 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE, s. 1576 - 1585

2025 [01/20] / **USA** - Ando, Yuriko - Miyakage, Takumi - Phuekphong, Alisa - Anzai, Akihiko - Huang, Mengwen - Fakir, Abdellah Ait El - Toyao, Takashi - Ogawa, Makoto - Kolganov, Alexander A. - Pidko, Evgeny A. - Shimizu, Ken ichi. **Hydrocracking of Polypropylene to Light Alkanes over HMFI Zeolite Catalysts under H2** [elektronický dokument]. DOI 10.1002/cctc.202500512 In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2025, Roč. 17, č. 16, art. no. e00512 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. e00512

2025 [01/20] / **DEU** - Jammee, Ratchawi - Kolganov, Alexander - Groves, Marc C. - Pidko, Evgeny A. - Sydora, Orson L. - Conley, Matthew P. **C−H Bond Activation by Sulfated Zirconium Oxide is Mediated by a Sulfur-Centered Lewis Superacid** [elektronický dokument]. DOI 10.1002/anie.202421699 In: **Angewandte Chemie**: International Edition. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 64, č. 11, art. no. e202421699 [tlačená forma] [online]. ISSN 1433-7851. ISSN (online) 1521-3773. - SCO ; CCC ; WOS CC ; SCIE ; OA, s.

2025 [01/20] / **DEU** - Zhao, Shangxun - Wen, Shuo - Chen, Hongrun - Zhan, Kewei - Weng, Jiawei - Ding, Danli - Cai, Xingwei - Song, Heng - Xu, Chen. **ortho-Selective Suzuki Coupling of Dichlorophenol and Dichlorobenzylalcohol in Water under Palladium Catalysis Directed by Noncovalent Interactions and Computational Analysis** [elektronický dokument]. DOI 10.1002/ajoc.202400581 In: **Asian Journal of Organic Chemistry**. Weinheim: John Wiley & Sons. Wiley-VCH, 2025, Roč. 14, č. 3, art. no. e202400581 [tlačená forma] [online]. ISSN 2193-5807. ISSN (online) 2193-5815. - SCO ; CCC ; WOS CC ; SCIE ; IC, s.

2025 [01/20] / **NLD** - Zhang, Jiapeng - Kong, Lingxin - Yang, Bin - Xu, Baoqiang. **Molecular dynamic simulation and experimental study on vacuum decomposition of InP scrap** [elektronický dokument]. DOI 10.1016/j.seppur.2025.134355 In: **Separation and Purification Technology**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 377, art. no. 134355 [tlačená forma] [online]. ISSN 1383-5866. ISSN (online) 1873-3794. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 134355

2025 [01/20] / **GBR** - Liu, Fengqing - Yi, Xianfeng - Yuan, Jiamin - Xing, Youdong - Xiao, Yao - Liu, Zhiqiang - Zheng, Anmin. **Microenvironment engineering unveils surface methoxy species origination in zeolite-catalyzed methanol chemistry under mild conditions** [elektronický dokument]. DOI 10.1038/s41467-025-64524-6 In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2025, Roč. 16, č. 1, art. no. 9519 [online]. ISSN (online) 2041-1723. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 9519

2025 [01/20] / **USA** - Yuan, Fan - Hou, Xueyang - Wang, Kaili - Zhu, Yi - Chen, Guoli - Hao, Yi - Yang, Jingxiu - Han, Jingfeng - Jia, Rongrong - Pimbaotham, Pimjai - Injongkol, Yuwanda - Jungsuttiwong, Siriporn - Shi, Liyi - Cheng, Ping - Huang, Lei. **Impact of Acid Sites in ZSM-5 Zeolites on the Selective Catalytic Oxi-Upcycling of High-Density Polyethylene to Dicarboxylic Acid under Mild Conditions** [elektronický dokument]. DOI 10.1021/acscatal.4c04987 In: **ACS Catalysis**. Washington: American Chemical Society, 2025, Roč. 15, č. 18, s. 15780-15791 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC ; SCIE, s. 15780 - 15791

2024 [01/20] / **GBR** - Qie, Guanyu - Deng, Quanzheng - Deng, Donghao - Zhai, Miao - Ding, Hongxin - Liu, Wei - Han, Lu - Zhu, Kake. **Generating zeolite crystals with mesoscopic aperiodic structure to promote catalytic hydroisomerization** [elektronický dokument]. DOI 10.1039/d4ta01303d In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2024, Roč. 12, č. 32, s. 21066-21078 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 21066 - 21078

2024 [01/20] / **NLD** - Dai, Leilei - Lata, Suman - Cobb, Kirk - Zou, Rongge - Lei, Hanwu - Chen, Paul - Ruan, Roger. **Recent advances in polyolefinic plastic pyrolysis to produce fuels and chemicals** [elektronický dokument]. DOI 10.1016/j.jaap.2024.106551 In: **Journal of Analytical and Applied Pyrolysis**. Amsterdam: Elsevier, 2024, Roč. 180, art. no. 106551 [tlačená forma] [online]. ISSN 0165-2370. ISSN (online) 1873-250X. - SCO ; CCC ; WOS CC, s. art. no. 106551

2024 [01/20] / **USA** - Moreira, V. M. **Carbocations**. DOI 10.1002/9781119716846.ch5 In: **Organic Reaction Mechanisms 2020**. New Jersey: John Wiley & Sons, 2024, s. 205-235 [online]. ISBN [9781119716839, 9781119716846]. - SCO, s. 205 - 235

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2023 [01/20] / **USA** - Chen, Wei - Huang, Mengdi - Yi, Xianfeng - Hui, Yu - Gao, Pan - Hou, Guangjin - Stepanov, Alexander G. - Qin, Yucai - Song, Lijuan - Liu, Shang Bin - Chen, Zhongfang - Zheng, Anmin. **Protonated methylcyclopropane is an intermediate providing complete 13C-label scrambling at C4 olefin isomerization in zeolite** [elektronický dokument]. DOI 10.1016/j.checat.2022.100503 In: **Chem Catalysis**. Philadelphia: Elsevier, 2023, Roč. 3, č. 2, art. no. 100503 [tlačená forma] [online]. ISSN 2667-1107. ISSN (online) 2667-1093. - SCO ; WOS CC, s.

2023 [01/20] / **USA** - Schmidt, Joel E. - Smit, Berend - Chen, Cong Yan - Xie, Dan - Maesen, Theo L.M. **Toward Superior Hydroisomerization Catalysts through Thermodynamic Optimization** [elektronický dokument]. DOI 10.1021/acscatal.3c00391 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 10, s. 6710-6720 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 6710 - 6720

2023 [01/20] / **USA** - Peng, Yan - Wang, Xuelin - Wang, Congxin - Bi, Wentao - Jiang, Qike - Tian, Zhijian. **Boosting catalytic performance via electron transfer effect for hydroisomerization on a low-Pt-content PtCeOX/zeolite catalyst** [elektronický dokument]. DOI 10.1016/j.checat.2023.100505 In: **Chem Catalysis**. Philadelphia: Elsevier, 2023, Roč. 3, č. 2, art. no. 100505 [tlačená forma] [online]. ISSN 2667-1107. ISSN (online) 2667-1093. - SCO ; WOS CC, s. art. no. 100505

2022 [01/20] / **NLD** - Kollias, Loukas - Collinge, Gregory - Zhang, Difan - Allec, Sarah I. - Gurunathan, Pradeep Kumar -

Piccini, Giovanni Maria - Yuk, Simuck F. - Nguyen, Manh Thuong - Lee, Mal Soon - Glezakou, Vassiliki Alexandra - Rousseau, Roger. **Assessing entropy for catalytic processes at complex reactive interfaces** [elektronický dokument]. DOI 10.1016/bs.arcc.2022.09.004 In: **Annual Reports in Computational Chemistry**. Amsterdam: Elsevier, 2022, s. 3-51 [tlačená forma] [online]. ISBN 978-0-323-99092-9. ISBN (online) 978-0-323-99093-6. ISSN 1574-1400. ISSN (online) 1875-5232. - SCO, s. 3 - 51

2022 [01/20] / **USA** - Zhang, Mingwei - Liu, Linlin - Wang, Li - Zhang, Xiangwen - Li, Guozhu. **Four-Carbon Segmented Discrete Hydrocracking of Long-Chain Paraffins in MTT Channels Following a Pore-Mouth Mechanism** [elektronický dokument]. DOI 10.1021/acscatal.2c03090 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 16, s. 10313-10325 [online]. ISSN (online) 2155-5435. - SCO, s. 10313 - 10325

2022 [01/20] / **GBR** - Piccini, Giovannimaria - Lee, Mal Soon - Yuk, Simuck F. - Zhang, Difan - Collinge, Greg - Kollias, Loukas - Nguyen, Manh Thuong - Glezakou, Vassiliki Alexandra - Rousseau, Roger. **Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis** [elektronický dokument]. DOI 10.1039/d1cy01329g In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 12, č. 1, s. 12-37 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO, s. 12 - 37

2022 [01/20] / **GBR** - Chen, Wei - Yi, Xianfeng - Liu, Zhiqiang - Tang, Xiaomin - Zheng, Anmin. **Carbocation chemistry confined in zeolites: spectroscopic and theoretical characterizations** [elektronický dokument]. DOI 10.1039/d1cs00966d In: **Chemical Society Reviews**. Cambridge: The Royal Society of Chemistry, 2022, Roč. 51, č. 11, s. 4337-4385 [tlačená forma] [online]. ISSN 0306-0012. ISSN (online) 1460-4744. - SCO, s. 4337 - 4385

2022 [01/20] / **USA** - Dong, Zhongwen - Chen, Wenjun - Xu, Keqing - Liu, Yue - Wu, Jing - Zhang, Fan. **Understanding the Structure-Activity Relationships in Catalytic Conversion of Polyolefin Plastics by Zeolite-Based Catalysts: A Critical Review** [elektronický dokument]. DOI 10.1021/acscatal.2c04915 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 24, s. 14882-14901 [online]. ISSN (online) 2155-5435. - SCO, s. 14882 - 14901

2022 [01/20] / **CHE** - Zhai, Miao - Wu, Wenxue - Xing, Enhui - Zhang, Yunfeng - Ding, Hongxin - Zhou, Jinghua - Luo, Yibin - Liu, Jichang - Zhu, Kake - Zhu, Xuedong. **Generating TON zeolites with reduced [0 0 1] length through combined mechanochemical bead-milling and porogen-directed recrystallization with enhanced catalytic property in hydroisomerization** [elektronický dokument]. DOI 10.1016/j.cej.2022.135874 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2022, č. 440, art. no. 135874 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO, s. art. no. 135874

2021 [01/20] / **GBR** - Fečík, Michal - Plessow, Philipp N. - Studt, Felix. **Theoretical investigation of the side-chain mechanism of the MTO process over H-SSZ-13 using DFT and: Ab initio calculations** [elektronický dokument]. DOI 10.1039/d1cy00433f In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2021, Roč. 11, č. 11, s. 3826-3833 [tlačená forma] [online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 3826 - 3833

ADC_066: / Silva, Manoj (Autor) (19%) - Barčauskaite, Karolina (Autor) (19%) - Drapanauskaite, Donata (Autor) (19%) - Tian, Huijie (Autor) (19%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (5%) - Baltrušaitis, Jonas (Autor) (19%): **Relative humidity facilitated urea particle reaction with salicylic acid: a combined in situ spectroscopy and DFT study**. – text, ilustr., graf. – [recenzované]. – DOI 10.1021/acsearthspacechem.0c00051. – SCO ; CCC ; WOS CC.
In: *ACS Earth and Space Chemistry* [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN (online) 2472-3452. – Roč. 4, č. 7 (2020), s. 1018-1028 [online]
Počet všetkých autorov: 6
[článok]

Lit.: 93
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 3,475 - 2020
SNIP: 0,949 - 2020
SJR: 0,876 - 2020
CiteScore: 4,1 - 2020
AIS: 0.998 - 2020
Kvartil Q:
2020, AIS - Chemistry, multidisciplinary - Q2; **2020, AIS** - Geochemistry & geophysics - Q2; **2020, JIF** - Chemistry, multidisciplinary - Q2; **2020, JIF** - Geochemistry & geophysics - Q2; **2020, Scimago** - Atmospheric science - Q2; **2020, Scimago** - Geochemistry and petrology - Q2; **2020, Scimago** - Space and planetary science - Q2

Ohlasy (15):
2025 [01/20] / **CHE** - Cao, Yuechao - Qu, Haibin - Wan, Xuxing - Guo, Shengzheng - Li, Kangli - Wu, Songgu - Gong, Junbo. **Spherical cocrystal as a fertilizer slow-release platform for improved nitrogen cycle management** [elektronický dokument]. DOI 10.1016/j.cej.2025.160288 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2025, Roč. 506, art. no. 160288 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 160288

2025 [01/20] / **ETH** - Fakhree, Falah M. - Yousif, Thana Y. **Syntheses and characterization of new complexes Cu(II), Co(II), Mn(II), Zn(II) from ligand preparing irradiation microwaves and their use as antibacterial drugs** [elektronický dokument]. DOI 10.4314/bcse.v39i11.1 In: **Bulletin of the Chemical Society of Ethiopia**. Addis Ababa: The Society, 2025, Roč. 39, č. 11, s. 2083-2091 [tlačená forma] [online]. ISSN 1011-3924. ISSN (online) 1726-801X. - SCO ; WOS CC ; SCIE ; OA, s. 2083 - 2091

2025 [01/20] / **NLD** - Baruah, Jubaraj B. **An overview of progress on synthesis, complexes, composites, detections, and decomposition of urea** [elektronický dokument]. DOI 10.1016/j.rechem.2025.102778 In: **Results in Chemistry**. Amsterdam: Elsevier, 2025, Roč. 18, art. no. 102778. ISSN (online) 22117156. - SCO ; WOS CC ; ESCI ; OA, s. art. no. 102778

2025 [01/20] / **NLD** - Müller-Kiedrowski, Carolin B.M. - Görs, Solvig - Mittermeier-Kleßinger, Verena K. - Dawid, Corinna - Wrage-Mönnig, Nicole - Kuhla, Björn. **Feeding salicylates containing willow leaves to cattle modulates urea metabolism and mitigates urine-derived ammonia and nitrous oxide emissions from soil** [elektronický dokument]. DOI 10.1016/j.agee.2025.109671 In: **Agriculture, Ecosystems & Environment**. Amsterdam: Elsevier, 2025, Roč. 388, art. no. 109671 [tlačená forma]. ISSN 0167-8809. ISSN (online) 1873-2305. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 109671

2024 [01/20] / **GBR** - Nagaraju, Vidya - Jange, Camila - Wassgren, Carl - Ambrose, Kingsly. **Understanding urea polymorphism and cocrystallization to develop enhanced fertilizers: A review** [elektronický dokument]. DOI 10.1016/j.jece.2024.114308 In: **Journal of Environmental Chemical Engineering**. Oxford: Elsevier, 2024, Roč. 12, č. 6, art. no. 114308 [tlačená forma] [online]. ISSN 2213-2929. ISSN (online) 2213-3437. - SCO ; CCC ; WOS CC, s. art. no. 114308

2024 [01/20] / **NLD** - de Castro, Saulo Augusto Quassi - Schjoerring, Jan Kofod. **Foliar nitrogen and phosphorus fertilization**. DOI 10.1016/bs.agron.2024.05.002 In: **Advances in Agronomy**. Amsterdam: Elsevier. Elsevier Science, 2024, s. 109-169. ISBN [9780443295300]. ISSN 00652113. - SCO, s. 109 - 169

2024 [01/20] / **USA** - Zhao, Jiang - Jia, Caiyun - Fang, Xiaoxia - Xiao, Anni - Zhang, Haijun. **Utilization of industrial by-product gypsum to prepare urea gypsum cocrystals as a sustained release fertilizer: A review** [elektronický dokument]. DOI 10.1002/apj.3066 In: **Asia-Pacific Journal of Chemical Engineering**. Hoboken: John Wiley & Sons, 2024, Roč. 19, č.

4, art. no. e3066. ISSN 1932-2135. ISSN (online) 1932-2143. - SCO ; WOS CC, s. art. no. e3066

2023 [01/20] / **GBR** - Song, Yong - Jin, Zhiyuan - Zhang, Jiawei - Jin, Bo - Peng, Rufang. **Manufacturing of urea co-crystals by spiral gas-solid two-phase flow (S-GSF) based on spiral jet mills: a continuous, solvent-free, and scalable mechanochemical method**. DOI 10.1039/d3ce00833a In: **CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2023, Roč. 25, č. 44, s. 6215-6224 [tlačená forma] [online]. ISSN 1466-8033. - SCO ; CCC ; WOS CC, s. 6215 - 6224

2023 [01/20] / **NLD** - MacEachern, L. - Kermanshahi-pour, A. - Mirmehrabi, Mahmoud - Ajiboye, L. - Trivedi, V. - Rohani, S. - He, Q. **Cocrystal formation of niclosamide and urea in supercritical CO2 and impact of cosolvent** [elektronický dokument]. DOI 10.1016/j.supflu.2023.106029 In: **Journal of Supercritical Fluids**. Amsterdam: Elsevier, 2023, Roč. 201, art. no. 106029 [tlačená forma] [online]. ISSN 0896-8446. ISSN (online) 1872-8162. - SCO ; CCC ; WOS CC, s. art. no. 106029

2023 [01/20] / **USA** - Xiao, Yuntian - Wu, Chuanhua - Cui, Pingping - Zhou, Ling - Yin, Qiuxiang. **Pursuing Green and Efficient Agriculture from Molecular Assembly: A Review of Solid-State Forms on Agrochemicals** [elektronický dokument]. DOI 10.1021/acs.jafc.3c01084 In: **Journal of agricultural and food chemistry**. Washington: American Chemical Society, 2023, Roč. 71, č. 28, s. 10500-10524 [tlačená forma] [online]. ISSN 0021-8561. ISSN (online) 1520-5118. - SCO ; CCC ; WOS CC, s. 10500 - 10524

2023 [01/20] / **GBR** - Rajbongshi, Trishna - Parakatawella, Shalika - Gogoi, Diptajyoti - Deka, Poonam - Adassooriya, Nadeesh M. - Thakuria, Ranjit. **Mechanosynthesis of urea-hydroxybenzoic acid cocrystals as sustained-release nitrogen fertilizer** [elektronický dokument]. DOI 10.1039/d3su00021d In: **RSC Sustainability**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 1, č. 6, s. 1416-1422 [online]. ISSN (online) 2753-8125. - SCO ; WOS CC, s. 1416 - 1422

2023 [01/20] / **CHN** - Xiao, Yuntian - Yin, Qiuxiang - Wu, Chuanhua - Cui, Pingping - Zhou, Ling. **Application of organic cocrystal engineering strategy in sustained-release of agrochemicals**. DOI 10.13353/j.issn.1004.9533.20220830 In: **Chemical Industry and Engineering**. Tianjin: Tianjin University, 2023, Roč. 40, č. 1, s. 15-24. ISSN 1004-9533. - SCO, s. 15 - 24

2022 [01/20] / **USA** - Qin, Jiangzhou - Liu, Nengsheng - Chen, Liuzhou - Wu, Kun - Zhao, Quanlin - Liu, Baojun - Ye, Zhengfang. **Selective Electrochemical Urea Synthesis from Nitrate and CO2 Using in Situ Ru Anchoring onto a Three-Dimensional Copper Electrode** [elektronický dokument]. DOI 10.1021/acssuschemeng.2c05110 In: **ACS Sustainable Chemistry & Engineering**. Washington: American Chemical Society, 2022, Roč. 10, č. 48, s. 15869-15875 [online]. ISSN (online) 2168-0485. - SCO, s. 15869 - 15875

2022 [01/20] / **USA** - Jing, Jianyuan - Zhang, Shuiqin - Yuan, Liang - Li, Yanting - Zhang, Yingqiang - Wen, Yanchen - Zhao, Bingqiang. **Humic acid complex formation with urea alters its structure and enhances biomass production in hydroponic maize** [elektronický dokument]. DOI 10.1002/jsfa.11710 In: **Journal of the science of food and agriculture**. Hoboken: John Wiley & Sons, 2022, Roč. 102, č. 9, s. 3636-3643 [tlačená forma] [online]. ISSN 0022-5142. ISSN (online) 1097-0010. - SCO, s. 3636 - 3643

2022 [01/20] / **GBR** - Adassooriya, Nadeesh M. - Mahanta, Sanjeev Pran - Thakuria, Ranjit. **Mechanochemistry as an emerging tool for the preparation of sustained release urea cocrystals as a nitrogen source**. DOI 10.1039/d1ce01713f In: **CrystEngComm**: Design and understanding of solid-state and crystalline materials. Londýn: The Royal Society of Chemistry, 2022, Roč. 24, č. 9, s. 1679-1689 [tlačená forma] [online]. ISSN 1466-8033. - SCO, s. 1679 - 1689

2021 - spolu : **6**

ADC_067: / Said, Halima (Autor) [Interný doktorand] [UKOPRCFZ] (50%) - Novotný, Michal (Autor) (5%) - Černušák, Ivan (Autor) [UKOPRCFZ] (5%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%): **Ab initio molecular dynamics investigation of Cs adsorption on Mo(001): Beyond a single monolayer coverage**. – text, graf. – SCO ; CCC ; WOS CC.
In: *Applied Surface Science* [textový dokument (print)] [elektronický dokument] : a journal devoted to applied physics and chemistry of surfaces and interfaces. – Amsterdam (Holandsko) : Elsevier. – ISSN 0169-4332. – ISSN (online) 1873-5584. – č. 559 (2021), art. no. 149822, s. [1-9] [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 45
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 7.392 - 2021
SNIP: 1,262 - 2021
SJR: 1,147 - 2021
CiteScore: 12,1 - 2021
AIS: 0.848 - 2021
Kvartil Q:
2021, AIS - Chemistry, physical - Q2; **2021, AIS** - Materials science, coatings & films - Q1; **2021, AIS** - Physics, applied - Q1; **2021, AIS** - Physics, condensed matter - Q2; **2021, JIF** - Chemistry, physical - Q2; **2021, JIF** - Materials science, coatings & films - Q1; **2021, JIF** - Physics, applied - Q1; **2021, JIF** - Physics, condensed matter - Q1; **2021, Scimago** - Chemistry (miscellaneous) - Q1; **2021, Scimago** - Condensed matter physics - Q1; **2021, Scimago** - Physics and astronomy (miscellaneous) - Q1; **2021, Scimago** - Surfaces and interfaces - Q1; **2021, Scimago** - Surfaces, coatings and films - Q1

Ohlasy (8):
2025 [01/20] / **NLD** - Ma, Yubo - Li, Wei - Hu, Jun - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Geng, Shaofei - Liu, Haifeng - Wang, Xianqu - Huang, Jie - Liu, Hai - Cheng, Jun - Tang, Changjian. **Investigating the stability and work function effects of Ba atoms adsorption on the Mo (110) surface** [elektronický dokument]. DOI 10.1016/j.nme.2025.101984 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2025, Roč. 45, art. no. 101984 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101984

2025 [01/20] / **NLD** - Zhang, Xin - Li, Heng - Tsumori, Katsuyoshi - Xu, Yuhong - Isobe, Mitsutaka - Lei, Guangjiu - Liu, Sanqiu - Osakabe, Masaki - Nakano, Haruhisa - Shimizu, Akihiro - Okamura, Shoichi - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Liu, Xiaoqiao - Zheng, Huaqing - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Chen, Jun. **The influence of hydrogen and impurities on the work function of multilayer Cs atoms on the plasma grid: An ab-initio molecular dynamics study about negative hydrogen ion sources for neutral beam injection systems** [elektronický dokument]. DOI 10.1016/j.nme.2025.101897 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2025, Roč. 42, art. no. 101897 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 101897

2024 [01/20] / **USA** - Xue, Feng - Zuo, Chen - Xia, Haohua - Li, Zengshan - Li, Dong - Chen, Dezhi. **Research of Cesium Adsorption on Mo and Ni Based on Temperature-Controlled Quartz Microbalance** [elektronický dokument]. DOI 10.1109/TIM.2024.3412206 In: **IEEE Transactions on instrumentation and measurement**: a publication of the IEEE Instrumentation and measurement society. Piscataway: Institute of Electrical and Electronics Engineers, 2024, Roč. 73, art. no. 1005811 [tlačená forma] [online]. ISSN 0018-9456. ISSN (online) 1557-9662. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Tsumori, Katsuyoshi - Nakano, Haruhisa - Osakabe, Masaki - Isobe, Mitsutaka - Okamura, Shoichi - Shimizu, Akihiro - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Zheng, Huaqing - Liu, Xiaoqiao - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **Effect of oxygen or copper impurities on the work function of cesiated surfaces under co-existence with hydrogen: A study about negative hydrogen ion sources for neutral beam injection systems** [elektronický dokument]. DOI 10.1016/j.nme.2024.101792 In: **Nuclear Materials and**

Energy. Amsterdam: Elsevier, 2024, Roč. 41, art. no. 101792 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC, s. art. no. 101792

2024 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Tsumori, Katsuyoshi - Nakano, Haruhisa - Osakabe, Masaki - Isobe, Mitsutaka - Okamura, Shoichi - Shimizu, Akihiro - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Zheng, Huaqing - Liu, Xiaoqiao - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **Effect of metal impurities on the adsorption energy of cesium and work function of the cesiated Mo (0 0 1) surface** [elektronický dokument]. DOI 10.1016/j.nme.2024.101619 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2024, Roč. 38, art. no. 101619 [online]. ISSN (online) 2352-1791. - SCO ; WOS CC, s. art. no. 101619

2024 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Liu, Xiaoqiao - Zheng, Huaqing - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **A new attempt to further reduce the work function of the cesiated surface: The strongest electronegative element fluorine co-adsorption with cesium on Mo (001) surface** [elektronický dokument]. DOI 10.1016/j.nme.2024.101738 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2024, Roč. 41, art. no. 101738 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC, s. art. no. 101738

2023 [01/20] / **NLD** - Li, Heng - Zhang, Xin - Xu, Yuhong - Lei, Guangjiu - Liu, Sanqiu - Tsumori, Katsuyoshi - Nakano, Haruhisa - Osakabe, Masaki - Isobe, Mitsutaka - Okamura, Shoichi - Shimizu, Akihiro - Ogawa, Kunihiro - Takahashi, Hiromi - Cui, Zilin - Hu, Jun - Zhu, Yiqin - Li, Xiaolong - Zheng, Huaqing - Liu, Xiaoqiao - Geng, Shaofei - Chen, Xiaochang - Liu, Haifeng - Wang, Xianqu - Liu, Hai - Tang, Changjian. **Effect of H atoms and O impurities on the adsorption stability and work function of the cesiated Mo(0 0 1) surface: A study about negative hydrogen ion sources for neutral beam injection systems** [elektronický dokument]. DOI 10.1016/j.nme.2023.101550 In: **Nuclear Materials and Energy**. Amsterdam: Elsevier, 2023, Roč. 37, art. no. 101550 [online]. ISSN (online) 2352-1791. - SCO ; CCC ; WOS CC, s. art. no. 101550

2023 [01/20] / **NLD** - Xia, Sihao - Wang, Yuyan - Diao, Yu - Shi, Hongkai - Kan, Caixia - Shi, Daning. **Surface evolution of AlGaN nanowire decorated by cesium atoms: A first principle study** [elektronický dokument]. DOI 10.1016/j.rinp.2023.106957 In: **Results in Physics**: The new online only, open access journal in Physics. Amsterdam: Elsevier, 2023, Roč. 53, art. no. 106957 [online]. ISSN (online) 2211-3797. - SCO ; CCC ; WOS CC, s. art. no. 106957

ADC_068: / Amsler, Jonas (Autor) (20%) - Plessow, Philipp N. (Autor) (15%) - Studt, Felix (Autor) (15%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (50%): **Anharmonic Correction to Adsorption Free Energy from DFT-Based MD Using Thermodynamic Integration**. – text, graf., tab., obr. – [recenzované]. – DOI 10.1021/acs.jctc.0c01022. – SCO ; CCC ; WOS CC ; SCIE.
In: *Journal of Chemical Theory and Computation* [textový dokument (print)] [elektronický dokument] . – Washington (USA) : American Chemical Society. – ISSN 1549-9618. – ISSN (online) 1549-9626. – Roč. 17, č. 2 (2021), s. 1155-1169 [tlačená forma] [online]
Počet všetkých autorov: 4
[článok]
Lit.: 129
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 6.578 - 2021
SNIP: 1,475 - 2021
SJR: 1,619 - 2021
CiteScore: 10 - 2021

AIS: 1.512 - 2021
Kvartil Q:
2021, AIS - Chemistry, physical - Q1; **2021, AIS** - Physics, atomic, molecular & chemical - Q1; **2021, JIF** - Chemistry, physical - Q2; **2021, JIF** - Physics, atomic, molecular & chemical - Q1; **2021, Scimago** - Computer science applications - Q1; **2021, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (29):
2025 [01/20] / **NLD** - Islam, Md Aminul - Hossain, Nayem - Ahsan, Zahid - Rana, Masud - Rahman, Mustafizur - Abdullah, Md. **DFT insights into the mechanical properties of NMs** [elektronický dokument]. DOI 10.1016/j.rsurfi.2025.100417 In: **Results in Surfaces and Interfaces**. Amsterdam: Elsevier, 2025, Roč. 18, art. no. 100417 [online]. ISSN (online) 2666-8459. - SCO ; WOS CC ; ESCI ; OA, s. art. no. 100417

2025 [01/20] / **USA** - Lei, Yanhua - Liu, Lei - Zhang, Erjun. **Calculation of Adsorbate Free Energy Using the Damping Function Method** [elektronický dokument]. DOI 10.1021/acs.jctc.4c01079 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2025, Roč. 21, č. 1, s. 46-57 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 46 - 57

2025 [01/20] / **NLD** - Karamanis, Ioannis - Marchal, Mathieu - Guillet-Nicolas, Rémy - Badawi, Michael - Monnier, Hubert. **Investigations of NO, CO and H2O adsorption on faujasites NaY and NaX to treat the exhaust gas diesel: Isotherm experiments, equilibrium modelling and DFT calculation** [elektronický dokument]. DOI 10.1016/j.apsusc.2025.164016 In: **Applied Surface Science**: a journal devoted to applied physics and chemistry of surfaces and interfaces. Amsterdam: Elsevier, 2025, Roč. 711, art. no. 164016 [tlačená forma] [online]. ISSN 0169-4332. ISSN (online) 1873-5584. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 164016

2025 [01/20] / **USA** - Singh, Madhur Babu - Narang, Garima - Singh, Prashant. **A Comparative Study of Graphynes for Sensing of Gasses (SO2 & Acetylene) Using DFT Calculations and MD Simulations** [elektronický dokument]. DOI 10.1007/s12088-024-01289-4 In: **Indian Journal of Microbiology**. New York: Springer Nature, 2025, Roč. 65, č. 1, s. 359-374 [tlačená forma]. ISSN 0046-8991. ISSN (online) 0973-7715. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 359 - 374

2025 [01/20] / **USA** - Wander, Brook - Musielewicz, Joseph - Cheula, Raffaele - Kitchin, John R. **Accessing Numerical Energy Hessians with Graph Neural Network Potentials and Their Application in Heterogeneous Catalysis** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c07477 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2025, Roč. 129, č. 7, s. 3510-3521 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. 3510 - 3521

2025 [01/20] / **NLD** - Qi, Yuechao - Qiu, Xianyang - Wang, Chenghang - Wei, Dezhou - Dai, Zilin - Zhang, Faming. **Lattice defects and surface adsorption properties of gold-bearing chalcopyrite: A theoretical study based on DFT** [elektronický dokument]. DOI 10.1016/j.colsurfa.2024.135484 In: **Colloids and Surfaces A: Physicochemical and Engineering Aspects**: an international journal devoted to the principles and applications of colloid and interface science. Amsterdam: Elsevier, 2025, Roč. 704, art. no. 135484 [tlačená forma] [online]. ISSN 0927-7757. ISSN (online) 1873-4359. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 135484

2025 [01/20] / **USA** - Joutsuka, Tatsuya - Itagaki, Yoshiteru. **Computational Evaluation of Molecular Binding on Metal Surfaces in Temperature Programmed Desorption: Accuracy of DFT Functionals and Neural Network Potentials** [elektronický dokument]. DOI 10.1002/jcc.70279 In: **Journal of computational chemistry**. Hoboken: John Wiley & Sons, 2025, Roč. 46, č. 31, art. no. e70279 [tlačená forma] [online]. ISSN 0192-8651. ISSN (online) 1096-987X. - SCO ; CCC ; WOS CC, s. art. no. e70279

2024 [01/20] / **USA** - Fang, Siyuan - Hu, Yun Hang. **Temperature, pressure, and adsorption dependent redox potentials: III. Processes of CO conversion to value-added compounds** [elektronický dokument]. DOI 10.1002/ese3.1399

In: **Energy Science and Engineering**. Hoboken: John Wiley & Sons, 2024, Roč. 12, č. 2, s. 362-393. ISSN (online) 2050-0505. - SCO ; CCC ; WOS CC, s. 362 - 393

2024 [01/20] / **USA** - Chen, Wei - Liu, Zhiqiang - Yi, Xianfeng - Zheng, Anmin. **Confinement-Driven Dimethyl Ether Carbonylation in Mordenite Zeolite as an Ultramicroscopic Reactor** [elektronický dokument]. DOI 10.1021/acs.accounts.4c00389 In: **Accounts of Chemical Research**. Washington: American Chemical Society, 2024, Roč. 57, č. 19, s. 2804-2815 [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCO ; CCC ; WOS CC, s. 2804 - 2815

2024 [01/20] / **GBR** - Jørgensen, Mikkel - Grönbeck, Henrik. **Kinetic Monte Carlo Simulations to Study Reactions over Nanoparticles** [elektronický dokument]. DOI 10.1039/9781839163296-00119 In: **RSC Catalysis Series**. Londýn: The Royal Society of Chemistry, 2024, s. 119-150. ISSN 17576725. ISSN (online) 17576733. - SCO, s. 119 - 150

2023 [01/20] / **CHE** - Jia, Zhenggang - Zhang, Xuexi - Qian, Mingfang - Ma, Siyao - Jin, Yingmin - Xiong, Yueping. **Design of ultra-thick graphene-molybdenum disulfide electrodes to reduce volume expansion and capacity fading by first principles** [elektronický dokument]. DOI 10.1016/j.jallcom.2022.168623 In: **Journal of Alloys and Compounds**: an interdisciplinary journal of materials science and solid-state chemistry and physics. Lausanne: Elsevier. Elsevier Science, 2023, Roč. 939, art. no. 168623 [tlačená forma] [online]. ISSN 0925-8388. ISSN (online) 1873-4669. - SCO ; CCC ; WOS CC, s. art. no. 168623

2023 [01/20] / **USA** - Fang, Siyuan - Hu, Yun Hang. **Temperature, pressure, and adsorption-dependent redox potentials: II. Processes of CH4 oxidation to value-added compounds** [elektronický dokument]. DOI 10.1002/ese3.1361 In: **Energy Science and Engineering**. Hoboken: John Wiley & Sons, 2023, Roč. 11, č. 2, s. 762-782. ISSN (online) 2050-0505. - SCO ; CCC ; WOS CC, s. 762 - 782

2023 [01/20] / **DEU** - Rybakov, A. A. - Trubnikov, D. N. - Vercauteren, D. P. - Larin, A. V. **Periodic DFT computation of rotational barriers for linear molecules in zeolites: Validation via zero-point energies and isotopic heat difference values of adsorbed H2/D2** [elektronický dokument]. DOI 10.1016/j.matchemphys.2022.126929 In: **Materials Chemistry and Physics**: including materials science communications: an international interdisciplinary journal on science, characterization and processing of advanced materials: The International Journal of the Materials Research Society-Taiwan (MRS-T). Berlín: Elsevier, 2023, Roč. 294, art. no. 126929 [tlačená forma] [online]. ISSN 0254-0584. ISSN (online) 1879-3312. - SCO ; CCC ; WOS CC, s. art. no. 126929

2023 [01/20] / **USA** - Blöndal, Katrín - Sargsyan, Khachik - Bross, David H. - Ruscic, Branko - Goldsmith, C. Franklin. **Configuration Space Integration for Adsorbate Partition Functions: The Effect of Anharmonicity on the Thermophysical Properties of CO-Pt(111) and CH3OH-Cu(111)** [elektronický dokument]. DOI 10.1021/acscatal.2c04246 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 1, s. 19-32 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 19 - 32

2023 [01/20] / **DEU** - Yook, Hyunwoo - Hwang, Jinwoo - Yeo, Woonsuk - Bang, Jungup - Kim, Jaeyoung - Kim, Tae Yong - Choi, Jae Soon - Han, Jeong Woo. **Design Strategies for Hydroxyapatite-Based Materials to Enhance Their Catalytic Performance and Applicability** [elektronický dokument]. DOI 10.1002/adma.202204938 In: **Advanced Materials**. Weinheim: John Wiley & Sons. Wiley-VCH, 2023, Roč. 35, č. 43, art. no. 2204938 [tlačená forma] [online]. ISSN 0935-9648. ISSN (online) 1521-4095. - SCO ; CCC ; WOS CC, s.

2023 [01/20] / **USA** - Berger, Fabian - Rybicki, Marcin - Sauer, Joachim. **Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites** [elektronický dokument]. DOI 10.1021/acscatal.2c05493 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 3, s. 2011-2024 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 2011 - 2024

2022 [01/20] / **NLD** - Kollias, Loukas - Collinge, Gregory - Zhang, Difan - Allec, Sarah I. - Gurunathan, Pradeep Kumar -

Piccini, Giovanni Maria - Yuk, Simuck F. - Nguyen, Manh Thuong - Lee, Mal Soon - Glezakou, Vassiliki Alexandra - Rousseau, Roger. **Assessing entropy for catalytic processes at complex reactive interfaces** [elektronický dokument]. DOI 10.1016/bs.arcc.2022.09.004 In: **Annual Reports in Computational Chemistry**. Amsterdam: Elsevier, 2022, s. 3-51 [tlačená forma] [online]. ISBN 978-0-323-99092-9. ISBN (online) 978-0-323-99093-6. ISSN 1574-1400. ISSN (online) 1875-5232. - SCO, s. 3 - 51

2022 [01/20] / **USA** - Yang, Yichang - Meng, Xiangyu - Zhu, Longfeng - Yang, Jinghuai - Zhang, Guoliang - Shen, Hongxia - Cao, Xuebo. **Rapid Synthesis of Si-Rich SSZ-13 Zeolite under Fluoride-Free Conditions** [elektronický dokument]. DOI 10.1021/acs.inorgchem.2c03749 In: **Inorganic Chemistry**. Washington: American Chemical Society, 2022, Roč. 61, č. 51, s. 21115-21122 [tlačená forma] [online]. ISSN 0020-1669. ISSN (online) 1520-510X. - SCO, s. 21115 - 21122

2022 [01/20] / **USA** - Fang, Siyuan - Hu, Yun Hang. **Temperature, pressure, and adsorption-dependent redox potentials: I. Processes of CO2> reduction to value-added compounds** [elektronický dokument]. DOI 10.1002/ese3.1287 In: **Energy Science and Engineering**. Hoboken: John Wiley & Sons, 2022, Roč. 10, č. 12, s. 4520-4543. ISSN (online) 2050-0505. - SCO, s. 4520 - 4543

2022 [01/20] / **USA** - Bocus, Massimo - Van Speybroeck, Veronique. **Insights into the Mechanism and Reactivity of Zeolite-Catalyzed Alkylphenol Dealkylation** [elektronický dokument]. DOI 10.1021/acscatal.2c03844 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 22, s. 14227-14242 [online]. ISSN (online) 2155-5435. - SCO, s. 14227 - 14242

2022 [01/20] / **USA** - Li, Shih Cheng - Lin, Yen Chun - Li, Yi Pei. **Comparative Analysis of Uncoupled Mode Approximations for Molecular Thermochemistry and Kinetics** [elektronický dokument]. DOI 10.1021/acs.jctc.2c00664 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 11, s. 6866-6877 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 6866 - 6877

2022 [01/20] / **USA** - Rybicki, Marcin - Sauer, Joachim. **Rigid Body Approximation for the Anharmonic Description of Molecule-Surface Vibrations** [elektronický dokument]. DOI 10.1021/acs.jctc.2c00597 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2022, Roč. 18, č. 9, s. 5618-5635 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO, s. 5618 - 5635

2022 [01/20] / **USA** - Bhan, Aditya - Delgass, W. Nicholas. **Best practices in catalysis: A perspective** [elektronický dokument]. DOI 10.1016/j.jcat.2021.12.014 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2022, č. 405, s. 419-429 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO, s. 419 - 429

2021 [01/20] / **USA** - Mortén, Magnus - Cordero-Lanzac, Tomás - Cnudde, Pieter - Redekop, Evgeniy A. - Svelle, Stian - van Speybroeck, Veronique - Olsbye, Unni. **Acidity effect on benzene methylation kinetics over substituted H-MeAlPO-5 catalysts** [elektronický dokument]. DOI 10.1016/j.jcat.2021.11.002 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2021, Roč. 404, s. 594-606 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. 594 - 606

2021 [01/20] / **USA** - Borodin, Dmitriy - Rahinov, Igor - Galparsoro, Oihana - Fingerhut, Jan - Schwarzer, Michael - Golibrzuch, Kai - Skoulatakis, Georgios - Auerbach, Daniel J. - Kandratsenka, Alexander - Schwarzer, Dirk - Kitsopoulos, Theofanis N. - Wodtke, Alec M. **Kinetics of NH<inf>3</inf>Desorption and Diffusion on Pt: Implications for the Ostwald Process** [elektronický dokument]. DOI 10.1021/jacs.1c09269 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2021, Roč. 143, č. 43, s. 18305-18316 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO, s. 18305 - 18316

2021 [01/20] / **USA** - Waitt, Craig - Miles, Audrey R. - Schneider, William F. **Adsorbate Free Energies from DFT-Derived Translational Energy Landscapes** [elektronický dokument]. DOI 10.1021/acs.jpcc.1c05917 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and

Hard Matter. Washington: American Chemical Society, 2021, Roč. 125, č. 37, s. 20331-20342 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 20331 - 20342

2021 [01/20] / **USA** - Galimberti, Daria Ruth - Sauer, Joachim. **Chemically Accurate Vibrational Free Energies of Adsorption from Density Functional Theory Molecular Dynamics: Alkanes in Zeolites** [elektronický dokument]. DOI 10.1021/acs.jctc.1c00519 In: **Journal of Chemical Theory and Computation**. Washington: American Chemical Society, 2021, Roč. 17, č. 9, s. 5849-5862 [tlačená forma] [online]. ISSN 1549-9618. ISSN (online) 1549-9626. - SCO ; CCC ; WOS CC, s. 5849 - 5862

2021 [01/20] / **USA** - Lee, Elizabeth M.Y. - Ludwig, Thomas - Yu, Boyuan - Singh, Aayush R. - Gygi, François - Nørskov, Jens K. - De Pablo, Juan J. **Neural Network Sampling of the Free Energy Landscape for Nitrogen Dissociation on Ruthenium** [elektronický dokument]. DOI 10.1021/acs.jpclett.1c00195 In: **The Journal of Physical Chemistry Letters**. Washington: American Chemical Society, 2021, Roč. 12, č. 11, s. 2954-2962 [online]. ISSN (online) 1948-7185. - SCO ; CCC ; WOS CC, s. 2954 - 2962

2021 [01/20] / **GBR** - Dahri, Mohammad - Abolmaali, Samira Sadat - Abedanzadeh, Mozhgan - Salmanpour, Mohsen - Maleki, Reza. **Composition and surface chemistry engineering of graphene grafting chitosan for stimuli-responsive cancer therapy: An in-silico study** [elektronický dokument]. DOI 10.1016/j.imu.2021.100627 In: **Informatics in medicine unlocked**. Londýn: Elsevier, 2021, Roč. 24, [online]. ISSN (online) 2352-9148. - SCO, s.

ADC_069: / Boje, Astrid (Autor) (16.67%) - Taifan, William E. (Autor) (16.666%) - Ström, Henrik (Autor) (16.666%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (16.666%) - Baltrušaitis, Jonas (Autor) (16.666%) - Hellman, Anders (Autor) (16.666%): **First-principles-informed energy span and microkinetic analysis of ethanol catalytic conversion to 1,3-butadiene on MgO**. – text, graf., tab. – [recenzované]. – DOI 10.1039/d1cy00419k. – SCO ; CCC ; WOS CC.
In: *Catalysis Science and Technology* [textový dokument (print)] [elektronický dokument] . – Cambridge (Veľká Británia) : The Royal Society of Chemistry. – ISSN 2044-4753. – ISSN (online) 2044-4761. – Roč. 11, č. 20 (2021), s. 6682-6694 [tlačená forma] [online]
Počet všetkých autorov: 6
[článok]
Lit.: 65
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 6.177 - 2021
SNIP: 1,043 - 2021
SJR: 1,299 - 2021
CiteScore: 9,2 - 2021
AIS: 1.055 - 2021
Kvartil Q:
2021, AIS - Chemistry, physical - Q2; **2021, JIF** - Chemistry, physical - Q2; **2021, Scimago** - Catalysis - Q1

Ohlasy (8):
2024 [01/20] / **USA** - Plucksacholatarn, Aunyamanee - Tharat, Bunrat - Faungnawakij, Kajornsak - Suthirakun, Suwit - Thongkham, Somprasong - Praserthdam, Piyasan - Junkaew, Anchalee. **Unraveling selectivity in non-noble metal-catalyzed hydrogenation of 5-hydroxymethylfurfural (HMF) through mechanistic insights** [elektronický dokument]. DOI 10.1016/j.jcat.2024.115531 In: **Journal of Catalysis**. San Diego: Elsevier. Academic Press, 2024, Roč. 434, art. no. 115531 [tlačená forma] [online]. ISSN 0021-9517. ISSN (online) 1090-2694. - SCO ; CCC ; WOS CC, s. art. no. 115531

2024 [01/20] / **NLD** - Chung, Sang–Ho –H - de Miguel, Juan Carlos Navarro - Li, Teng - Lavrik, Polina - Komaty, Sarah -

Yuan, Youyou - Poloneeva, Daria - Anbari, Wejdan H. - Hedhili, Mohamed Nejib - Zaarour, Moussa - Martín, Cristina - Shoinkhorova, Tuiana - Abou–Hamad, Edy - Gascon, Jorge - Ruiz–Martínez, Javier. **Core–shell structured magnesia–silica as a next generation catalyst for one-step ethanol-to-butadiene Lebedev process**. DOI 10.1016/j.apcatb.2023.123628 In: **Applied Catalysis B: Environmental**. Amsterdam: Elsevier, 2024, Roč. 344, art. no. 123628 [tlačená forma]. ISSN 0926-3373. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **NLD** - Cui, Tianxiao - Chen, Qicheng - Zhang, Yingjin - Nie, Binjian - Yang, Boting. **The promotion mechanisms of Mo for the dry reforming of methane reaction over a Mo-doped Ni(2 1 1) bimetallic catalyst** [elektronický dokument]. DOI 10.1016/j.comptc.2024.114827 In: **Computational and Theoretical Chemistry**. Amsterdam: Elsevier, 2024, Roč. 1240, art. no. 114827 [tlačená forma] [online]. ISSN 2210-271X. ISSN (online) 1872-7999. - SCO ; WOS CC, s. art. no. 114827

2024 [01/20] / **USA** - Zhang, Yin Sheng - Gou, Jin Tao - Liu, Ting Hao - Zhang, Ming Hui - Hu, Chang Wei - Yang, Hua Qing. **Theoretical Mechanism Exploration of Highly Selective Reductive Amination of Furfural to Furfurylamine over a Single-Atom Ru1-N3/C Catalyst** [elektronický dokument]. DOI 10.1021/acs.jpcc.4c04113 In: **The Journal of Physical Chemistry C**: Energy Conversion and Storage, Optical and Electronic Devices, Interfaces, Nanomaterials, and Hard Matter. Washington: American Chemical Society, 2024, Roč. 128, č. 37, s. 15431-15442 [tlačená forma] [online]. ISSN 1932-7447. ISSN (online) 1932-7455. - SCO ; CCC ; WOS CC, s. 15431 - 15442

2023 [01/20] / **CHE** - Bojang, Adama A. - Wu, Ho Shing. **1,3-Butadiene Production Using Ash-Based Catalyst**. DOI 10.3390/catal13020258 In: **Catalysts**. Bazilej: Multidisciplinary Digital Publishing Institute, 2023, Roč. 13, č. 2, art. no. 258 [online]. ISSN 2073-4344. - SCO ; CCC ; WOS CC, s. art. no. 258

2023 [01/20] / **BGR** - Oyegoke, T. - Peter, E. E. - Igwebuike, C. M. - El-Yakubu Jibril, B. **Current opinion on the significance of promoting molecular modeling and simulation applications in Nigeria's future experimental catalysis and reaction engineering studies** [elektronický dokument]. DOI 10.34049/bcc.55.1.5521 In: **Izvestija po chimija**. Sofia: Balgarska akademiya na naukite. Institute of Chemical Engineering, 2023, Roč. 55, č. 1, s. 32-39 [tlačená forma] [online]. ISSN 0861-9808. ISSN (online) 0324-1130. - SCO, s. 32 - 39

2022 [01/20] / **DEU** - Tai, Wei - Fu, Shuai - Liu, Ting Hao - Yang, Hua Qing - Hu, Chang Wei. **Mechanism of Preferential Hydrogenation of Hydroxymethyl Group to Aldehyde Group in 5-Hydroxymethylfurfural over W2C-Based Catalyst** [elektronický dokument]. DOI 10.1002/cssc.202200174 In: **ChemSusChem**. Weinheim: John Wiley & Sons. Wiley-VCH, 2022, Roč. 15, č. 13, art. no. e202200174 [tlačená forma] [online]. ISSN 1864-5631. ISSN (online) 1864-564X. - SCO, s.

2022 [01/20] / **DEU** - Kayanuma, Megumi - Shinke, Yu - Miyazawa, Tomohisa - Fujitani, Tadahiro - Choe, Yoong Kee. **Theoretical study of the side reactions of ethanol-to-butadiene conversion on MgO catalyst: formation of diethyl ether, ethyl acetal, 1,3-butanediol, methyl ethyl ketone, n-butanol, butanal, and acetone** [elektronický dokument]. DOI 10.1007/s00214-022-02927-0 In: **Theoretical Chemistry Accounts**: Theory, Computation, and Modeling. Berlín: Springer Nature. Springer International Publishing AG, 2022, Roč. 141, č. 11, art. no. 63 [tlačená forma] [online]. ISSN 1432-881X. ISSN (online) 1432-2234. - SCO, s. art. no. 63

ADC_070: / Casier, Bastien (Autor) (14.29%) - da Silva, Mauricio Chagas (Autor) (14.285%) - Badawi, Michael (Autor) (14.285%) - Pascale, Fabien (Autor) (14.285%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (14.285%) - Lebegue, Sebastien (Autor) (14.285%) - Rocca, Dario (Autor) (14.285%): **Hybrid localized graph kernel for machine learning energy-related properties of molecules and solids**. – text, ilustr., graf., tab. – [recenzované]. – DOI 10.1002/jcc.26550. – SCO ; CCC ; WOS CC ; SCIE.
In: *Journal of computational chemistry* [textový dokument (print)] [elektronický dokument] . – Hoboken (USA) : John Wiley & Sons. – ISSN 0192-8651. – ISSN (online) 1096-987X. – Roč. 42, č. 20 (2021), s. 1390-1401 [tlačená forma] [online]

Počet všetkých autorov: 7
[článok]
Lit.: 72
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 3.672 - 2021
SNIP: 0,977 - 2021
SJR: 0,778 - 2021
CiteScore: 6 - 2021
AIS: 0.866 - 2021
Kvartil Q:
2021, AIS - Chemistry, multidisciplinary - Q2; **2021, JIF** - Chemistry, multidisciplinary - Q2; **2021, Scimago** - Chemistry (miscellaneous) - Q1; **2021, Scimago** - Computational mathematics - Q2

Ohlasy (2):
2024 [01/20] / **GBR** - Liu, Yutong - Dong, Yawen - Wu, Hua. **Comprehensive overview of machine learning applications in MOFs: from modeling processes to latest applications and design classifications** [elektronický dokument]. DOI 10.1039/d4ta06740a In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2024, Roč. 13, č. 4, s. 2403-2440 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; WOS CC, s. 2403 - 2440

2022 [01/20] / **NLD** - Pinheiro, Max - Dral, Pavlo O. **Kernel methods** [elektronický dokument]. DOI 10.1016/B978-0-323-90049-2.00009-3 In: **Quantum Chemistry in the Age of Machine Learning**. Amsterdam: Elsevier, 2022, s. 205-232 [tlačená forma] [online]. ISBN 978-0-323-90049-2. ISBN (online) 978-0-323-88604-8. - SCO, s. 205 - 232

ADC_071: / Gešvandtnerová, Monika (Autor) [Interný doktorand] [UKOPRCFZ] (50%) - Rocca, Dario (Autor) (10%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (40%): **Methanol carbonylation over acid mordenite: Insights from ab initio molecular dynamics and machine learning thermodynamic perturbation theory**. – text, graf., tab. – [recenzované]. – DOI 10.1016/j.jcat.2021.02.011. – CCC ; SCO ; WOS CC.
In: *Journal of Catalysis* [textový dokument (print)] [elektronický dokument] . – San Diego (USA) : Elsevier. Academic Press. – ISSN 0021-9517. – ISSN (online) 1090-2694. – č. 396 (2021), s. 166-178 [tlačená forma] [online]
Počet všetkých autorov: 3
[článok]
Lit.: 111
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 8.047 - 2021
SNIP: 1,442 - 2021
SJR: 1,936 - 2021
CiteScore: 13 - 2021
AIS: 1.510 - 2021
Kvartil Q:
2021, AIS - Chemistry, physical - Q1; **2021, AIS** - Engineering, chemical - Q1; **2021, JIF** - Chemistry, physical - Q1; **2021, JIF** - Engineering, chemical - Q1; **2021, Scimago** - Catalysis - Q1; **2021, Scimago** - Physical and theoretical chemistry - Q1

Ohlasy (10):
2025 [01/20] / **NLD** - Rosli, Nur Ayshah - Yusoff Azudin, Nurhazwani - Ishak, Noor Fauziyah. **Methanol to Acetic Acid and Vinyl Acetates: Plant, Process, Operation, and Equipment**. DOI 10.1016/B978-0-443-15740-0.00147-6 In:

Comprehensive Methanol Science Production Applications and Emerging Technologies. Amsterdam: Elsevier. Elsevier Science, 2025, s. 644-665 [tlačená forma] [online]. ISBN [9780443157400, 9780443157417]. - SCO, s. 644 - 665

2025 [01/20] / **GBR** - Vacek, Jaroslav - Vrška, Dávid - Manna, Debashree - Lo, Rabindranath - Hobza, Pavel. **Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches** [elektronický dokument]. DOI 10.1039/D5SC06336A In: **Chemical Science**. Cambridge: The Royal Society of Chemistry, 2025, Roč. 16, č. 48, s. 23129-23138 [tlačená forma] [online]. ISSN 2041-6520. ISSN (online) 2041-6539. - SCO ; WOS CC ; CCC ; SCIE ; Nature Index ; OA, s. 23129 - 23138

2024 [01/20] / **USA** - Chen, Wei - Liu, Zhiqiang - Yi, Xianfeng - Zheng, Anmin. **Confinement-Driven Dimethyl Ether Carbonylation in Mordenite Zeolite as an Ultramicroscopic Reactor** [elektronický dokument]. DOI 10.1021/acs.accounts.4c00389 In: **Accounts of Chemical Research**. Washington: American Chemical Society, 2024, Roč. 57, č. 19, s. 2804-2815 [tlačená forma] [online]. ISSN 0001-4842. ISSN (online) 1520-4898. - SCO ; CCC ; WOS CC, s. 2804 - 2815

2023 [01/20] / **USA** - Chizallet, Céline - Bouchy, Christophe - Larmier, Kim - Pirngruber, Gerhard. **Molecular Views on Mechanisms of Brønsted Acid-Catalyzed Reactions in Zeolites** [elektronický dokument]. DOI 10.1021/acs.chemrev.2c00896 In: **Chemical Reviews**. Washington: American Chemical Society, 2023, Roč. 123, č. 9, s. 6107-6196 [tlačená forma] [online]. ISSN 0009-2665. ISSN (online) 1520-6890. - SCO ; CCC ; WOS CC, s. 6107 - 6196

2023 [01/20] / **USA** - Van Speybroeck, Veronique - Bocus, Massimo - Cnudde, Pieter - Vanduyfhuys, Louis. **Operando Modeling of Zeolite-Catalyzed Reactions Using First-Principles Molecular Dynamics Simulations** [elektronický dokument]. DOI 10.1021/acscatal.3c01945 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 17, s. 11455-11493 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 11455 - 11493

2022 [01/20] / **USA** - Ma, Sicong - Liu, Zhi Pan. **The Role of Zeolite Framework in Zeolite Stability and Catalysis from Recent Atomic Simulation** [elektronický dokument]. DOI 10.1007/s11244-021-01473-6 In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, s. 59-68 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 59 - 68

2022 [01/20] / **USA** - Chizallet, Céline. **Achievements and Expectations in the Field of Computational Heterogeneous Catalysis in an Innovation Context** [elektronický dokument]. DOI 10.1007/s11244-021-01489-y In: **Topics in Catalysis**. New York: Springer Nature. Springer International Publishing AG, 2022, Roč. 65, s. 69-81 [tlačená forma]. ISSN 1022-5528. ISSN (online) 1572-9028. - SCO, s. 69 - 81

2022 [01/20] / **GBR** - Chen, Wei - Tarach, Karolina A. - Yi, Xianfeng - Liu, Zhiqiang - Tang, Xiaomin - Góra-Marek, Kinga - Zheng, Anmin. **Charge-separation driven mechanism via acylium ion intermediate migration during catalytic carbonylation in mordenite zeolite** [elektronický dokument]. DOI 10.1038/s41467-022-34708-5 In: **Nature communications**. Londýn: Springer Nature. Nature Publishing Group, 2022, Roč. 13, č. 1, art. no. 7106 [online]. ISSN (online) 2041-1723. - SCO, s. art. no. 7106

2021 [01/20] / **USA** - Wang, Haifeng - Hu, P. - Lai, Zhuangzhuang - Sun, Ningling - Jin, Jiamin - Chen, Jianfu. **Resolving the intricate mechanism and selectivity of syngas conversion on reduced ZnCr2Ox: A quantitative study from DFT and microkinetic simulations** [elektronický dokument]. DOI 10.1021/acscatal.1c03579 In: **ACS Catalysis**. Washington: American Chemical Society, 2021, Roč. 11, č. 21, s. 12977-12988 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 12977 - 12988

2021 [01/20] / **USA** - Chen, Wei - Li, Guangchao - Yi, Xianfeng - Day, Sarah J. - Tarach, Karolina A. - Liu, Zhiqiang - Liu, Shang Bin - Edman Tsang, Shik Chi - Góra-Marek, Kinga - Zheng, Anmin. **Molecular Understanding of the Catalytic Consequence of Ketene Intermediates under Confinement** [elektronický dokument]. DOI 10.1021/jacs.1c08036 In: **Journal of the American Chemical Society**. Washington: American Chemical Society, 2021, Roč. 143, č. 37, s. 15440-

15452 [tlačená forma] [CD-ROM] [online]. ISSN 0002-7863. ISSN 1943-2984. ISSN (online) 1520-5126. - SCO ; CCC ; WOS CC, s. 15440 - 15452

ADC_072: / Qin, Zhengxing (Autor) (6.676%) - Zeng, Shu (Autor) (6.666%) - Melinte, Georgian (Autor) (6.666%) - Bučko, Tomáš (Autor) [UKOPRCFZ] (6.666%) - Badawi, Michael (Autor) (6.666%) - Shen, Yanfeng (Autor) (6.666%) - Gilson, Jean-Pierre (Autor) (6.666%) - Ersen, Ovidiu (Autor) (6.666%) - Wei, Yingxu (Autor) (6.666%) - Liu, Zhongmin (Autor) (6.666%) - Liu, Xinmei (Autor) (6.666%) - Yan, Zifeng (Autor) (6.666%) - Xu, Shutao (Autor) (6.666%) - Valtchev, Valentin (Autor) (6.666%) - Mintova, Svetlana (Autor) (6.666%): **Understanding the Fundamentals of Microporosity Upgrading in Zeolites: Increasing Diffusion and Catalytic Performances**. – text, ilustr., graf. – [recenzované]. – DOI 10.1002/advs.202100001. – SCO ; CCC ; WOS CC.
In: *Advanced Science* [elektronický dokument] . – Hoboken (USA) : John Wiley & Sons. Wiley Blackwell. – ISSN (online) 2198-3844. – Roč. 8, č. 17 (2021), art. no. 2100001, s. [1-9] [online]
Počet všetkých autorov: 15
[článok]
Lit.: 43
[OV 120 Chémia, chemická technológia a biotechnológie]
Indikátor časopisu:
IF: 17.521 - 2021
SNIP: 2,238 - 2021
SJR: 3,984 - 2021
CiteScore: 20,8 - 2021
AIS: 3.539 - 2021
Kvartil Q:
2021, AIS - Chemistry, multidisciplinary - Q1; **2021, AIS** - Materials science, multidisciplinary - Q1; **2021, AIS** - Nanoscience & nanotechnology - Q1; **2021, JIF** - Chemistry, multidisciplinary - Q1; **2021, JIF** - Materials science, multidisciplinary - Q1; **2021, JIF** - Nanoscience & nanotechnology - Q1; **2021, Scimago** - Biochemistry, genetics and molecular biology (miscellaneous) - Q1; **2021, Scimago** - Chemical engineering (miscellaneous) - Q1; **2021, Scimago** - Engineering (miscellaneous) - Q1; **2021, Scimago** - Materials science (miscellaneous) - Q1; **2021, Scimago** - Medicine (miscellaneous) - Q1; **2021, Scimago** - Physics and astronomy (miscellaneous) - Q1

Ohlasy (32):

2025 [01/20] / **DEU** - Lu, Fangjun - Zong, Kai - Wang, Jiayi - Zhang, Xiaoyu - Chen, Zhen - luo, Dan - Yan, Zhangyong - Yan, Jinliang - Xiong, Haoyang - Zhang, Ruizhen - Wang, Xin - Chen, Zhongwei. **Efficient Zeolite Electrocatalysts for Lithium-Sulfur Batteries: Synergistic Catalysis of Co Single Atom and CoO Nanoparticles Regulated by Pore Structure** [elektronický dokument]. DOI 10.1002/smll.202507900 In: **Small**. Weinheim: John Wiley & Sons, 2025, Roč. 21, č. 50, art. no. e07900 [tlačená forma] [online]. ISSN 1613-6810. ISSN (online) 1613-6829. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. e07900

2025 [01/20] / **DEU** - Stefani, Maria - Lunardi, Valentino Bervia - Go, Alchris Woo - Cheng, Kuan Chen - Hsu, Hsien Yi - Lin, Shin Ping - Angkawijaya, Artik Elisa - Lin, Hui Wen - Simanullang, Wiyanti Fransisca - Hsieh, Chang Wei - Santoso, Shella Permatasari - Ismadji, Suryadi. **Transforming spent coffee grounds into sulfonated char: an eco-innovative method using a refined simultaneous sulfonation-carbonization process** [elektronický dokument]. DOI 10.1007/s13399-025-06881-2 In: **Biomass conversion and biorefinery**. Berlin : Springer Nature, 2025, Roč. 15, č. 24, s. 30775-30794 [tlačená forma] [online]. ISSN 2190-6815. ISSN (online) 2190-6823. - SCO ; CCC ; WOS CC ; SCIE, s. 30775 - 30794

2025 [01/20] / **USA** - Liu, Yi - Niu, Zhao wei - Wang, Miaomiao - Luo, Xin - Li, Wei - Wang, Bohong - Wang, Peng - He, Lu - Zhang, Ji - Chen, Shangxing - Wang, Zongde - Li, Xiang. **Synergistic Effect of Hierarchical ZSM-5 Zeolites Promotes Synthesis of Bioderived 4-Hydroxy-2-Cyclopentenones and p-Xylene** [elektronický dokument]. DOI 10.1002/cctc.202500942 In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2025, Roč. 17, č. 22, art. no. e00942 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. e00942

2025 [01/20] / **USA** - Yuan, Jiamin - Fan, Yuzhou - Tang, Xiaomin - Wang, Jiujiang - Liu, Honghai - Zhao, Hongjuan - Liu, Zhiqiang - Zheng, Anmin. **Impact of Coke Distribution on the Diffusion of Alkanes in the MFI Zeolite** [elektronický dokument]. DOI 10.1021/acs.iecr.5c02173 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2025, Roč. 64, č. 45, s. 21850-21860 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO ; CCC ; WOS CC ; SCIE, s. 21850 - 21860

2025 [01/20] / **USA** - Nuno Almeida, José - Song, Lu - Askarli, Sohrab - Chung, Sang Ho - Ruiz-Martínez, Javier. **Zeolite–Water Chemistry: Characterization Methods to Unveil Zeolite Structure**. DOI 10.1002/cmtd.202400076 In: **Chemistry-methods**. Hoboken: John Wiley & Sons, 2025, Roč. 5, č. 4, art. no. e202400076 [online]. ISSN 2628-9725. - SCO ; WOS CC ; ESCI ; OA, s.

2025 [01/20] / **CHE** - Segneanu, Adina Elena - Herea, Dumitru Daniel - Buema, Gabriela - Bradu, Ionela Amalia - Cepan, Melinda - Grozescu, Ioan. **Advanced Aerogels for Water Remediation: Unraveling Their Potential in Fats, Oils, and Grease Sorption—A Comprehensive Review** [elektronický dokument]. DOI 10.3390/gels11040268 In: **Gels**. Bazilej: Multidisciplinary Digital Publishing Institute, 2025, Roč. 11, č. 4, art. no. 268 [online]. ISSN (online) 2310-2861. - SCO ; CCC ; WOS CC ; SCIE ; OA, s. art. no. 268

2025 [01/20] / **NLD** - Gao, Xu - Feng, Aihu - Mi, Le - Yu, Yang - Yu, Yun. **Fabrication and adsorption properties of hierarchical NaY zeolite with mesopores in the range of 2–5 nm** [elektronický dokument]. DOI 10.1016/j.cplett.2024.141732 In: **Chemical Physics Letters**: a Frontier Research in Molecular Sciences, Materials and Biological Systems. Amsterdam: Elsevier, 2025, Roč. 858, art. no. 141732 [tlačená forma] [online]. ISSN 0009-2614. ISSN (online) 1873-4448. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 141732

2025 [01/20] / **NLD** - Li, Xuhan - Sun, Fei - Qu, Zhibin - Wang, Jingjie - Xu, Yanhui - Gao, Jihui - Zhao, Guangbo. **A review of porous catalysts for low-temperature selective catalytic reduction of NOx with NH3: Insights into the role of mass transfer within nanopores** [elektronický dokument]. DOI 10.1016/j.seppur.2024.130678 In: **Separation and Purification Technology**. Amsterdam: Elsevier. Elsevier Science, 2025, Roč. 359, art. no. 130678 [tlačená forma] [online]. ISSN 1383-5866. ISSN (online) 1873-3794. - SCO ; CCC ; WOS CC ; SCIE, s. art. no. 130678

2025 [01/20] / **USA** - Hullfish, Cole W. - Tan, Jun Zhi - Adawi, Hayat I. - Sarazen, Michele L. **Toward Intrinsic Catalytic Rates and Selectivities of Zeolites in the Presence of Limiting Diffusion and Deactivation**. DOI 10.1021/acscatal.3c03559 In: **Aiche Annual Meeting Conference Proceedings**. New York: AIChE, 2025, s. 13140-13150 [tlačená forma]. ISBN [9798331332143]. - SCO ; CCC ; WOS CC ; SCIE, s. 13140 - 13150

2025 [01/20] / **NLD** - Dai, Leilei - Lata, Suman - Chen, Junhui - Cobb, Kirk - Lei, Hanwu - Chen, Paul - Ruan, Roger. **Pyrolysis of municipal solid waste for bio-oil production**. DOI 10.1016/B978-0-443-29291-0.00003-X In: **Thermochemical Conversion of Biomass Feedstock and Solid Waste into Biofuels Production and Pollutant Control**. Amsterdam: Elsevier. Elsevier Science, 2025, s. 43-61 [tlačená forma] [online]. ISBN [9780443292927, 9780443292910]. - SCO, s. 43 - 61

2024 [01/20] / **USA** - Li, Qian - Ding, Yan - Cong, Erli - Xu, Shijia - Li, Lanxin - Ma, Xinchi - Xiao, Songtao - Gao, Chenyu - Yang, Libin. **Regulation pore size distribution of FAU deposited by Ag-oxide nanoparticles with F anions corrosion for the adsorption of CH3I** [elektronický dokument]. DOI 10.1007/s10853-024-09738-7 In: **Journal of Materials Science**. Norwell: Springer Nature. Springer International Publishing AG, 2024, Roč. 59, č. 21, s. 9276-9290 [tlačená forma] [online]. ISSN 0022-2461. ISSN (online) 1573-4803. - SCO ; CCC ; WOS CC, s. 9276 - 9290

2024 [01/20] / **USA** - Xiao, Yuehua - Wang, Chengtao - Xiao, Jiale - Li, Hangjie - Cui, Zhengxing - Wang, Yeqing - Wang, Liang - Xiao, Feng Shou. **Isoamylene Dimerization over Mesoporous Y Zeolites** [elektronický dokument]. DOI 10.1021/acs.iecr.4c03390 In: **Industrial & Engineering Chemistry Research**. Washington: American Chemical Society, 2024, Roč. 63, č. 51, s. 22320-22327 [tlačená forma] [online]. ISSN 0888-5885. ISSN (online) 1520-5045. - SCO ; CCC ; WOS CC, s. 22320 - 22327

2024 [01/20] / **USA** - Schwarz, Fabian - Barthel, Senja - Mace, Amber. **Understanding Mobile Particles in Solid-State Materials: From the Perspective of Potential Energy Surfaces** [elektronický dokument]. DOI 10.1021/acs.chemmater.4c01822 In: **Chemistry of Materials**: a Publication of the American Chemical Society. Washington: American Chemical Society, 2024, Roč. 36, č. 23, s. 11359-11376 [tlačená forma] [online]. ISSN 0897-4756. ISSN (online) 1520-5002. - SCO ; CCC ; WOS CC, s. 11359 - 11376

2024 [01/20] / **NLD** - Qi, Ying - Yang, Huaming - Li, Chunli - Li, Hao. **Trace ethylene adsorbents Ag/F-Z5(X) for improved preservation of fruits and vegetables: Enhanced adsorption and water resistance** [elektronický dokument]. DOI 10.1016/j.seppur.2024.127634 In: **Separation and Purification Technology**. Amsterdam: Elsevier. Elsevier Science, 2024, Roč. 347, art. no. 127634 [tlačená forma] [online]. ISSN 1383-5866. ISSN (online) 1873-3794. - SCO ; CCC ; WOS CC, s. art. no. 127634

2024 [01/20] / **USA** - Dong, Qi - Li, Ruifeng - Jiao, Haijun. **Zeolite Catalysts for Selective Hydrocracking of Polycyclic Aromatic Hydrocarbons – Structures and Mechanisms** [elektronický dokument]. DOI 10.1002/cctc.202400117 In: **ChemCatChem**: Heterogeneous & Homogeneous & Bio- & Nano- Catalysis: Chemical Catalysis Catalytical Chemistry. Hoboken: John Wiley & Sons, 2024, Roč. 16, č. 21, art. no. e202400117 [tlačená forma] [online]. ISSN 1867-3880. ISSN (online) 1867-3899. - SCO ; CCC ; WOS CC, s.

2024 [01/20] / **GBR** - Palčić, Ana - Bosnar, Damir - Hršak, Patricija - Bronić, Josip - Bosnar, Sanja. **Comparative analysis of parent and modified ZSM-5 zeolites: Insights from positron annihilation lifetime spectroscopy**. DOI 10.1016/j.radphyschem.2024.111919 In: **Radiation Physics and Chemistry**: The Journal for Radiation Physics, Radiation Chemistry and Radiation Processing. Oxford: Elsevier. Pergamon Press, 2024, Roč. 223, art. no. 111919 [tlačená forma]. ISSN 0969-806X. ISSN 1879-0895. - SCO ; CCC ; WOS CC, s. art. no. 111919

2024 [01/20] / **NLD** - Guo, Xiaonan - Zhang, Runduo - Di, Zhaoying - Kang, Bin - Wei, Ying - Jia, Jingbo. **Rational design on hierarchically porous Cu/ZSM-5 zeolite for promoting low-temperature NH3-SCR performance based on protectively alkali-etching strategy** [elektronický dokument]. DOI 10.1016/j.cattod.2024.114656 In: **Catalysis Today**.

Amsterdam: Elsevier. Elsevier Science, 2024, Roč. 433, art. no. 114656 [tlačená forma]. ISSN 0920-5861. ISSN (online) 1873-4308. - SCO, s. art. no. 114656

2024 [01/20] / **USA** - Zhou, Xinru - Han, Xinlei - Qu, Zhengyan - Zhang, Jiuxuan - Zeng, Feng - Tang, Zhenchen - Chen, Rizhi. **Hierarchical FAU Zeolites Boosting the Hydrocracking of Polyolefin Waste into Liquid Fuels** [elektronický dokument]. DOI 10.1021/acssuschemeng.4c01097 In: **ACS Sustainable Chemistry & Engineering**. Washington: American Chemical Society, 2024, Roč. 12, č. 15, s. 6013-6022 [online]. ISSN (online) 2168-0485. - SCO ; CCC ; WOS CC, s. 6013 - 6022

2024 [01/20] / **NLD** - Aumond, Thibaud - Compère, Steven - Sachse, Alexander. **Impact of thermal ethylene degradation in zeolite-templated carbon synthesis** [elektronický dokument]. DOI 10.1016/j.micromeso.2023.112967 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2024, Roč. 367, art. no. 112967 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO ; CCC ; WOS CC, s. art. no. 112967

2024 [01/20] / **USA** - Jarrin, Thomas - de Bruin, Theodorus - Chizallet, Céline. **Impact of Point Defects, External Surfaces Sites, and Si/Al Ratio on Al-O Bonds Hydrolysis Kinetics at the Initiation of Faujasite Dealumination** [elektronický dokument]. DOI 10.1021/acscatal.3c05517 In: **ACS Catalysis**. Washington: American Chemical Society, 2024, Roč. 14, č. 3, s. 1639-1652 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 1639 - 1652

2023 [01/20] / **GBR** - Zhang, Dexin - Li, Kang - Chen, Junli - Sun, Changyu - Li, Zhi - Lei, Jie - Ma, Qinlan - Zhang, Pan - Liu, Yong - Yang, Lin. **Improved catalytic performance in gas-phase dimethyl ether carbonylation over facile NH4F etched ferrierite** [elektronický dokument]. DOI 10.1039/d3ra07084k In: **RSC advances**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 50, s. 35379-35390 [online]. ISSN (online) 2046-2069. - SCO ; CCC ; WOS CC, s. 35379 - 35390

2023 [01/20] / **USA** - Hullfish, Cole W. - Tan, Jun Zhi - Adawi, Hayat I. - Sarazen, Michele L. **Toward Intrinsic Catalytic Rates and Selectivities of Zeolites in the Presence of Limiting Diffusion and Deactivation** [elektronický dokument]. DOI 10.1021/acscatal.3c03559 In: **ACS Catalysis**. Washington: American Chemical Society, 2023, Roč. 13, č. 19, s. 13140-13150 [online]. ISSN (online) 2155-5435. - SCO ; CCC ; WOS CC, s. 13140 - 13150

2023 [01/20] / **USA** - Li, Tingting - Ho, Chengen - Han, Mengxi - Peng, Pai - Chen, Junjie - Huang, Yong - Li, Bin - Chen, Qiang. **Zeolite Encapsulation of Indole as an Antibacterial with Controllable Release Property** [elektronický dokument]. DOI 10.1021/acs.langmuir.3c01063 In: **Langmuir**: the ACS Journal of Surfaces and Colloids. Washington: American Chemical Society, 2023, Roč. 39, č. 29, s. 10122-10132 [tlačená forma] [online]. ISSN 0743-7463. ISSN (online) 1520-5827. - SCO ; CCC ; WOS CC, s. 10122 - 10132

2023 [01/20] / **CHE** - Yu, Qiang - Li, Junjie - Liu, Wen - Wang, Yanan - Chu, Weifeng - Zhang, Xinbao - Xu, Longya - Zhu, Xiangxue - Li, Xiujie. **Rational design of a novel Silica-Based material with abundant open micropores for efficient VOC removal** [elektronický dokument]. DOI 10.1016/j.cej.2022.140077 In: **Chemical engineering journal**. Lausanne: Elsevier. Elsevier Science, 2023, č. 454, art. no. 140077 [tlačená forma] [online]. ISSN 1385-8947. ISSN (online) 1873-3212. - SCO ; CCC ; WOS CC, s. art. no. 140077

2023 [01/20] / **NLD** - Liu, Peng - Yu, Chengqu - Li, Weixue - Shen, Baojian. **A facile strategy of preparing nanosized NaY zeolite by stimulating negative crystals to accelerate the formation of D6R units** [elektronický dokument]. DOI 10.1016/j.micromeso.2022.112341 In: **Microporous and Mesoporous Materials**. Amsterdam: Elsevier, 2023, Roč. 347, art. no. 112341 [tlačená forma] [online]. ISSN 1387-1811. ISSN (online) 1873-3093. - SCO ; CCC ; WOS CC, s. art. no. 112341

2023 [01/20] / **GBR** - Hong, Zhe - Li, Lei - Miao, Lei - Zhao, Guoqing - Zhu, Zhirong. **Opening sodalite cages of X zeolite for boosting toluene side-chain alkylation performance** [elektronický dokument]. DOI 10.1039/d2cy01970a In: **Catalysis Science and Technology**. Cambridge: The Royal Society of Chemistry, 2023, Roč. 13, č. 7, s. 1991-1995 [tlačená forma]

[online]. ISSN 2044-4753. ISSN (online) 2044-4761. - SCO ; CCC ; WOS CC, s. 1991 - 1995

2022 [01/20] / **GBR** - Yan, Puxiang - Wang, Haiyong - Liao, Yuhe - Sun, Pengyao - Wang, Chenguang. **Introducing mesopore and regulating Al distribution for improving catalytic performances of ZSM-5 in furfuryl alcohol to levulinic acid** [elektronický dokument]. DOI 10.1016/j.fuel.2022.125213 In: **Fuel**: the science and technology of fuel and energy. Oxford: Elsevier, 2022, Roč. 329, art. no. 125213 [tlačená forma] [online]. ISSN 0016-2361. ISSN (online) 1873-7153. - SCO, s. art. no. 125213

2022 [01/20] / **USA** - Li, Shaojie - Liutkova, Anna - Kosinov, Nikolay - Hensen, Emiel J.M. **Zeolite Nanocrystals (MOR, EU-1, and ZSM-12) Synthesized Using a Versatile Diquaternary Ammonium Template as Robust Catalysts** [elektronický dokument]. DOI 10.1021/acsanm.2c03805 In: **ACS applied nano materials**. Washington: American Chemical Society, 2022, Roč. 5, č. 11, s. 16862-16871 [online]. ISSN (online) 2574-0970. - SCO, s. 16862 - 16871

2022 [01/20] / **GBR** - Ni, Wenjuan - Zhang, Peiyu - Long, Liangkun - Ding, Shaojun. **Engineering and linker-mediated co-immobilization of carotenoid cleavage oxygenase with phenolic acid decarboxylase for efficiently converting ferulic acid into vanillin** [elektronický dokument]. DOI 10.1016/j.procbio.2022.08.020 In: **Process Biochemistry**. Kidlington,Oxford: Elsevier, 2022, č. 122, s. 67-77 [tlačená forma] [online]. ISSN 1359-5113. ISSN (online) 1873-3298. - SCO, s. 67 - 77

2022 [01/20] / **USA** - Dong, Zhongwen - Chen, Wenjun - Xu, Keqing - Liu, Yue - Wu, Jing - Zhang, Fan. **Understanding the Structure-Activity Relationships in Catalytic Conversion of Polyolefin Plastics by Zeolite-Based Catalysts: A Critical Review** [elektronický dokument]. DOI 10.1021/acscatal.2c04915 In: **ACS Catalysis**. Washington: American Chemical Society, 2022, Roč. 12, č. 24, s. 14882-14901 [online]. ISSN (online) 2155-5435. - SCO, s. 14882 - 14901

2021 [01/20] / **GBR** - Awala, Hussein - Kunjir, Shrikant M. - Aurélie Vicente - Gilson, Jean Pierre - Valtchev, Valentin - Seblani, Hussein - Retoux, Richard - Lakiss, Louwanda - Fernandez, Christian - Bedard, Robert - Abdo, Suheil - Bricker, Jeffery - Mintova, Svetlana. **Crystallization pathway from a highly viscous colloidal suspension to ultra-small FAU zeolite nanocrystals** [elektronický dokument]. DOI 10.1039/d1ta02781f In: **Journal of Materials Chemistry A**: Materials for Energy and Sustainability. Cambridge: The Royal Society of Chemistry, 2021, Roč. 9, č. 32, s. 17492-17501 [tlačená forma] [online]. ISSN 2050-7488. ISSN (online) 2050-7496. - SCO ; CCC ; WOS CC, s. 17492 - 17501

2021 [01/20] / **CHE** - Pacana, Andrzej - Siwiec, Dominika. **Universal model to support the quality improvement of industrial products** [elektronický dokument]. DOI 10.3390/ma14247872 In: **Materials**. Bazilej: Multidisciplinary Digital Publishing Institute, 2021, Roč. 14, č. 24, art. no. 7872, s. [1-19] [online]. ISSN (online) 1996-1944. - SCO ; CCC ; WOS CC, s. [1 - 19]

ŠTATISTIKA ZÁZNAMOV: 95

Podľa kategórie EPC od roku 2022
Počet všetkých záznamov: 23
V3 - Vedecký výstup publikačnej činnosti z časopisu: 22
P1 - Pedagogický výstup publikačnej činnosti ako celok: 1

Podľa kategórie EPC do roku 2021
Počet všetkých záznamov: 72
ADC - Vedecké práce v zahraničných karentovaných časopisoch: 72

Podľa typu dokumentu
článok: 94
učebnica pre vysoké školy: 1

Podľa krajiny vydania
Počet domácich vydaní: 1
Počet zahraničných vydaní: 94

Podľa oblasti výskumu
120 Chémia, chemická technológia a biotechnológie: 93

Podľa študijného odboru
1420 chémia: 26

Podľa projektov
Počet publikácií s naviazaným projektom: 61

Podľa databáz a citačných indexov
CCC Current Content Connect: 86
MEDLINE®: 2
Nature Index: 2
OA Open access: 9
SCO SCOPUS: 91
WOS CC Web of Science Core Collection: 93
CPCI-S Conference Proceedings Citation Index - Science: 1
SCIE Science Citation Index Expanded: 30

Podľa metrík
AIS: 30
CiteScore: 64
IF: 48
Nordic List: 19
SJR: 64
SNIP: 63

Podľa kvartilov
Počet záznamov s kvartilom AIS: 31
Z toho Q1: 24
Z toho Q2: 18

Z toho Q3: 1
Počet záznamov s kvartilom JCI: 21
Z toho Q1: 17
Z toho Q2: 8
Z toho Q3: 2
Počet záznamov s kvartilom JIF: 44
Z toho Q1: 29
Z toho Q2: 22
Z toho Q3: 6
Z toho Q4: 1
Počet záznamov s kvartilom Scimago: 40
Z toho Q1: 36
Z toho Q2: 11
Z toho Q3: 1

ŠTATISTIKA OHLASOV: 4154
Počet publikácií s ohlasom: 90

Podľa kategórie ohlasov
Počet ohlasov kategorizovaných podľa vyhlášky č. 456/2012: 2380
Z toho bez autocitácií: **2380**
01 Citácie v zahraničných publikáciách registrované v citačných indexoch WOS CC a SCOPUS: **2378**
Z toho bez autocitácií: **2378**
03 Citácie v zahraničných publikáciách neregistrované v citačných indexoch: **2**
Z toho bez autocitácií: **2**

Počet ohlasov kategorizovaných podľa vyhlášky č. 397/2020: 1774
Z toho bez autocitácií: **1774**
01 Citácia v publikácii registrovaná v citačných indexoch: **1774**
Z toho bez autocitácií: **1774**

Počet indexovaných ohlasov
CCC Current Content Connect: 945
OA Open access: 194
SCO SCOPUS: 1283
WOS CC Web of Science Core Collection: 1040
ESCI Emerging Sources Citation Index: 14
IC Index Chemicus: 1
SCIE Science Citation Index Expanded: 352
Ostatné: Ostatné: 6

Počet ohlasov podľa teritoriality
Počet zahraničných vydaní: 3279
Počet bez krajiny vydania: 875

Vypracovala: Eliška Matejíková
Verifikovala: Mgr. Ingrida Švecová

V Bratislave 27.10.2026