

**UNIVERZITA KOMENSKÉHO  
FAKULTA MATEMATIKY, FYZIKY A INFORMATIKY**

**Zoznam publikačnej činnosti**

**Doc. Ing. Roman Martoňák, DrSc.**

**ABC Kapitoly vo vedeckých monografiách vydané v zahraničných vydavateľstvách**

ABC01 Martoňák, Roman 100 %: Simulation of structural phase transitions in crystals: The metadynamics approach  
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In: Modern Methods of Crystal Structure Prediction. - Weinheim : WILEY-VCH Verlag, 2011. - S. 107-130. -  
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**ADC Vedecké práce v zahraničných karentovaných časopisoch**

ADC01 Martoňák, Roman - Tosatti, Erio : Ultraviolet and soft X-ray photon-photon elastic scattering in an electron  
gas  
Lit. 12 záz. n., 11 obr., 1 tab.  
In: Zeitschrift für Physik B - Condensed Matter. - Vol. 92, No. 4 (1993), s. 417-429

ADC02 Martoňák, Roman - Tosatti, Erio : Path-integral Monte Carlo study of a model two-dimensional quantum  
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Lit. 41 záz. n., 16 obr., 2 tab.  
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Lit. 42 zázň., 8 obr.

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Lit. 21 zázň., 2 obr.

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Lit. 46 zázn.  
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Lit. 31 zázň., 8 obr., 1 tab.

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Lit. 39 zázň.

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Lit. 31 zázň., 4 obr.

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Lit. 7 zázn., 1 obr.

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Lit. 61 zázn., 11 obr.

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Lit. 58 zázn.  
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- [o1] 2011 Zwijnenburg, M. A. - Bromley, S. T.: Structural richness of ionic binary materials: An exploration of the energy landscape of magnesium oxide. In: Physical Review B - Condensed Matter and Materials Physics, Vol. 83, No. 2, 2011, Art.No. 024104 - SCI ; SCOPUS
- [o1] 2012 Akdogan, E. K. - Savkliyildiz, I. - Berke, B. - Zhong, Z. - Wang, L. - Weidner, D. - Croft, M. C. - Tsakalakos, T.: Pressure effects on phase equilibria and solid solubility in MgO-Y<sub>2</sub>O<sub>3</sub> nanocomposites. In: Journal of Applied Physics, Vol. 111, No. 5, 2012, Art. No. 053506 - SCI ; SCOPUS
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- [o1] 2012 Joshi, K. B. - Sharma, B. K. - Paliwal, U. - Barbiellini, B.: Pressure-dependent electronic properties of MgO polymorphs: A first-principles study of Compton profiles and autocorrelation functions. In: Journal of Materials Science, Vol. 47, No. 21, 2012, s. 7549-7557 - SCI ; SCOPUS

- [o1] 2012 McWilliams, R. S. - Spaulding, D. K. - Eggert, J. H. - Celliers, P. M. - Hicks, D. G. - Smith, R. F. - Collins, G. W. - Jeanloz, R.: Phase transformations and metallization of magnesium oxide at high pressure and temperature. In: *Science*, Vol. 338, No. 6112, 2012, s. 1330-1333 - SCI
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- [o1] 2013 Boates, B. - Bonev, S. A.: Demixing instability in dense molten MgSiO<sub>3</sub> and the phase diagram of MgO. In: *Physical Review Letters*, Vol. 110, No. 13, 2013, Art. No. 135504 - SCI ; SCOPUS
- [o1] 2013 Sokolova, T. S. - Dorogokupets, P. I. - Litasov, K. D.: Self-consistent pressure scales based on the equations of state for ruby, diamond, MgO, B<sub>2</sub>-NaCl, as well as Au, Pt, and other metals to 4 Mbar and 3000 K. In: *Russian Geology and Geophysics*, Vol. 54, No. 2, 2013, s. 181-199 - SCI ; SCOPUS
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ADC48 Yao, Yansun - Martoňák, Roman 95% - Patchkovskii, Serguei - Klug, Dennis D. : Stability of simple cubic calcium at high pressure: A first-principles study

Lit. 40 zázň., 7 obr.

In: *Physical Review B*. - Vol. 82, No. 9 (2010), Art. No. 094107, [8 s.]

*Ohlasy (7):*

[o1] 2011 Sakata, M. - Nakamoto, Y. - Shimizu, K. - Matsuoka, T. - Ohishi, Y.: Superconducting state of Ca-VII below a critical temperature of 29 K at a pressure of 216 GPa. In: *Physical Review B - Condensed Matter and Materials Physics*, Vol.83, No. 22, 2011, Art. No. 220512 - SCI ; SCOPUS

[o1] 2012 Ishikawa, T. - Nagara, H. - Suzuki, N., Shimizu, K.: First-principles molecular dynamics study on simple cubic calcium: Comparison with simple cubic phosphorus. In: *High Pressure Research*, Vol. 32, No. 1, 2012, s. 11-17 - CPCI-S ; SCOPUS

[o1] 2012 Ishikawa, T. - Nagara, H. - Suzuki, N., Shimizu, K.: First-principles molecular dynamics simulation for calcium under high-pressure: Thermodynamic effect on simple cubic structure. In: *Journal of the Physics Society of Japan*, Vol.81, No. 12, 2012, Art. No. 124601 - SCI

[o1] 2012 Li, B. - Ding, Y. - Yang, W. G. - Wang, L. - Zou, B. - Shu, J. F. - Sinogeikin, S. - Park, C. - Zou, G. T. - Mao, H. K.: Calcium with the beta-tin structure at high pressure and low temperature. In: *Proceedings of the National Academy of Sciences of the United States of America*, Vol. 109, No. 41, 2012, s. 16459-16462 - SCI ; SCOPUS

[o1] 2012 Liu, H. - Cui, W. - Ma, Y.: Hybrid functional study rationalizes the simple cubic phase of calcium at high pressures. In: *Journal of Chemical Physics*, Vol. 137, No. 18, 2012, Art. No. 184502 - SCI ; SCOPUS

[o1] 2012 Szczesniak, R. - Szczesniak, D.: Characterization of the high-pressure superconductivity in the Pnma phase of calcium. In: *Physica Status Solidi B - Basic Solid State Physics*, Vol. 249, No. 11, 2012, s. 2194-2201 - SCI

[o1] 2012 Tse, J. S. - Desgreniers, S. - Ohishi, Y. - Matsuoka, T.: Large amplitude fluxional behaviour of elemental calcium under high pressure. In: *Scientific Reports*, Vol. 2, 2012, Art. No. srep00372 - SCI ; SCOPUS

ADC49 Yao, Yansun - Klug, Dennis D. - Sun, Jian - Martoňák, Roman 95%: Comment On "Structural Prediction and Phase Transformation Mechanisms in Calcium at High Pressure" Reply

Lit. 5 zázň.

In: *Physical Review Letters*. - Vol. 104, No. 20 (2010), Art. No. 209602, [1 s.]

ADC50 Hromadová, Liliana 50% - Martoňák, Roman 50%: Pressure-induced structural transitions in BN from ab initio metadynamics

Lit. 39 zázn., 10 obr., 1 tab.

In: Physical Review B. - Vol. 84, No. 22 (2011), Art. No. 224108, [7 s.]

*Ohlasy (5):*

[o1] 2012 He, C. - Sun, L. - Zhang, C. - Peng, X. - Zhang, K. - Zhong, J.: Z-BN: A novel superhard boron nitride phase. In: Physical Chemistry Chemical Physics, Vol. 14, No. 31, 2012, s. 10967-10971 - SCI ; SCOPUS

[o1] 2012 He, Ch. - Sun, L. Z. - Zhong, J.: Prediction of superhard carbon allotropes from the segment combination method. In: Journal of Superhard Materials, Vol. 34, No. 6, 2012, s. 386-399 - SCI ; SCOPUS

[o1] 2012 Huang, Q. - Yu, D. L. - Zhao, Z. S. - Fu, S. W. - Xiong, M. - Wang, Q. Q. - Gao, Y. F. - Luo, K. - He, J. L. - Tian, Y. J.: First-principles study of O-BN: A sp<sup>3</sup>-bonding boron nitride allotrope. In: Journal of Applied Physics, Vol. 112, No. 5, 2012, Art. No. 053518 - SCI ; SCOPUS

[o1] 2013 Jiang, X. - Zhao, J. - Ahuja, R.: A novel superhard BN allotrope under cold compression of h-BN. In: Journal of Physics Condensed Matter, Vol. 25, No. 12, 2013, Art. No. 122204 - SCI ; SCOPUS

[o1] 2013 Zhang, X. - Wang, Y. - Lv, J. - Li, Q. - Zhu, C. - Li, Q., Zhang, M. - Ma, Y.: First-principles structural design of superhard materials. In: Journal of Chemical Physics, Vol. 138, No. 11, 2013, Art. No. 114101 - SCI ; SCOPUS

ADC51 Martoňák, Roman 100 %: Atomistic simulations of pressure-induced structural transformations in solids  
Lit. 100 zázn.

In: The European Physical Journal B. - Vol. 79, No. 3 (2011), s. 241-252

*Ohlasy (4):*

[o1] 2012 Cartwright, J. H. E. - Piro, O. - Sánchez, P. A. - Sintès, T.: Ice polymorphism in the minimal Mercedes-Benz model of water. In: Journal of Chemical Physics, Vol. 137, No. 24, 2012, Art. No. 244503 - SCI ; SCOPUS

[o1] 2012 Grunwald, M. - Zayak, A. - Neaton, J. B. - Geissler, P. L. - Rabani, E.: Transferable pair potentials for CdS and ZnS crystals. In: Journal of Chemical Physics, Vol. 136, No. 23, 2012, Art. No. 234111 - SCI ; SCOPUS

[o1] 2012 Yao, Y. - Klug, D. D.: Structural phase transitions in Si under hydrostatic and uniaxial compression. In: Physical Review B - Condensed Matter and Materials Physics, Vol. 85, No. 21, 2012, Art. No. 214122 - SCI ; SCOPUS

[o1] 2012 Yao, Y. - Klug, D. D.: Reconstructive structural phase transitions in dense Mg. In: Journal of Physics - Condensed Matter, Vol. 24, No. 26, 2012, Art. No. 265401 - SCI

ADC52 Selli, Daniele 25% - Baburin, Igor A. 25% - Martoňák, Roman 25% - Leoni, Stefano 25%: Superhard sp<sup>3</sup> carbon allotropes with odd and even ring topologies

Lit. 34 zázn., 5 obr., 2 tab.

In: Physical Review B. - Vol. 84, No. 16 (2011), Art. No. 161411 [5 s.]

*Ohlasy (19):*

[o1] 2012 Botti, S. - Flores-Livas, J. A. - Amsler, M. - Goedecker, S. - Marques, M. A. L.: Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. In: Physical Review B - Condensed Matter and Materials Physics, Vol. 86, No. 12, 2012, Art. No. 121204 - SCI ; SCOPUS

[o1] 2012 Boufelfel, S. E. - Zhu, Q. - Oganov, A. R.: Novel sp<sup>3</sup> forms of carbon predicted by evolutionary metadynamics and analysis of their synthesizability using transition path sampling. In: Journal of Superhard Materials, Vol. 34, No. 6, 2012, s. 350-359 - SCI ; SCOPUS

[o1] 2012 Boufelfel, S. E. - Oganov, A. R. - Leoni, S.: Understanding the nature of "superhard graphite". In: Scientific Reports, Vol. 2, 2012, Art. No. 471 - SCOPUS

[o1] 2012 Flores-Livas, J. A. - Lehtovaara, L. - Amsler, M. - Goedecker, S. - Pailhes, S. - Botti, S. - San Miguel, A. - Marques, M. A. L.: Raman activity of sp<sup>3</sup> carbon allotropes under pressure: A density functional theory study. In: Physical Review B - Condensed Matter and Materials Physics, Vol. 85, No. 15, 2012, Art. No. 155428 - SCI ; SCOPUS

[o1] 2012 He, C. - Sun, L. - Zhang, C. - Peng, X. - Zhang, K. - Zhong, J.: Z-BN: A novel superhard boron nitride phase. In: Physical Chemistry Chemical Physics, Vol. 14, No. 31, 2012, s.10967-10971 - SCI ; SCOPUS

- [o1] 2012 He, C. - Sun, L. - Zhang, C. - Peng, X. - Zhang, K. - Zhong, J.: New superhard carbon phases between graphite and diamond. In: Solid State Communications, Vol. 152, No. 16, 2012, s.1560-1563 - SCI ; SCOPUS
- [o1] 2012 He, Ch. - Sun, L. Z. - Zhong, J.: Prediction of superhard carbon allotropes from the segment combination method. In: Journal of Superhard Materials, Vol. 34, No. 6, 2012, s. 386-399 - SCI ; SCOPUS
- [o1] 2012 He, C. Y. - Sun, L. Z. - Zhang, C. X. - Peng, X. Y. - Zhang, K. W. - Zhong, J. X.: Four superhard carbon allotropes: a first-principles study. In: Physical Chemistry Chemical Physics, Vol. 14, No. 23, 2012, s. 8410-8414 - SCI
- [o1] 2012 Huang, Q. - Yu, D. - Zhao, Z. - Fu, S. - Xiong, M. - Wang, Q. - Gao, Y. - Luo, K. - He, J. - Tian, Y.: First-principles study of O-BN: A sp<sup>3</sup>-bonding boron nitride allotrope. In: Journal of Applied Physics, Vol. 112, No. 5, 2012, s.Art. No. 053518 - SCI ; SCOPUS
- [o1] 2012 Li, D. - Bao, K. - Tian, F. - Zeng, Z. - He, Z. - Liu, B. - Cui, T.: Lowest enthalpy polymorph of cold-compressed graphite phase. In: Physical Chemistry Chemical Physics, Vol. 14, No. 13, 2012, s. 4347-4350 - SCI ; SCOPUS
- [o1] 2012 Niu, H. - Chen, X. Q. - Wang, S. - Li, D. - Mao, W. L. - Li, Y.: Families of superhard crystalline carbon allotropes constructed via cold compression of graphite and nanotubes. In: Physical Review Letters, Vol. 108, No. 13, 2012, s.Art. No. 135501 - SCI ; SCOPUS
- [o1] 2012 Zhai, J. - Yu, D. - Luo, K. - Wang, Q. - Zhao, Z. - He, J. - Tian, Y.: Metastable C-centered orthorhombic Si 8 and Ge 8. In: Journal of Physics Condensed Matter, Vol. 24, No. 40, 2012, Art. No. 405803 - SCI ; SCOPUS
- [o1] 2012 Zhao, Z. S. - Zhou, X. F. - Hu, M. - Yu, D. L. - He, J. L. - Wang, H. T. - Tian, Y. J. - Xu, B.: High-pressure behaviors of carbon nanotubes. In: Journal of Superhard Materials, Vol. 34, No. 6, 2012, s. 371-385 - SCI ; SCOPUS
- [o1] 2012 Zhao, Z. S. - Tian, F. - Dong, X. - Li, Q. - Wang, Q. Q. - Wang, H. - Zhong, X. - Xu, B. - Yu, D. L. - He, J. L. - Wang, H. T. - Ma, Y. M. - Tian, Y. J.: Tetragonal allotrope of group 14 elements. In: Journal of the American Chemical Society, Vol. 134, No. 30, 2012, s. 12362-12365 - SCI
- [o1] 2012 Zhou, R. - Zeng, X. C.: Polymorphic phases of sp<sup>3</sup>-hybridized carbon under cold compression. In: Journal of the American Chemical Society, Vol. 134, No. 17, 2012, s. 7530-7538 - SCI ; SCOPUS
- [o1] 2012 Zhu, Q. - Zeng, Q. - Oganov, A. R.: Systematic search for low-enthalpy sp<sup>3</sup> carbon allotropes using evolutionary metadynamics. In: Physical Review B - Condensed Matter and Materials Physics, Vol. 85, No. 20, 2012, Art. No. 201407 -SCI ; SCOPUS
- [o1] 2013 He, C. Y. - Sun, L. Z. - Zhang, C. X. - Zhong, J. X.: Two viable three-dimensional carbon semiconductors with an entirely sp<sup>2</sup> configuration. In: Physical Chemistry Chemical Physics, Vol. 15, No. 2, 2013, s. 680-684 - SCI
- [o1] 2013 Ivanovskii, A. L.: Search for superhard carbon: Between graphite and diamond. In: Journal of Superhard Materials, Vol. 35, No. 1, 2013, s. 1-14 - SCI ; SCOPUS
- [o1] 2013 Zhang, X. - Wang, Y. - Lv, J. - Li, Q. - Zhu, C. - Li, Q. - Zhang, M. - Ma, Y.: First-principles structural design of superhard materials. In: Journal of Chemical Physics, Vol. 138, No. 11, 2013, Art. No. 114101 - SCI ; SCOPUS

ADC53 Yao, Yansun 2% - Klug, Dennis D. 2% - Martoňák, Roman 95% - Patchkovskii, Serguei 1%: Dimerization of boron triiodide at high pressure

Lit. 34 zázn.

In: Physical Review B. - Vol. 83, No. 21 (2011), Art. No. 214105, [9 s.]

*Ohlasy (1):*

[o1] 2011 Zhang, J. - Li, Y. L. - Lin, H. - Zeng, Z.: Pressure-induced structural phase transition in wide-gap molecular solid CF<sub>4</sub>. In: Chemical Physics Letters, Vol. 512, No. 4-6, 2011, s. 223-226 - SCI ; SCOPUS

ADC54 Plašienka, Dušan, ml. 50% - Martoňák, Roman 50%: Study of pressure-induced amorphization in sulfur using ab initio molecular dynamics

Lit. 63 zázn.

In: Physical Review B. - Vol. 85, No. 9 (2012), Art. No. 094112, [9 s.]

*Ohlasy (2):*

[o1] 2013 Andrikopoulos, K. S. - Gorelli, F. A. - Santoro, M. - Yannopoulos, S. N.: Elemental sulfur under high hydrostatic pressure. An up-to-date Raman study. In: High Pressure Research, Vol. 33, No. 1, 2013, s. 134-140 - SCI ; SCOPUS

[o1] 2013 Zhou, D. W. - Pu, C. Y. - Szczeniak, D. - Zhang, G. F. - Lu, C. - Li, G. Q. - Song, J. F.: The predicted fcc superconducting phase for compressed Se and Te. In: Chinese Physics Letters, Vol. 30, No. 2, 2013, Art. No. 027401 - SCI ; SCOPUS

ADC55 Hromadová, Liliana 34% - Martoňák, Roman 33% - Tosatti, Erio 33%: Structure change, layer sliding, and metallization in high-pressure MoS<sub>2</sub>

Lit. 35 zázň.

In: Physical Review B. - Vol. 87, No. 14 (2013), Art. No. 144105, [6 s.]

[SMEC 2013 : Study of Matter at Extreme Conditions. Miami, 23.-30.3.2013]

POZNÁMKA: Vyšlo aj ako abstrakt - SMEC 2013 Conference. - Miami : HIPSSA, 2013. - S. 24. -

#### **ADE Vedecké práce v zahraničných nekarentovaných časopisoch**

ADE01 Martoňák, Roman - Paul, W. - Binder, K. : Constant-volume and constant-pressure Monte Carlo simulation of crystalline polyethylene

Lit. 16 zázň., 6 obr.

In: Journal of Computer-Aided Materials Design. - Vol. 4, No. 1 (1997), s. 9-18

#### **ADM Vedecké práce v zahraničných časopisoch registrovaných v databázach Web of Science alebo SCOPUS**

ADM01 Selli, Daniele 25% - Baburin, Igor A. 25% - Martoňák, Roman 25% - Leoni, Stefano 25%: Novel metastable metallic and semiconducting germaniums

Lit. 48 zázň.

In: Scientific Reports [elektronický zdroj]. - Vol. 3 (2013), Art. No. 1713, s. 1-6 [online]

URL: <http://www.scopus.com/record/display.url?eid=2-s2.0-84876551562&origin=resultslist&sort=plf-f&src=s&st1=novel+metastable+metallic&sid=4E38DA4DCA1C5BA635C5B02C05D88698.53bsOu7mi7A1NSY7fPJf1g%3a20&sot=b&sdt=b&sl=40&s=TITLE-ABS-KEY%28novel+metastable+metallic%29&relpos=0&relpos=0&searchTerm=TITLE-ABS-KEY%28novel+metastable+metallic%29>

KEY%28novel+metastable+metallic%29&relpos=0&relpos=0&searchTerm=TITLE-ABS-

KEY%28novel+metastable+metallic%29<http://www.nature.com/srep/2013/130315/srep01466/full/srep01466.html>

#### **AFE Abstrakty pozvaných príspevkov zo zahraničných konferencií**

AFE01 Martoňák, Roman 100%: Metadynamics simulations of structural phase transitions

Lit. 10 zázň.

In: Pressure Effects on Materials. - Santa Barbara : University of California, 2010. - [nestr., 1 s.]

[Pressure Effects on Materials : Conference. Santa Barbara, 22.-27.8.2010]

AFE02 Hromadová, Liliana 50% - Martoňák, Roman 50%: Ab initio metadynamics study of sp<sup>2</sup> to sp<sup>3</sup> transitions in boron nitride [elektronický dokument]

Popis urobený 4.5.2012

Lit. 5 zázň.

In: SMEC 2011 Conference. - Miami : HIPSSA, 2011. - S. 70

[SMEC 2011 : Study of Matter at Extreme Conditions. Miami, 27.3.-2.4.2011]

URL: <http://hipssa.org/smec2011/abstract/040-abs-abstract.doc>

AFE03 Hreha, J. 34% - Hromadová, Liliana 33% - Martoňák, Roman 33%: Structural transitions in silica at Mbar pressures from ab initio metadynamics

In: European Mineralogical Conference [elektronický zdroj]. - [s.l.] : [s.n.], 2012. - EMC2012-664, s. 1 [online]

[EMC 2012 : European Mineralogical Conference. Frankfurt, 2.-6.9.2012]

URL: <http://meetingorganizer.copernicus.org/EMC2012/EMC2012-664.pdf>



AFE04 Plašienka, Dušan, ml. 50% - Martoňák, Roman 50%: Ab initio molecular dynamics study of pressure-induced amorphization in sulfur  
Lit. 3 záz. n.  
In: 50th European High Pressure Research Group Meeting [elektronický dokument]. - Thessaloniky : Aristotle University of Thessaloniki, 2012. - S. 218 [online]  
[EHPRG Meeting 2012 : European High Pressure Research Group Meeting. 50th, Thessaloniki, 16.-21.9.2012]  
URL: <http://ehprg2012.web.auth.gr/>

AFE05 Plašienka, Dušan, ml. 50% - Martoňák, Roman 50%: Pressure-induced amorphization in sulfur: an ab initio molecular dynamics study  
In: E-MRS Fall Meeting 2012 [elektronický zdroj]. - [Strasbourg] : [European Materials Research Society], 2012. - [nestr., 1 s.], [online]  
[E-MRS Fall Meeting 2012 : Symposium : Computer modelling in nanoscience and nanotechnology: an atomic-scale perspective II. Warsaw, 17.-21.9.2012]  
[SMEC 2013 : Study of Matter at Extreme Conditions. Miami, 23.-30.3.2013]  
URL: [http://www.emrs-strasbourg.com/files/FALL%2012/symposium\\_i.pdf](http://www.emrs-strasbourg.com/files/FALL%2012/symposium_i.pdf)  
POZNÁMKA: Vyšlo aj - SMEC 2013 Conference. - Miami : HIPSSA, 2013. - S.14. -

#### **AFG Abstrakty príspevkov zo zahraničných konferencií**

AFG01 Martoňák, Roman 100%: Polymorphism and structural phase transitions in crystals: Computer simulation by metadynamics  
Lit. 5 záz. n.  
In: 21 Congress of the International Union of Crystallography. - Osaka : International Union of Crystallography, 2008. - S. C42  
[IUCr 2008 : International Union of Crystallography : Congress and General Assembly. 21th, Osaka, 23.-31.8.2008]

AFG02 Martoňák, Roman 100%: Crystal polymorphism and structural transformation: Computer simulations by metadynamics  
Lit. 7 záz. n.  
In: Frontiers towards Predictive Simulations and Computations. - Tsukuba : Research Institute for Computational Sciences, 2008. - S. 13  
[CSW 2008 : Computational Science Workshop: Frontiers towards Predictive Simulations and Computations. Tsukuba, 8.-10.12.2008]

AFG03 Martoňák, Roman 100%: Exploration of free-energy landscapes of crystals by metadynamics-study of polymorphism and structural transformations  
Lit. 5 záz. n.  
In: Energy Landscape of Solids: from (hypothetical) topologies to material properties. - Lausanne : CECAM, 2008. - S. 20  
[Energy Landscape of Solids: from (hypothetical) topologies to material properties: CECAM Workshop. Lausanne, 22.-25.7.2008]

AFG04 Martoňák, Roman 100%: Study of structural transformations in crystals by metadynamics simulations: some applications  
Lit. 9 záz. n.  
In: SMEC 2009 Conference. - Miami : HIPSSA, 2009. - S. 61-62  
[SMEC 2009 : Study of Matter at Extreme Conditions. Miami, 28.3.-2.4.2009]

AFG05 Sun, Jian - Klug, Dennis D. - Martoňák, Roman 30%: Structural transformations of carbon under high pressure: Beyond diamond  
In: Structural Transitions in Solids: Theory, Simulations, Experiments and Visualization Techniques. - Lausanne : CECAM, 2009. - S. 32

[Structural Transitions in Solids: Theory, Simulations, Experiments and Visualization Techniques. Lugano, 8.-11.7.2009]

### **AFH Abstrakty príspevkov z domácich konferencií**

AFH01 Martoňák, Roman 100 %: Heuristické optimalizačné metódy [elektronický dokument]

Recenzované. - Popis urobený 29.10.2009

In: Matematický kaleidoskop pre fyzikov : Texty zo Zimnej školy poriadanej KTFDF FMFI UK. - Bratislava : Knižničné a edičné centrum FMFI UK, 2009. - S. 117. - ISBN 978-80-89186-56-3

[Zimná škola z vybraných kapitol matematiky pre fyzikov. Bratislava, 2.-4.2.2009]

URL: [http://sophia.dtp.fmph.uniba.sk/~fecko/referaty/ZS\\_2009-1.pdf](http://sophia.dtp.fmph.uniba.sk/~fecko/referaty/ZS_2009-1.pdf)

AFH02 Martoňák, Roman 100%: Simulácie štruktúrnych fázových prechodov v kryštáloch

In: 17. Konferencia slovenských fyzikov : Zborník abstraktov. - Bratislava : FMFI UK, 2009. - S. 26

[Konferencia slovenských fyzikov 2009. 17., Bratislava, 16.-19.9.2009]

### **BFA Abstrakty odborných prác zo zahraničných podujatí (konferencie...)**

BFA01 Plašienka, Dušan, ml. 50% - Martoňák, Roman 50%: Study of polyamorphism in CO<sub>2</sub> by ab initio molecular dynamics

Lit. 5 záz. n.

In: SMEC 2013 Conference. - Miami : HIPSSA, 2013. - S. 26

[SMEC 2013 : Study of Matter at Extreme Conditions. Miami, 23.-30.3.2013]

### **DAI Dizertačné a habilitačné práce**

DAI01 Martoňák, Roman : Models of quantum paraelectric behaviour of Perovskites. - Trieste : [s.n.], 1993. - 121 s.

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### **GAI Výskumné štúdie a priebežné správy**

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Záverečná správa,

### **Štatistika kategórií (Záznamov spolu: 76):**

ABC Kapitoly vo vedeckých monografiách vydané v zahraničných vydavateľstvách (1)

ADC Vedecké práce v zahraničných karentovaných časopisoch (55)  
ADE Vedecké práce v zahraničných nekarentovaných časopisoch (1)  
ADM Vedecké práce v zahraničných časopisoch registrovaných v databázach Web of Science alebo SCOPUS (1)  
AFE Abstrakty pozvaných príspevkov zo zahraničných konferencií (5)  
AFG Abstrakty príspevkov zo zahraničných konferencií (5)  
AFH Abstrakty príspevkov z domácich konferencií (2)  
BFA Abstrakty odborných prác zo zahraničných podujatí (konferencie...) (1)  
DAI Dizertačné a habilitačné práce (2)  
EDJ Prehľadové práce, odborné preklady v časopisoch a zborníkoch (2)  
GAI Výskumné štúdie a priebežné správy (1)

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