

Zoznam publikačnej činnosti

Mgr. Michal Pitoňák, PhD.

ABC Kapitoly vo vedeckých monografiách vydané v zahraničných vydavateľstvách

ABC01 Urban, Miroslav 34% [0,88 AH] - Pitoňák, Michal 33% [0,86 AH] - Neogrády, Pavel 33% [0,86 AH] : Optimized virtual orbital space (OVOS) as a tool for more efficient correlated and relativistic calculations of molecular properties and interactions.

Lit.: 63 zázň.

In: Trends and perspectives in Modern Computational Science. - Leiden : Brill Academic Publishers, 2006. - S. 265-285 [2,6 AH]. - ISBN-10: 90-04-15541-4, ISBN-13: 978-90-04-15541-1. - (Lecture Series on Computer and Computational Sciences ; Vol. 265)

ABC02 Neogrády, Pavel 30% [0,75 AH] - Pitoňák, Michal 30% [0,75 AH] - Granatier, Jaroslav 15% [0,37 AH] - Urban, Miroslav 25% [0,63 AH] : Coupled cluster calculations: OVOS as an alternative avenue towards treating still larger molecules

Lit.: 90 zázň., 6 obr., 5 tab.

In: Challenges and Advances in Computational Chemistry and Physics, Vol. 11. Recent Progress in Coupled Cluster Methods. Theory and applications. - [S.l.] : Springer, 2010. - S. 429-454 [2,5 AH]. - ISBN 978-90-481-2884-6

ACB Vysokoškolské učebnice vydané v domácich vydavateľstvách

ACB01 Čerňušák, Ivan 1% [0,06 AH] - Neogrády, Pavel 48% [3 AH] - Noga, Jozef 1% [0,06 AH] - Iliáš, Miroslav 2% [0,15 AH] - Pitoňák, Michal 48% [3 AH] : Základy numerickej matematiky pre prírodovedcov : s príkladmi v Microsoft Excel 2010. - 2. vyd. - Banská Bystrica : Univerzita Mateja Bela, 2012. - 119 s. [6,27 AH]

Lit.: 37 zázň., obr., tabuľky, grafy v texte

ISBN 978-80-557-0277-3

ADC Vedecké práce v zahraničných karentovaných časopisoch

ADC01 Neogrády, Pavel - Pitoňák, Michal - Urban, Miroslav : Optimized virtual orbitals for correlated calculations: an alternative approach

Lit.: 69 zázň.

In: Molecular Physics. - Vol. 103, No. 15-16 (2005), s. 2141-2157

Ohlasy (14):

[o1] 2006 Kowalski, K. - Valiev, M.: Journal of Physical Chemistry A, Vol. 110, No. 48, 2006, s. 13106-13111 - SCI

[o1] 2006 Kohn, A. - Olsen, J.: Journal of Chemical Physics, Vol. 125, No. 17, 2006, Art. No. 174110 - SCI

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[o1] 2008 Sponer, J. - Riley, K.E. - Hobza, P.: Physical Chemistry Chemical Physics, Vol. 10, No. 19, 2008, s. 2595-2610 - SCI

[o1] 2008 Taube, A.G. - Bartlett, R.J.: Journal of Chemical Physics, Vol. 128, No. 16, 2008, Art. No. 164101 - SCI

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- [o1] 2012 Hohenstein, E.G. - Sherrill, C.D.: Wiley Interdisciplinary Reviews-Computational Molecular Science, Vol. 2, No. 2, 2012, s. 304-326 - SCI

ADC02 Pitoňák, Michal - Lischka, Hans : Excited-state potential energy surfaces of silaethylene: a MRCI investigation

Lit.: 47 zázň., 8 obr., 4 tab.

In: Molecular Physics. - Vol. 103, No. 6-8 (2005), s. 855-862

Ohlasy (2):

[o1] 2009 Blancafort, L.: Photochemistry and Photobiology, Vol. 83, No. 3, 2007, s. 603-610 - SCI

[o1] 2012 West, A.C. - Windus, T.L.: Theoretical Chemistry Accounts, Vol. 131, No. 8, 2012, Art. No. 1251 - SCI

ADC03 Uhlár, Milan - Pitoňák, Michal - Černušák, Ivan : A study of H₂S . . . NO⁺ complex

Lit.: 51 zázň.

In: Molecular Physics. - Vol. 103, No. 15-16 (2005), s. 2309-2319

ADC04 Pitoňák, Michal - Holka, Filip - Neogrady, Pavel - Urban, Miroslav : Optimized virtual orbitals for correlated calculations: Towards large scale CCSD(T) calculations of molecular dipole moments and polarizabilities

Lit.: 55 zázň.

In: Journal of Molecular Structure-Theochem. - Vol. 768, No. 1-3 (2006), s. 79-89

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ADC05 Pitoňák, Michal - Neogrady, Pavel - Kellö, Vladimír - Urban, Miroslav : Optimized virtual orbitals for relativistic calculations: an alternative approach to the basis set construction for correlation calculations

Lit.: 74 zázň.

In: Molecular Physics. - Vol. 104, No. 13-14 (2006), s. 2277-2292

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ADC06 Wang, Weizhou - Pitoňák, Michal - Hobza, Pavel : C-H stretching vibrational shift of benzene dimer: Consistency of experiment and calculation

Lit.: 23 zázň., 2 obr., 2 tab.

In: ChemPhysChem. - Vol. 8, No. 14 (2007), s. 2107-2111

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ADC07 Dedíková, Pavlína 30% - Pitoňák, Michal 10% - Neogrady, Pavel 20% - Černušák, Ivan 15% - Urban, Miroslav 25% : Toward more efficient CCSD(T) calculations of intermolecular interactions in model hydrogen-bonded and stacked dimers

Lit.: 55 zázň., 8 obr., 5 tab.

In: Journal of Physical Chemistry A. - Vol. 112, No. 30 (2008), s. 7115-7123

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ADC08 Pitoňák, Michal - Neogrady, Pavel 17% - Řezáč, J. - Jurečka, P. - Urban, Miroslav 17% - Hobza, P. : Benzene Dimer: High-Level Wave Function and Density Functional Theory Calculations

Lit.: 33 zázň., 2 obr., 3 tab.

In: Journal of Chemical Theory and Computation. - Vol. 4, No. 11 (2008), s. 1829-1834

Ohlasy (62):

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