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<b>Pozícia na projekte</b>	Vedecko-výskumný pracovník
<b>Vedecké identifikátory</b>	<b>WoS (Researcher ID): C-3944-2012, Scopus (AuthorID): 24759724000, ORCID: 0000-0002-2492-4377</b>
<b>Vedecké zameranie</b>	počítačové modelovania atomárnych štruktúr
<b>Publikačná činnosť s ohlasmí (aktuálne k 31.10.2022)</b>	
<b>V2 Vedecký výstup publikačnej činnosti ako časť editovanej knihy alebo zborníka</b>	
V2_01	ŠULKA, Martin - ŠULKOVÁ, Katarína. Properties of atomically precise nanoclusters. In <i>Bulletin vedeckých príspevkov : Bulletin vedeckých príspevkov z projektu Vedeckovýskumné centrum excelentnosti Slovákion pre materiálový a interdisciplinárny výskum</i> . 1. vyd. Bratislava : Spektrum, 2022, S. 64-67. ISBN 978-80-227-5220-6. Typ výstupu: príspevok; Výstup: domáci; Kategória publikácie do 2021: AED
<b>V3 Vedecký výstup publikačnej činnosti z časopisu</b>	
V3_01	ANTUŠEK, Andrej - ŠULKA, Martin. Ab initio calculations of NMR shielding of Sc <sup>3+</sup> , Y <sup>3+</sup> and La <sup>3+</sup> ions in the water solution and <sup>45</sup> Sc, <sup>89</sup> Y, <sup>138</sup> La and <sup>139</sup> La nuclear magnetic dipole moments. In <i>Chemical Physics Letters</i> . Vol. 660, (2016), s. 127-131. ISSN 0009-2614 (2016: 1.815 - IF, Q2 - JCR Best Q, 0.718 - SJR, Q2 - SJR Best Q). V databáze: DOI: <a href="http://dx.doi.org/10.1016/j.cplett.2016.08.002">http://dx.doi.org/10.1016/j.cplett.2016.08.002</a> ; SCOPUS ; WOS ; MLJ : CCC:000384787600023. Kategória publikácie do 2021: ADC Ohlasy: 1. [1] OLEJNICZAK, Malgorzata - BAST, Radovan - GOMES, Andre Severo Pereira. On the calculation of second-order magnetic properties using subsystem approaches in a relativistic framework. In <i>PHYSICAL CHEMISTRY CHEMICAL PHYSICS</i> , 2017, vol. 19, no. 12, pp. 8400-8415. ISSN 1463-9076., Registrované v: SCOPUS, CC, WOS Ohlas: zahraničný 2. [1] DE OLIVEIRA, A. Z. - CAMPOS, C. T. - JORGE, F. E. - FERREIRA, I. B. - FANTIN, P. A. All-electron triple zeta basis sets for the actinides. In <i>Computational and Theoretical Chemistry</i> , 2018, 1135, pp. 28-33. ISSN 2210-271X., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 3. [1] JORGE, Francisco E. - DA COSTA VENANCIO, Jose R. Structure, stability, catalytic activity, and polarizabilities of small iridium clusters. In <i>CHINESE PHYSICS B</i> , 2018, vol. 27, no. 6, pp. ISSN 1674-1056., Registrované v: SCOPUS, CC, WOS Ohlas: zahraničný 4. [1] DE OLIVEIRA, A. Z. - FERREIRA, I. B. - CAMPOS, C. T. - JORGE, F. E. - FANTIN, P. A. Segmented all-electron basis sets of triple zeta quality for the lanthanides: application to structure calculations of lanthanide monoxides. In <i>Journal of Molecular Modeling</i> , 2019, 25, 2, pp. ISSN 16102940., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 5. [1] PRASETYO, Niko. The effect of electron correlation in unraveling the hydration properties of Sc <sup>3+</sup> in aqueous solution: A rigid body quantum mechanics/molecular mechanics simulation study. In <i>Journal of Molecular Liquids</i> , 2021, 331, pp. ISSN 01677322., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 6. [1] BAI, S. W. - KOSZORÚS - HU, B. S. - YANG, X. F. - BILLOWES, J. - BINNERSLEY, C. L. - BISSELL, M. L. - BLAUM, K. - CAMPBELL, P. - CHEAL, B. - COCOLIOS, T. E. - DE GROOTE, R. P. - DEVLIN, C. S. - FLANAGAN, K. T. - GARCIA RUIZ, R. F. - HEYLEN, H. - HOLT, J. D. - KANELAKOPOULOS, A. - KRÄMER, J. - LAGAKI, V. - MAAß, B. - MALBRUNOT-ETTENAUER, S. - MIYAGI, T. - NEUGART, R. - NEYENS, G. - NÖRTERSCHÄUSER, W. - RODRÍGUEZ, L. V. - SOMMER, F. - VERNON, A. R. - WANG, S. J. - WANG, X. B. - WILKINS, S. G. - XU, Z. Y. - YUAN, C. X. Electromagnetic moments of scandium isotopes and N = 28 isotones in the distinctive 0f <sub>7/2</sub> /inf orbit. In <i>Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics</i> , 2022-06-10, 829, pp. ISSN 03702693., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný
V3_02	LABANC, Daniel - ŠULKA, Martin - PITOŇÁK, Michal - ČERNUŠÁK, Ivan - URBAN, Miroslav - NEOGRÁDY, Pavel. Benchmark CCSD(T) and DFT study of binding energies in Be <sub>7</sub> -12: in search of reliable DFT functional for beryllium clusters. In <i>Molecular Physics</i> . Vol. 116, iss. 10 (2018), s. 1259-1274. ISSN 0026-8976 (2018: 1.571 - IF, Q4 - JCR Best Q, 0.635 - SJR, Q2 - SJR Best Q). V databáze: WOS ; MLJ ; CC: 000430503800001 ; SCOPUS: 2-s2.0-85040978280. Kategória publikácie do 2021: ADC Ohlasy: 1. [1] GRIBANOVA, Tatyana N. - MINYAEV, Ruslan M. - MINKIN, Vladimir I. Stabilization of non-typical forms of boron clusters by beryllium doping. In <i>Chemical Physics</i> , 2019, 522, pp. 44-54. ISSN 03010104., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 2. [1] FIORESSI, Silvina E. - DUCHOWICZ, Pablo - BACELO, Daniel E. DFT Study on the Structures and Stability of Be <sub>n</sub> S <sub>n</sub> (n=1-5) and Be <sub>2n</sub> S <sub>n</sub> (n=1-4) Clusters. In <i>ChemistrySelect</i> , 2018, 3, 46, pp. 13017-13024., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 3. [1] MONTERO-CAMPILLO, M. Merced - MÓ, Otilia - YÁÑEZ, Manuel - ALKORTA, Ibon - ELGUERO, José. The beryllium bond. In <i>Advances in Inorganic Chemistry</i> , 2019, 73, pp. 73-121. ISSN 08988838., Registrované v: SCOPUS, WOS Ohlas: zahraničný 4. [1] SHARIPOV, Alexander S. - LOUKHOVITSKI, Boris I. Small atomic clusters: quantum chemical research of

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Ohlas: zahraničný

V3\_03

SAAB, Mohamed - REAL, Florent - ŠULKA, Martin - CANTREL, Laurent - VIROT, Francois - VALLET, Valerie. Facing the challenge of predicting the standard formation enthalpies of n-butyl-phosphate species with ab initio methods. In *Journal of Chemical Physics*. Vol. 146, iss. 24 (2017), s. 1-7. ISSN 0021-9606 (2017: 2.843 - IF, Q2 - JCR Best Q, 1.252 - SJR, Q1 - SJR Best Q). V databáze: WOS: CCC:000404302600027 ; SCOPUS ; MLJ.

Katégória publikácie do 2021: ADC

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Ohlas: zahraničný

V3\_04

ŠULKA, Martin - CANTREL, L. - VALLET, V. Theoretical study of plutonium(IV) complexes formed within the PUREX process: A proposal of a plutonium surrogate in fire conditions. In *Journal of Physical Chemistry A*. Vol. 118, iss. 43 (2014), s. 10073-10080. ISSN 1089-5639 (P) (2014: 2.693 - IF, Q2 - JCR Best Q, 1.159 - SJR, Q1 - SJR Best Q). V databáze: CC ; SCOPUS ; WOS.

Katégória publikácie do 2021: ADC

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Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

7. [1] RYZHKOV, Mikhail V. - ENYASHIN, Andrei N. - DELLEY, Bernard. Plutonium complexes in water: New approach to ab initio modeling. In Radiochimica Acta, 2021, 109, 5, pp. 327-342. ISSN 00338230., Registrované v: SCOPUS, WOS, CC

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Ohlas: zahraničný

9. [1] RYZHKOV, Mikhail V. - ENYASHIN, Andrei N. - DELLEY, Bernard. First-principles study on the plutonium ions interaction with diamide molecules in acid solutions. In International Journal of Quantum Chemistry, 2021, 121, 16, pp. ISSN 00207608., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

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Ohlas: zahraničný

V3\_05 ŠULKA, Martin - DUBECKÝ, Matúš. Fragmentation of natural orbital occupation numbers-based diagnostic of differential multireference character in complexes with hydrogen bonds. In *Journal of Computational Chemistry*. Vol. 42, iss. 7 (2021), s. 475-483. ISSN 0192-8651 (2021: 3.672 - IF, Q2 - JCR Best Q, 0.778 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1002/jcc.26470 ; SCOPUS: 2-s2.0-85097564119 ; WOS: 000598674400001 ; CC: 000612509100002.  
Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC

V3\_06 ŠULKA, Martin - ŠULKOVÁ, Katarína - ANTUŠEK, Andrej. Exploring water adsorption and reactivity in a series of doped aluminum cluster anions. In *Physical Chemistry Chemical Physics*. Vol. 23, iss. 41 (2021), s. 896-908. ISSN 1463-9076 (2021: 3.945 - IF, Q1 - JCR Best Q, 0.899 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1039/d1cp03104j ; SCOPUS: 2-s2.0-85118452282 ; WOS: 000707408500001 ; CC: 000711558600001.  
Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC

## I2 Iný výstup publikačnej činnosti ako časť publikácie alebo zborníka

I2\_01 ŠULKA, Martin - ŠULKOVÁ, Katarína - DUBECKÝ, Matúš. Assessing the accuracy of quantum Monte Carlo in hydrogen-bonded and strongly correlated systems. In *CESTC 2022 : 18th Central European Symposium on Theoretical Chemistry 2022, 7-10 September 2022, Balatonszárszó, Hungary*. 1. vyd. Budapešť : Hungarian Chemical Society, 2022, S. 90. ISBN 978-615-6018-10-6.  
Typ výstupu: časti, ktoré nemožno zaradiť do kategórie V, O, P, U alebo D; Výstup: zahraničný; Kategória publikácie do 2021: AFK

I2\_02 ŠULKOVÁ, Katarína - ŠULKA, Martin - ANTUŠEK, Andrej. Exploring water adsorption and reactivity in a series of doped aluminum cluster anions. In *CESTC 2022 : 18th Central European Symposium on Theoretical Chemistry 2022, 7-10 September 2022, Balatonszárszó, Hungary*. 1. vyd. Budapešť : Hungarian Chemical Society, 2022, S. 91. ISBN 978-615-6018-10-6.  
Typ výstupu: časti, ktoré nemožno zaradiť do kategórie V, O, P, U alebo D; Výstup: zahraničný; Kategória publikácie do 2021: AFK

## XXX XXX

\_01 ŠULKA, Martin - PITOŇÁK, Michal - NEOGRÁDY, Pavel - URBAN, Miroslav. Electron affinity of the O<sub>2</sub> molecule: CCSD(T) calculations using the optimized virtual orbitals space approach. In *International Journal of Quantum Chemistry*. Vol. 108, Iss. 12 (2008), s.2159-2171. ISSN 0020-7608 (2008: 1.317 - IF, Q2 - JCR Best Q, 0.809 - SJR, Q2 - SJR Best Q). V databáze: SCOPUS ; WOS.

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6. [1] WANG, F. - UEDA, W. - XU, J. Detection and measurement of surface electron transfer on reduced molybdenum oxides (MoO<sub>x</sub>) and catalytic activities of Au/MoO<sub>x</sub>. In *Angewandte Chemie-International edition*, 2012, vol. 51, iss. 16, s.3883-3887.  
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7. [1] DANG, Zheng - SONG, Le Xin - YANG, Jun - CHEN, Jie - TENG, Yue. The physical properties and unusual pyrolysis behaviour of a supramolecular complex of beta-cyclodextrin and potassium ferrioxalate. In *Dalton Transactions*, 2012, vol. 41, iss. 10, s.3006-3013.  
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8. [1] KRIVETSKIY, V. - RUMYANTSEVA, M. - GASKOV, A. Chemical modification of nanocrystalline tin dioxide for selective gas sensors. In *Russian Chemical Reviews*, 2013, vol. 82, iss. 10, s.917-941.  
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9. [1] CHIZHOV, A. S. - RUMYANTSEVA, M. N. - VASILIEV, R. B. - FILATOVA, D. G. - DROZDOV, K. A. - KRYLOV, I. V. - ABAKUMOV, A. M. - GASKOV, A. M. Visible light activated room temperature gas sensors based on nanocrystalline ZnO sensitized with CdSe quantum dots. In *Sensors and Actuators B: Chemical*, 2014, vol. 205, s.305-312., Registrované v: WOS, SCOPUS, CC  
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10. [1] GUTSEV, G. L. - BOZHENKO, K. V. - GUTSEV, L. G. - UTENYSHEV, A. N. - ALDOSHIN, S. M. Transitions from Stable to Metastable States in the Cr<sub>2</sub>O<sub>n</sub> and Cr<sub>2</sub>O<sub>n</sub>- Series, n=1-14. In *JOURNAL OF PHYSICAL CHEMISTRY A*, 2017, vol. 121, no. 4, pp. 845-854. ISSN 1089-5639., Registrované v: SCOPUS, CC, WOS  
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11. [1] SETVIN, Martin - HULVA, Jan - PARKINSON, Gareth S. - SCHMID, Michael - DIEBOLD, Ulrike. Electron transfer between anatase TiO<sub>2</sub> and an O<sub>2</sub> molecule directly observed by atomic force microscopy. In *Proceedings of the National Academy of Sciences of the United States of America*, 2017, 114, 13, pp. E2556-E2562. ISSN 0027-8424., Registrované v: WOS, CC, SCOPUS  
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13. [1] MIRZAEI, Ali - KANG, Sung Yong - CHOI, Sun Woo - KWON, Yong Jung - CHOI, Myung Sik - BANG, Jae Hoon - KIM, Sang Sub - KIM, Hyoun Woo. Fabrication and gas sensing properties of vertically aligned Si nanowires. In *Applied Surface Science*, 2018, 427, pp. 215-226. ISSN 0169-4332., Registrované v: WOS, CC, SCOPUS  
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16. [1] YANG, Huawei - LUO, Mingchuan - LU, Shiyu - ZHANG, Qinghua - CHAO, Yuguang - LV, Fan - ZHU, Lili - BAI, Liangjiu - YANG, Lixia - WANG, Wenxiang - WEI, Donglei - LIANG, Ying - GU, Lin - CHEN, Hou - GUO, Shaojun. Low-temperature aerobic oxidation of thiophenic sulfides over atomic Mo hosted by cobalt hydroxide sub-nanometer sheets. In: *Chem*, 2022-09-08, 8, 9, pp. 2460-2471. ISSN 24519308., Registrované v: SCOPUS, WOS, CC  
Ohlas: zahraničný

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