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Pozícia na projekte	Vedecko-výskumný pracovník
Vedecké identifikátory	WoS (Researcher ID): L-9517-2015 , Scopus (AuthorID): 8530185700 , ORCID: 0000-0002-4574-2943
Vedecké zameranie	počítačové modelovania elektrónovej štruktúry molekúl a materiálov
Publikačná činnosť s ohlasmí (aktuálne k 31.10.2022)	
V2 Vedecký výstup publikačnej činnosti ako časť editovanej knihy alebo zborníka	
V2_01	ANTUŠEK, Andrej - JASZUNSKI, Michal. Accurate non-relativistic calculations of NMR shielding constants. In <i>Gas phase NMR</i> . s. 187-217. V databáze: SCOPUS: DOI:10.1039/9781782623816-00186 ; WOS: WOS:000388328500007. Kategória publikácie do 2021: AEC Ohlasy: 1. [1] KRIVDIN, Leonid B. Calculation of sup15/supN NMR chemical shifts: Recent advances and perspectives. In <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2017, 102-103, pp. 98-119. ISSN 0079-6565., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 2. [1] MAKULSKI, Włodzimierz - WILCZEK, Marcin - JACKOWSKI, Karol. 17O and 1H NMR spectral parameters in isolated water molecules. In <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 35, pp. 22468-22476. ISSN 14639076., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 3. [1] MAKULSKI, Włodzimierz - JACKOWSKI, Karol. H-1, C-13 and Si-29 magnetic shielding in gaseous and liquid tetramethylsilane. In <i>JOURNAL OF MAGNETIC RESONANCE</i> , 2020, vol. 313, no., pp. ISSN 1090-7807., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný
V2_02	ANTUŠEK, Andrej. On the borderline between computational chemistry and nuclear physics. In <i>Bulletin vedeckých príspevkov : Bulletin vedeckých príspevkov z projektu Vedeckovýskumné centrum excelentnosti Slovákion pre materiálovú a interdisciplinárny výskum</i> . 1. vyd. Bratislava : Spektrum, 2022, S. 26-28. ISBN 978-80-227-5220-6. Typ výstupu: príspevok; Výstup: domáci; Kategória publikácie do 2021: AED
V3 Vedecký výstup publikačnej činnosti z časopisu	
V3_01	ADRJAN, B. - MAKULSKI, W. - JACKOWSKI, K. - DEMISSIE, T. B. - RUUD, K. - ANTUŠEK, Andrej - JASZUNSKI, Michal. NMR absolute shielding scale and nuclear magnetic dipole moment of 207-Pb. In <i>Physical Chemistry Chemical Physics</i> . Vol. 18, iss. 24 (2016), s. 16483-16490. ISSN 1463-9076 (2016: 4.123 - IF, Q1 - JCR Best Q, 1.685 - SJR, Q1 - SJR Best Q). V databáze: SCOPUS: DOI: 10.1039/c6cp01781a ; WOS: CCC:000381056500050 ; MLJ. Kategória publikácie do 2021: ADC Ohlasy: 1. [1] AUCAR, I. Agustín - GOMEZ, Sergio S. - GIRIBET, Claudia G. - AUCAR, Gustavo A. Toward an absolute NMR shielding scale using the spin-rotation tensor within a relativistic framework. In <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 34, pp. 23572-23586. ISSN 1463-9076., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 2. [1] AUCAR, Gustavo A. - MELO, Juan I. - AUCAR, Ignacio Agustín - MALDONADO, Alejandro F. Foundations of the LRESC model for response properties and some applications. In <i>International Journal of Quantum Chemistry</i> , 2018, 118, 1, pp. ISSN 0020-7608., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 3. [1] ALKORTA, Ibon - ELGUERO, José. A theoretical study of perovskites related to $\text{CHinF3/infNHinF3/infPbXinF3/inf(X = F, Cl, Br, I)}$. In <i>New Journal of Chemistry</i> , 2018, 42, 16, pp. 13889-13898. ISSN 1144-0546., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 4. [1] AUCAR, Gustavo A. - AUCAR, I. Agustín. Recent Developments in Absolute Shielding Scales for NMR Spectroscopy. In <i>Annual Reports on NMR Spectroscopy</i> , 2019, 96, pp. 77-141. ISSN 00664103., Registrované v: SCOPUS, WOS Ohlas: zahraničný 5. [1] KOZIOŁ, Karol - AGUSTÍN AUCAR, I. - AUCAR, Gustavo A. Relativistic and QED effects on NMR magnetic shielding constant of neutral and ionized atoms and diatomic molecules. In <i>Journal of Chemical Physics</i> , 2019, 150, 18, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 6. [1] BAUER, David - BLUMBERG, Markus - KÖCKERLING, Martin - MAMAT, Constantin. A comparative evaluation of calix[4]arene-1,3-crown-6 as a ligand for selected divalent cations of radiopharmaceutical interest. In <i>RSC Advances</i> , 2019, 9, 55, pp. 32357-32366., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 7. [1] INDELICATO, P. QED tests with highly charged ions. In <i>JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS</i> , 2019, vol. 52, no. 23, pp. ISSN 0953-4075., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 8. [1] VICHA, Jan - NOVOTNY, Jan - KOMOROVSKY, Stanislav - STRAKA, Michal - KAUPP, Martin - MAREK, Radek. Relativistic Heavy-Neighbor-Atom Effects on NMR Shifts: Concepts and Trends Across the Periodic Table. In <i>CHEMICAL REVIEWS</i> , 2020, vol. 120, no. 15, pp. 7065-7103. ISSN 0009-2665., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 9. [1] CASTRO, Abril C. - SWART, Marcel. Chapter 2: Recent Advances in Computational NMR Spectrum

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Ohlas: zahraničný

V3_02

ANTUŠEK, Andrej - JASZUNSKI, Michal - OLEJNICZAK, Maja. Ab initio study of NMR shielding constants and spin-rotation constants in N, P and As diatomic molecules. In *Computational and Theoretical Chemistry*. Vol. 970, iss. 1-3 (2011), s.54-60. ISSN 2210-271X (2011: Q4 - JCR Best Q, 0.586 - SJR, Q2 - SJR Best Q). V databáze: SCOPUS ; WOS.

Kategória publikácie do 2021: ADC

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Ohlas: zahraničný

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V3_03

ANTUŠEK, Andrej - KEDZIERA, Dariusz - KACZMAREK-KEDZIERA, Anna - JASZUNSKI, Michal. Coupled cluster study of NMR shielding of alkali metal ions in water complexes and magnetic moments of alkali metal nuclei. In *Chemical Physics Letters*. Vol. 532 (2012), s.1-8. ISSN 0009-2614 (2012: 2.145 - IF, Q2 - JCR Best Q, 0.951 - SJR, Q1 - SJR Best Q). V databáze: WOS ; SCOPUS.

Kategória 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

V3_04

ANTUŠEK, Andrej - RODZIEWICZ, Pawel - KACZMAREK-KEDZIERA, Anna - JASZUNSKI, Michal. Ab initio study of NMR shielding of alkali earth metal ions in water complexes and magnetic moments of alkali earth metal nuclei. In *Chemical Physics Letters*. Vol. 588 (2013), s.57-62. ISSN 0009-2614 (2013: 1.991 - IF, Q3 - JCR Best Q, 0.901 - SJR, Q2 - SJR Best Q). V databáze: WOS ; SCOPUS.

Kategória 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

V3_05

ANTUŠEK, Andrej - HOLKA, Filip. Absolute shielding scales for Al, Ga, and In and revised nuclear magnetic dipole moments of Al-27, Ga-69, Ga-71, In-113, and In-115 nuclei. In *Journal of Chemical Physics*. Vol. 143, iss. 7 (2015), article number 074301. ISSN 0021-9606 (2015: 2.894 - IF, Q2 - JCR Best Q, 1.255 - SJR, Q1 - SJR Best Q). V databáze: MLJ ; SCOPUS ; WOS ; DOI: DOI: 10.1063/1.4928592.

Kategória publikácie do 2021: ADC

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Ohlas: zahraničný

2. [1] MARTINEZ-BAEZ, Ernesto - FENG, Rulin - PEARCE, Carolyn I. - SCHENTER, Gregory K. - CLARK, Aurora E. Al27 NMR chemical shift of Al (OH)4 - Calculated from first principles: Assessment of error cancellation in chemically distinct reference and target systems. In *Journal of Chemical Physics*, 2020, 152, 13, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

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V3_06

ANTUŠEK, Andrej - ŠULKA, Martin. Ab initio calculations of NMR shielding of Sc³⁺, Y³⁺ and La³⁺ ions in the water solution and 45Sc, 89Y, 138La and 139La nuclear magnetic dipole moments. In *Chemical Physics Letters*. 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: <http://dx.doi.org/10.1016/j.cplett.2016.08.002> ; SCOPUS ; WOS ; MLJ: CCC:000384787600023.

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Ohlas: zahraničný
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- [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 *Journal of Molecular Modeling*, 2019, 25, 2, pp. ISSN 16102940., Registrované v: SCOPUS, WOS, CC
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Ohlas: zahraničný
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Ohlas: zahraničný

V3_07

ANTUŠEK, Andrej - BLAŠKO, M. - URBAN, Miroslav - NOGA, Pavol - KISIĆ, D. - NENADOVIĆ, M. - LONČAREVIĆ, D. - RAKOČEVIĆ, Z. Density functional theory modeling of C-Au chemical bond formation in gold implanted polyethylene. In *Physical Chemistry Chemical Physics*. Vol. 19, iss. 42 (2017), s. 28897-28906. ISSN 1463-9076 (2017: 3.906 - IF, Q1 - JCR Best Q, 1.686 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1039/c7cp05637k ; SCOPUS: 2-s2.0-85032816209 ; WOS: 000414243300041 ; CC: 000414243300041 ; MLJ.

Kategória publikácie do 2021: ADC

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- [1] GUPTA, Ritu - JASH, Priyajit - SACHAN, Pradeep - BAYAT, Akhtar - SINGH, Vikram - MONDAL, Prakash Chandra. Electrochemical Potential-Driven High-Throughput Molecular Electronic and Spintronic Devices: From Molecules to Applications. In *Angewandte Chemie International Edition*, 2021-12-20, 60, 52, pp. 26904-26921. ISSN 14337851., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
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Ohlas: zahraničný

V3_08

ANTUŠEK, Andrej - REPISKÝ, Michal - JASZUNSKI, Michal - JACKOWSKI, Karol - MAKULSKI, Włodzimierz - MISIAK, Maria. Nuclear magnetic dipole moment of Bi-209 from NMR experiments. In *Physical Review A*. Vol. 98, iss. 5 (2018), s. 052509(7). ISSN 2469-9926 (2018: 2.907 - IF, Q2 - JCR Best Q, 1.268 - SJR, Q1 - SJR Best Q). V databáze: DOI:

	<p>10.1103/PhysRevA.98.052509 ; WOS: 000450547000005 ; CC: 000450547000005 ; SCOPUS: 2-s2.0-85057176602.</p> <p>Kategória publikácie do 2021: ADC</p> <p>Ohlasy:</p> <ol style="list-style-type: none"> [1] INDELICATO, P. QED tests with highly charged ions. In <i>JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS</i>, 2019, vol. 52, no. 23, pp. ISSN 0953-4075., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný [1] FELLA, Verena - SKRIPNIKOV, Leonid, V - NOERTERSHAEUSER, Wilfried - BUCHNER, Magnus R. - DEUBNER, H. Lars - KRAUS, Florian - PRIVALOV, Alexei F. - SHABAEV, Vladimir M. - VOGEL, Michael. Magnetic moment of Pb-207 and the hyperfine splitting of Pb-207(81+). In <i>PHYSICAL REVIEW RESEARCH</i>, 2020, vol. 2, no. 1, pp., Registrované v: WOS Ohlas: zahraničný
V3_09	<p>ANTUŠEK, Andrej - REPISKÝ, Michal. NMR absolute shielding scales and nuclear magnetic dipole moments of transition metal nuclei. In <i>Physical Chemistry Chemical Physics</i>. Vol.22. iss. 13 (2020), s. 1-12. ISSN 1463-9076 (2020: 3.676 - IF, Q1 - JCR Best Q, 1.053 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1039/DOCP00115E ; SCOPUS: 2-s2.0-85083041509 ; WOS: 000524512700027 ; CC: 000524512700027.</p> <p>Kategória publikácie do 2021: ADC</p> <p>Ohlasy:</p> <ol style="list-style-type: none"> [1] MAKULSKI, Włodzimierz. Explorations of magnetic properties of noble gases: The past, present, and future. In <i>Magnetochemistry</i>, 2020, 6, 4, pp. 1-20., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný [1] PROSNYAK, S. D. - SKRIPNIKOV, L. V. Effect of nuclear magnetization distribution within the Woods-Saxon model: Hyperfine splitting in neutral Tl. In <i>Physical Review C</i>, 2021, 103, 3, pp. ISSN 24699985., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný
V3_10	<p>BLAŠKO, Martin - MACH, Pavel - ANTUŠEK, Andrej - URBAN, Miroslav. DFT Modeling of Cross-Linked Polyethylene: Role of Goll Atoms and Dispersion Interactions. In <i>Journal of Physical Chemistry A</i>. Vol. 122, Iss. 5 (2018), s. 1496-1503. ISSN 1089-5639 (P) (2018: 2.641 - IF, Q2 - JCR Best Q, 0.969 - SJR, Q1 - SJR Best Q). V databáze: CC: CCC:000424954700035 ; WOS ; SCOPUS ; MLJ.</p> <p>Kategória publikácie do 2021: ADC</p> <p>Ohlasy:</p> <ol style="list-style-type: none"> [1] AKBARIAN, Dooman - HAMED, Hossein - DAMIRCHI, Behzad - YILMAZ, Dundar E. - PENROD, Kathryn - WOODWARD, W. H. Hunter - MOORE, Jonathan - LANAGAN, Michael T. - VAN DUIN, Adri C.T. Atomistic-scale insights into the crosslinking of polyethylene induced by peroxides. In <i>Polymer</i>, 2019, 183, pp. ISSN 00323861., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný [1] THOMAS, Jince - JOSEPH, Blessy - JOSE, Josmin P. - MARIA, Hanna J. - MAIN, Priyanka - ALI RAHMAN, Azerai - FRANCIS, Bejoy - AHMAD, Zakiah - THOMAS, Sabu. Recent Advances in Cross-linked Polyethylene-based Nanocomposites for High Voltage Engineering Applications: A Critical Review. In <i>Industrial and Engineering Chemistry Research</i>, 2019, 58, 46, pp. 20863-20879. ISSN 08885885., Registrované v: SCOPUS, WOS Ohlas: zahraničný [1] AKBARIAN, Dooman - GANESHAN, Karthik - WOODWARD, W. H. Hunter - MOORE, Jonathan - VAN DUIN, Adri C.T. Atomistic-scale insight into the polyethylene electrical breakdown: An eReaxFF molecular dynamics study. In <i>Journal of Chemical Physics</i>, 2021, 154, 2, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný [1] MANNODI-KANAKITHODI, Arun - KUMAR, Rishi E. - FENNING, David P. - CHAN, Maria K.Y. First principles modeling of polymer encapsulant degradation in Si photovoltaic modules. In <i>Physical Chemistry Chemical Physics</i>, 2021, 23, 17, pp. 10357-10364. ISSN 14639076., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný
V3_11	<p>HARDING, R.D. - PALLADA, S. - CROESE, J. - ANTUŠEK, Andrej - BARANOWSKI, Michal - BISSELL, M.L. - CERATO, L. - DZIUBINSKA - KÜHN, K.M. - GINS, W. - GUSTAFSSON, F.P. - JAVAJI, A. - JOLIVET, R.B. - KANELAKOPOULOS, A. - KARG, B. - KEMPKA, M. - KOCMAN, V. - KOZÁK, M. - KULESZ, K. - MADURGA FLORES, M. - NEYENS, G. - PIETRZYK, R. - PLAVEC, J. - POMORSKI, M. - SKRZYPCZAK, Aleksandra - WAGENKNECHT, P. - WIENHOLTZ, F. - WOLAK, J. - XU, Z. - ZAKOUCKY, D. - KOWALSKA, M. Magnetic moments of short-lived nuclei with part-per-million accuracy. Paving the way for applications of β-detected NMR in chemistry and biology. In <i>PHYSICAL REVIEW X</i>. Vol. 10, iss. 4 (2020), s.1-15. ISSN 2160-3308 (2020: 15.762 - IF, Q1 - JCR Best Q, 7.940 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1103/PhysRevX.10.041061 ; SCOPUS: 2-s2.0-85098574792 ; WOS: 000602855000001 ; CC: 000602855000001.</p> <p>Kategória publikácie do 2021: ADC</p> <p>Ohlasy:</p> <ol style="list-style-type: none"> [1] NÖRTERSÄUSER, W. - SURZHYKOV, A. - SÁNCHEZ, R. - BOTERMANN, B. - GWINNER, G. - HUBER, G. - KARPUK, S. - KÜHL, T. - NOVOTNY, C. - REINHARDT, S. - SAATHOFF, G. - STÖHLKER, T. - WOLF, A. Polarization-dependent disappearance of a resonance signal: Indication for optical pumping in a storage ring? In <i>Physical Review Accelerators and Beams</i>, 2021, 24, 2, pp., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný [1] KIMURA, Y. - MIHARA, M. - MATSUTA, K. - FUKUDA, M. - OTANI, Y. - TAKAYAMA, G. - IZUMIKAWA, T. - NOGUCHI, N. - OGOSE, M. - SATO, M. - TAKATSU, K. - OHTSUBO, T. - TAKAHASHI, H. - MOMOTA, S. - OKUMURA, H. - MORIGUCHI, T. - OZAWA, A. - KITAGAWA, A. - SATO, S. Development of a small Beta-NMR system using Halbach Array permanent magnet. In <i>Hyperfine Interactions</i>, 2022-12-01, 243, 1, pp. ISSN 03043843., Registrované v: SCOPUS Ohlas: zahraničný

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Ohlas: zahraničný

V3_12

JACKOWSKI, K. - MAKULSKI, W. - SZYPROWSKA, Anna - ANTUŠEK, Andrej - JASZUNSKI, Michal - JUŠELIUS, Jonas. NMR shielding constants in BF₃ and magnetic dipole moments of B-11 and B-10 nuclei. In *Journal of Chemical Physics*. Vol. 130 (2009), s.044309. ISSN 0021-9606 (2009: 3.093 - IF, Q1 - JCR Best Q, 2.040 - SJR, Q1 - SJR Best Q). V databáze: WOS ; SCOPUS.

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Ohlas: zahraničný

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Ohlas: zahraničný

4. [1] OH, Se-Woung - WEISS, Joseph W. E. - KERNEGHAN, Phillip A. - KOROBKOV, Ilia - MALY, Kenneth E. - BRYCE, D. L. Solid-state ¹¹B and ¹³C NMR, IR and X-ray crystallographic characterization of selected arylboronic acids and their catechol cyclic esters. In *Magnetic resonance in chemistry*, 2012, vol. 50, iss. 5, s.388-401.

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

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Ohlas: zahraničný

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Ohlas: zahraničný

V3_13

JACKOWSKI, K. - MAKULSKI, W. - SZYPROWSKA, Anna - ANTUŠEK, Andrej - JASZUNSKI, Michal. Temperature dependence of the ¹J((BF)-B-11-F-19) spin-spin coupling in BF₃ molecule. In *Magnetic resonance in chemistry*. Vol. 47, Iss. 10 (2009), s.857-861. ISSN 0749-1581 (2009: 1.612 - IF, Q2 - JCR Best Q, 0.651 - SJR, Q2 - SJR Best Q). V databáze: SCOPUS ; WOS.

Katégoria publikácie do 2021: ADC

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Ohlas: zahraničný

2. [1] PERRAS, F. A. - BRYCE, D. L. A ZORA-DFT and NLMO study of the one-bond fluorine-X indirect nuclear spin-spin coupling tensors for various VSEPR geometries. In *Canadian journal of chemistry = JOURNAL CANADIEN DE CHIMIE*, 2011, vol. 89, iss. 7, s.789-802.

Ohlas: zahraničný

3. [1] FABER, Rasmus - KAMINSKY, Jakub - SAUER, Stephan P A. Rovibrational and temperature effects in theoretical studies of NMR parameters. In *New Developments in NMR*, 2016, Issue 6, pp. 218-266. ISSN 2044-253X., Registrované v: SCOPUS

Ohlas: zahraničný

4. [1] JAMESON, Cynthia J. Fundamental intramolecular and intermolecular information from NMR in the gas phase. In *New Developments in NMR*, 2016, Issue 6, pp. 1-51. ISSN 2044-253X., Registrované v: WOS, SCOPUS

Ohlas: zahraničný

5. [1] KRIVDIN, Leonid B. Computational aspects of F-19 NMR. In *RUSSIAN CHEMICAL REVIEWS*, 2020, vol. 89, no. 10, pp. 1040-1073. ISSN 0036-021X., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

JASZUNSKI, Michal - ANTUŠEK, Andrej - GARBACZEWSKI, Piort - JACKOWSKI, K. - MAKULSKI, W. - WILCZEK, M. The determination of accurate nuclear magnetic dipole moments and direct measurement of NMR shielding constants. In *Progress in Nuclear Magnetic Resonance Spectroscopy*. Vol. 67, November 2012 (2012), s.49-63. ISSN 0079-6565 (2012: 6.022 - IF, Q1 - JCR Best Q, 1.974 - SJR, Q1 - SJR Best Q). V databáze: WOS ; SCOPUS.

Kategória publikácie do 2021: ADC

Ohlasy:

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Ohlas: zahraničný

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Ohlas: zahraničný

3. [1] MALDONADO, Alejandro F. - AUCAR, Gustavo A. Relativistic and electron-correlation effects on the nuclear magnetic resonance shieldings of molecules containing tin and lead atoms. In *Journal of Physical Chemistry A*, 2014, vol. 118, iss. 36, s.7863-7875., Registrované v: CC

Ohlas: zahraničný

4. [1] MÜLLER, H. S. P. - SPEZZANO, S. - BIZZOCCHI, L. - GOTTLIEB, C. A. - DEGLI ESPOSTI, C. - MCCARTHY, M. C. Rotational spectroscopy of isotopologues of silicon monoxide, SiO, and spectroscopic parameters from a combined fit of rotational and rovibrational data. In *Journal of Physical Chemistry A*, 2013, vol. 117, iss. 50, s.13843-13854.

Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

7. [1] JAREMKO, Lukasz - Jaremko, Mariusz - Buczek, Aneta - Broda, Malgorzata A. - Kupka, Teobald - Jackowska, Karol. H-1 and C-13 shielding measurements in comparison with DFT calculations performed for two 2-(acetyloamino)-N,N-dimethyl-3-phenylacrylamide isomers. In *CHEMICAL PHYSICS LETTERS*, 2015, vol. 627, no., pp. 1-6. ISSN 0009-2614., Registrované v: CC, SCOPUS, WOS

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

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Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

17. [1] INDELICATO, P. QED tests with highly charged ions. In *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR*

AND OPTICAL PHYSICS, 2019, vol. 52, no. 23, pp. ISSN 0953-4075., Registrované v: WOS, CC, SCOPUS
 Ohlas: zahraničný

18. [1] HALBERT, Loïc - OLEJNICZAK, Małgorzata - VALLET, Valérie - SEVERO PEREIRA GOMES, André. Investigating solvent effects on the magnetic properties of molybdate ions (MoO₄²⁻) with relativistic embedding. In *International Journal of Quantum Chemistry*, 2020, 120, 21, pp. ISSN 00207608., Registrované v: SCOPUS, WOS, CC
 Ohlas: zahraničný

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 Ohlas: zahraničný

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 Ohlas: zahraničný

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 Ohlas: zahraničný

22. [1] KEHL, Annemarie - HILLER, Markus - HECKER, Fabian - TKACH, Igor - DECHERT, Sebastian - BENNATI, Marina - MEYER, Andreas. Resolution of chemical shift anisotropy in 19F ENDOR spectroscopy at 263 GHz/9.4 T. In *Journal of Magnetic Resonance*, 2021, 333, pp. ISSN 10907807., Registrované v: SCOPUS, WOS, CC
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 Ohlas: zahraničný

24. [1] COLOMBO JOFRÉ, Mariano T. - KOZIOL, Karol - AUCAR, I. Agustín - GAUL, Konstantin - BERGER, Robert - AUCAR, Gustavo A. Relativistic and QED corrections to one-bond indirect nuclear spin-spin couplings in X 2 2 + and X 3 2 + ions (X = Zn, Cd, Hg). In: *Journal of Chemical Physics*, 2022-08-14, 157, 6, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC
 Ohlas: zahraničný

V3_15 JASZUNSKI, Michal - ANTUŠEK, Andrej - DEMISSIE, T. B. - KOMOROVSKY, Stanislav - REPISKY, M. - RUUD, K. Indirect NMR spin-spin coupling constants in diatomic alkali halides. In *Journal of Chemical Physics*. Vol. 145, iss. 24 (2016), article number 244308. ISSN 0021-9606 (2016: 2.965 - IF, Q2 - JCR Best Q, 1.486 - SJR, Q1 - SJR Best Q). V databáze: DOI: DOI: 10.1063/1.4972892 ; SCOPUS ; WOS ; MLJ: CCC:000392174800025.

Kategória publikácie do 2021: ADC

Ohlasy:

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 Ohlas: zahraničný
2. [1] YOSHIZAWA, Terutaka. On the development of the exact two-component relativistic method for calculating indirect NMR spin-spin coupling constants. In *Chemical Physics*, 2019, 518, pp. 112-122. ISSN 03010104., Registrované v: SCOPUS, WOS, CC
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 Ohlas: zahraničný
4. [1] OLIVEIRA, João P.C. - RIVELINO, Roberto. Linear response of the indirect J-coupling alternation to the energy gap of increasing π -conjugated oligomers. In *International Journal of Quantum Chemistry*, 2021, 121, 4, pp. ISSN 00207608., Registrované v: SCOPUS
 Ohlas: zahraničný

V3_16 MÜLLER, Yann L. - JEURGENS, Lars P.H. - ANTUŠEK, Andrej - TURLO, Vladyslav. Atomistic Assessment of Melting Point Depression and Enhanced Interfacial Diffusion of Cu in Confinement with AlN. In *ACS Applied Materials & Interfaces*. Vol. 14, iss. 22 (2022), s. 26099-26115. ISSN 1944-8244 (2020: 9.229 - IF, Q1 - JCR Best Q, 2.535 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1021/acsmi.2c01347 ; SCOPUS: 2-s2.0-85131746480 ; WOS: 000810020300001 ; CC: 000810020300001.

Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC

V3_17 OLEJNICZAK, Małgorzata - ANTUŠEK, Andrej - JASZUNSKI, Michal. Relativistic frozen density embedding calculations of solvent effects on the nuclear magnetic resonance shielding constants of transition metal nuclei. In *International Journal of Quantum Chemistry*. Vol. 121, iss. 22 (2021), s. 1-13. ISSN 0020-7608 (2020: 2.444 - IF, Q2 - JCR Best Q, 0.484 - SJR, Q2 - SJR Best Q). V databáze: DOI: 10.1002/qua.26789 ; SCOPUS: 2-s2.0-85111864393 ; WOS: 000681364200001 ; CC: 000704902300002.

Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC

V3_18 PIGOZZI, G. - ANTUŠEK, Andrej - JANCZAK - RUSCH, J. - PARLINSKA - WOJTAN, M. - PASSERONE, D. - PIGNEDOLI, Antonio - BISSIG, V. - PATSCHEIDER, J. - JEURGENS, L.P.H. Phase constitution and interface structure of nano-sized Ag-Cu/AlN multilayers: Experiment and ab initio modeling. In *Applied Physics Letters*. s.81602-81602. ISSN 0003-6951 (2012: 3.794 -

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Ohlas: zahraničný

V3_19

RAAB, J. - ANTUŠEK, Andrej - BISKUPIČ, Stanislav - URBAN, Miroslav. A coupled cluster study of van der Waals interaction of the He atom with CN, NO and O2 radicals. In *Collection of Czechoslovak Chemical Communications*. 69 (2004), s.nestr. ISSN 0010-0765 (2004: 1.062 - IF, Q2 - JCR Best Q). V databáze: WOS ; SCOPUS.

Kategória publikácie do 2021: ADC

Ohlasy:

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Ohlas: domáci
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Ohlas: zahraničný

V3_20

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 (2020: 3.676 - IF, Q1 - JCR Best Q, 1.053 - 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

HURAJT, Andrej - ZNAVA, Martin - KARG, Beatrice - MADDAH, Mina - KOWALSKA, Magdalena - ANTUŠEK, Andrej. NMR shielding calculations of beta-NMR probe nuclei in ionic liquids. 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. 63. 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

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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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ANTUŠEK, Andrej - JASZUNSKI, Michal - RIZZO, Antonio. Ab initio study of interaction-induced NMR shielding constants in mixed rare gas dimers. In *Journal of Chemical Physics*. Vol. 126 (2007), s.074303-1/074303-9. ISSN 0021-9606 (2007: 3.044 - IF, Q1 - JCR Best Q, 2.245 - SJR, Q1 - SJR Best Q). V databáze: WOS ; SCOPUS.

Kategória 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

11. [1] Makulski, Włodzimierz S. 129Xe and 131Xe nuclear magnetic dipole moments from gas phase NMR spectra. In *Magnetic Resonance in Chemistry*, 2015, 53, 4, pp. 273-279. ISSN 0749-1581., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

17. [1] ZALESNY, Robert - MEDVED, Miroslav - GÓRA, Robert W. - REIS, Heribert - LUIS, Josep M. Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. In *Physical Chemistry Chemical Physics*, 2018, 20, 30, pp. 19841-19849. ISSN 1463-9076., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

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Ohlas: zahraničný

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Ohlas: zahraničný

20. [1] WEHRLI, Dominik - SPYSZKIEWICZ-KACZMAREK, Anna - PUCHALSKI, Mariusz - PACHUCKI, Krzysztof. QED Effect on the Nuclear Magnetic Shielding of He 3. In *Physical Review Letters*, 2021-12-24, 127, 26, pp. ISSN 00319007., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

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ANTUŠEK, Andrej - URBAN, Miroslav - SADLEJ, A.J. Lone pair interactions with coinage metal atoms: Weak van der Waals complexes of the coinage metal atoms with water and ammonia. In *Journal of Chemical Physics*. Vol. 119, iss.14 (2003), s.7247-7262. ISSN 0021-9606 (2003: 2.950 - IF, Q1 - JCR Best Q, 2.275 - SJR, Q1 - SJR Best Q). V databáze: WOS ; SCOPUS. Kategória 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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