

Riešiteľ	DERZSI Mariana
Pozícia na projekte	Vedecko-výskumný pracovník
Vedecké identifikátory	WoS (Researcher ID): S-9358-2017, Scopus (AuthorID): 26535817400, ORCID: 0000-0002-4404-0392
Vedecké zameranie	počítačové modelovanie kryštálovej, elektrónovej a fonónovej štruktúry komplexných materiálov z prvých princípov
Publikačná činnosť s ohlasmí (aktuálne k 31.10.2022)	
V2 Vedecký výstup publikačnej činnosti ako časť editovanej knihy alebo zborníka	
V2_01	FERENČÍK, Filip - HALANDA, Juraj - KUSÝ, Martin - SHEN, Tielong - VAŇA, Dušan - BEŇO, Matúš - DERZSI, Mariana - NOGA, Pavol. Ion beam synthesis of high oxidation state palladium oxide nanoparticles. In <i>Applied Nuclear Physics Conference 2021 : September 12-16, Prague, Czech Republic</i> . 1. vyd. Praha : AMCA, 2021, S. 81. Typ výstupu: abstrakt z podujatia; Výstup: zahraničný; Kategória publikácie do 2021: AFG
V2_02	TOKÁR, Kamil - UHLIAR, Matej - DERZSI, Mariana. The first silver chloride with rare silver clusters from ab initio study. In <i>CESTC 2022 : 18th Central European Symposium on Theoretical Chemistry 2022, 7-10 September 2022, Balatonszárszód, Hungary</i> . 1. vyd. Budapešť : Hungarian Chemical Society, 2022, S. 55. ISBN 978-615-6018-10-6. Typ výstupu: abstrakt z podujatia; Výstup: zahraničný; Kategória publikácie do 2021: AFG
V3 Vedecký výstup publikačnej činnosti z časopisu	
V3_01	BANDARU, Subrahmanyam - DERZSI, Mariana - GRZELAK, Adam - LORENZANA, Jose - GROCHALA, Wojciech. Fate of doped carriers in silver fluoride cuprate analogs. In <i>Physical Review Materials</i> . Vol. 5, iss. 6 (2021), s. 1-5. ISSN 2475-9953 (2021: 3.980 - IF, Q2 - JCR Best Q, 1.200 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1103/PhysRevMaterials.5.064801 ; WOS: 000661933600003 ; SCOPUS: 2-s2.0-85101522170 ; CC: 000661933600003. Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC Ohlasy: 1. [1] LIU, Xiaoqiang - PANDEY, Shishir K. - FENG, Ji. Silver(II) route to unconventional superconductivity. In <i>Physical Review B</i> , 2022-04-01, 105, 13, pp. ISSN 24699950., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný
V3_02	DERZSI, Mariana - GRZELAK, Adam - KONDRATIUK, Pawel - TOKÁR, Kamil - GROCHALA, Wojciech. Quest for Compounds at the Verge of Charge Transfer Instabilities: The Case of Silver(II) Chloride. In <i>NEW SZP GEN: Crystals</i> . Vol. 9, iss. 8 (2019), s. 1-19. ISSN 2073-4352 (2019: 2.404 - IF, Q2 - JCR Best Q, 0.594 - SJR, Q2 - SJR Best Q). V databáze: DOI: 10.3390/cryst9080423 ; WOS: 000482996000025 ; CC: 000482996000025 ; SCOPUS: 2-s2.0-85073295099. Kategória publikácie do 2021: ADC Ohlasy: 1. [1] HERMANN, Andreas - KURZYDŁOWSKI, Dominik. First-Principles Prediction of Structures and Properties in Crystals. In <i>CRYSTALS</i> , 2019, vol. 9, no. 9, pp. ISSN 2073-4352., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 2. [1] JOVEN-SANCHO, Daniel - BAYA, Miguel - FALVELLO, Larry R. - MARTÍN, Antonio - ORDUNA, Jesús - MENJÓN, Babil. Stability of AgIII towards Halides in Organosilver(III) Complexes. In <i>Chemistry A European Journal</i> , 2021, 27, 50, pp. 12796-12806. ISSN 09476539., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný 3. [1] ROSTAMI, Samare - GHASEMI, S. Alireza - GOEDECER, Stefan. Novel polymorphs and polytypes of lithium chloride from structure predictions based on charge equilibration via neural network technique. In <i>Physical Review Materials</i> , 2021, 5, 12, pp., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný
V3_03	DERZSI, Mariana - UHLIAR, M. - TOKÁR, Kamil. Ag6Cl4: the first silver chloride with rare Ag-6 clusters from an ab initio study. In <i>Chemical Communications</i> . Vol. 57, iss. 79 (2021), s. 186-189. ISSN 1359-7345 (2021: 6.065 - IF, Q2 - JCR Best Q, 1.513 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1039/d1cc03426j ; SCOPUS: 2-s2.0-85116612688 ; WOS: 000695618600001 ; CC: 000703714000001. Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC Ohlasy: 1. [1] GRZELAK, Adam - GROCHALA, Wojciech. Stability of hypothetical AgsupII/supClinf2/inf polymorphs under high pressure, revisited: a computational study. In <i>Scientific Reports</i> , 2022-12-01, 12, 1, pp., Registrované v: SCOPUS Ohlas: zahraničný
V3_04	DERZSI, Mariana - TOKÁR, Kamil - PIEKARZ, Przemyslaw - GROCHALA, Wojciech. Charge ordering mechanism in silver difluoride. In <i>Physical Review B</i> . Vol. 105, iss. 8 (2022), s.1-6. ISSN 2469-9950 (2021: 3.908 - IF, Q2 - JCR Best Q, 1.537 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1103/PhysRevB.105.L081113 ; SCOPUS: 2-s2.0-85126052416 ; WOS: 000766640700006 ; CC: 000766640700006. Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC Ohlasy: 1. [1] LIU, Xiaoqiang - PANDEY, Shishir K. - FENG, Ji. Silver(II) route to unconventional superconductivity. In <i>Physical Review B</i> , 2022-04-01, 105, 13, pp. ISSN 24699950., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

2. [1] PROSNIKOV, M. A. Magnons in AgF₂, AgCuF₄, and AgNiF₄. In *Journal of Magnetism and Magnetic Materials*, 2022-09-01, 557, pp. ISSN 03048853., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

V3_05

DOMANSKI, Mateusz - DERZSI, Mariana - GROCHALA, Wojciech. Theoretical study of ternary silver fluorides AgMF₄ (M = Cu, Ni, Co) formation at pressures up to 20 GPa. In *RSC Advances*. Vol. 11, iss. 41 (2021), s.801-810. ISSN 2046-2069 (2021: 4.036 - IF, Q2 - JCR Best Q, 0.667 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1039/d1ra04970d ; SCOPUS: 2-s2.0-85111614414 ; CC: 000678294800065 ; WOS: 000678294800065.

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

Ohlasy:

1. [1] PROSNIKOV, M. A. Magnons in AgF₂, AgCuF₄, and AgNiF₄. In *Journal of Magnetism and Magnetic Materials*, 2022-09-01, 557, pp. ISSN 03048853., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

V3_06

GAWRACZYŃSKI, Jakub - KURZYDŁOWSKI, Dominik - EWINGS, Russel A. - BANDARU, Subrahmanyam - GADOMSKI, Wojciech - MAZEJ, Zoran - RUANI, Giampiero - BERGENTI, Ilaria - JARON, Tomasz - OZAROWSKI, Andrew - HILL, Stephen - LESZCZYŃSKI, Piotr J. - TOKÁR, Kamil - DERZSI, Mariana - BARONE, Paolo - WOHLFELD, Krzysztof - LORENZANA, Jose - GROCHALA, Wojciech. Silver route to cuprate analogs. In *Proceedings of the national academy of sciences of the United States of America*. Vol. 116, iss. 5 (2019), s. 1495-1500. ISSN 0027-8424 (2019: 9.412 - IF, Q1 - JCR Best Q, 5.165 - SJR, Q1 - SJR Best Q). V databáze: CC: 000456944600011 ; WOS: 000456944600011 ; SCOPUS: 2-s2.0-85060803846 ; DOI: 10.1073/pnas.1812857116.

Kategória publikácie do 2021: ADC

Ohlasy:

1. [1] MILLER, Clark - BOTANA, Antia Sanchez. Cupratelike electronic and magnetic properties of layered transition-metal difluorides from first-principles calculations. In *PHYSICAL REVIEW B*, 2020, vol. 101, no. 19, pp. ISSN 2469-9950., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

2. [1] KIM, Bongjae - KHMELEVSKYI, Sergii - FRANCHINI, Cesare - MAZIN, I. I. - KIM, Kyoo. SrRuO₃-SrTiO₃ heterostructure as a possible platform for studying unconventional superconductivity in Sr₂RuO₄. In *PHYSICAL REVIEW B*, 2020, vol. 101, no. 22, pp. ISSN 2469-9950., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

3. [1] MATASOV, Anton - KRASAVINA, Varvara. Prediction of critical temperature and new superconducting materials. In *SN APPLIED SCIENCES*, 2020, vol. 2, no. 9, pp. ISSN 2523-3963., Registrované v: WOS, SCOPUS

Ohlas: zahraničný

4. [1] BERNARDINI, F. - OLEVANO, V - BLASE, X. - CANO, A. Infinite-layer fluoro-nickelates as a (9)model materials. In *JOURNAL OF PHYSICS-MATERIALS*, 2020, vol. 3, no. 3, pp., Registrované v: WOS

Ohlas: zahraničný

5. [1] ZHANG, Junjie - TAO, Xutang. Review on quasi-2D square planar nickelates. In *CrystEngComm*, 2021, 23, 18, pp. 3249-3264., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

6. [1] BOTANA, A. S. - BERNARDINI, F. - CANO, A. Nickelate Superconductors: An Ongoing Dialog between Theory and Experiments. In *Journal of Experimental and Theoretical Physics*, 2021, 132, 4, pp. 618-627. ISSN 10637761., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

7. [1] BERNARDINI, F. - DEMOURGUES, A. - CANO, A. Single-layer T'-type nickelates: Ni¹⁺ is Ni¹⁺. In *Physical Review Materials*, 2021, 5, 6, pp., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

8. [1] RYBIN, Nikita - NOVOSELOV, Dmitry Y. - KOROTIN, Dmitry M. - ANISIMOV, Vladimir I. - OGANOV, Artem R. Novel copper fluoride analogs of cuprates. In *Physical Chemistry Chemical Physics*, 2021, 23, 30, pp. 15989-15993. ISSN 14639076., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

9. [1] LILIA, Boeri - HENNIG, Richard - HIRSCHFELD, Peter - PROFETA, Gianni - SANNA, Antonio - ZUREK, Eva - PICKETT, Warren E. - AMSLER, Maximilian - DIAS, Ranga - EREMETS, Mikhail, I - HEIL, Christoph - HEMLEY, Russell J. - LIU, Hanyu - MA, Yanming - PIERLEONI, Carlo - KOLMOGOROV, Aleksey N. - RYBIN, Nikita - NOVOSELOV, Dmitry - ANISIMOV, Vladimir - OGANOV, Artem R. - PICKARD, Chris J. - BI, Tiange - ARITA, Ryotaro - ERREA, Ion - PELLEGRINI, Camilla - REQUIST, Ryan - GROSS, E. K. U. - MARGINE, Elena Roxana - XIE, Stephen R. - QUAN, Yundi - HIRE, Ajinkya - FANFARILLO, Laura - STEWART, G. R. - HAMLIN, J. J. - STANEV, Valentin - GONNELLI, Renato S. - PIATTI, Erik - ROMANIN, Davide - DAGHERO, Dario - VALENTI, Roser. The 2021 room-temperature superconductivity roadmap. In *JOURNAL OF PHYSICS-CONDENSED MATTER*, 2022, vol. 34, no. 18, pp. ISSN 0953-8984., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

10. [1] SANCHEZ-MOVELLAN, Ines - MORENO-CEBALLOS, Jorge - GARCIA-FERNANDEZ, Pablo - ARAMBURU, Jose Antonio - MORENO, Miguel. New Ideas for Understanding the Structure and Magnetism in AgF₂: Prediction of Ferroelasticity. In *CHEMISTRY-A EUROPEAN JOURNAL*, 2021, vol. 27, no. 54, pp. 13582-13590. ISSN 0947-6539., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

11. [1] NOMURA, Yusuke - ARITA, Ryotaro. Superconductivity in infinite-layer nickelates. In *REPORTS ON PROGRESS IN PHYSICS*, 2022, vol. 85, no. 5, pp. ISSN 0034-4885., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

12. [1] PROSNIKOV, M. A. Magnons in AgF₂, AgCuF₄, and AgNiF₄. In *Journal of Magnetism and Magnetic*

	<p>Materials, 2022-09-01, 557, pp. ISSN 03048853., Registrované v: SCOPUS, WOS, CC 13. [1] LIU, Xiaoqiang - PANDEY, Shishir K. - FENG, Ji. Silver(II) route to unconventional superconductivity. In <i>Physical Review B</i>, 2022-04-01, 105, 13, pp. ISSN 24699950., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný</p>
V3_07	<p>GROCHALA, Wojciech - DERZSI, Mariana. High-temperature superconductivity as viewed from the maximum hardness principle. In <i>Journal of molecular modeling</i>. Vol. 24, iss. 9 (2018), s. 1-7. ISSN 1610-2940 (2018: 1.335 - IF, Q3 - JCR Best Q, 0.370 - SJR, Q3 - SJR Best Q). V databáze: CC: 000441800200002 ; WOS: 000441800200002 ; MLJ ; SCOPUS. Kategória publikácie do 2021: ADC</p>
V3_08	<p>GRZELAK, Adam - DERZSI, Mariana - GROCHALA, Wojciech. Defect Trapping and Phase Separation in Chemically Doped Bulk AgF₂. In <i>Inorganic Chemistry</i>. Vol.60, iss. 3 (2021), s. 1561-1570. ISSN 0020-1669 (2021: 5.436 - IF, Q1 - JCR Best Q, 1.121 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1021/acs.inorgchem.0c02970 ; SCOPUS: 2-s2.0-85100252150 ; WOS: 000617925100034 ; CC: 000617925100034. Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC Ohlasy: 1. [1] YAMANAKA, Toshiro - OGUMI, Zempachi - ABE, Takeshi. Fluoride Shuttle Battery Reactions of CuF₂: Intermediate Phase for Defluorination. In: <i>JOURNAL OF PHYSICAL CHEMISTRY C</i>, 2022, vol. 126, no. 30, pp. 12361-12369. ISSN 1932-7447., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný</p>
V3_09	<p>GRZELAK, Adam - GAWRACZYŃSKI, Jakub - DERZSI, Mariana - STRUZHKIN, Viktor - SOMAYAZULU, Maddury - GROCHALA, Wojciech. Observation of a New Polyhalide Phase in Ag-Cl₂ System at High Pressure. In <i>Crystals</i>. Vol. 11, iss. 12 (2021), s. 1-9. ISSN 2073-4352 (2021: 2.670 - IF, Q2 - JCR Best Q, 0.459 - SJR, Q2 - SJR Best Q). V databáze: DOI: 10.3390/cryst11121565 ; SCOPUS: 2-s2.0-85121585302 ; WOS: 000741891600001 ; CC: 000741891600001. Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC</p>
V3_10	<p>KOTERAS, Kacper - GAWRACZYŃSKI, Jakub - DERZSI, Mariana - MAZEJ, Zoran - GROCHALA, Wojciech. Lattice Dynamics of KAgF₃ Perovskite, Unique 1D Antiferromagnet. In <i>Chemistry</i>. Vol. 3, iss. 1 (2021), s. 94-103. ISSN 2624-8549 (2021). V databáze: DOI: 10.3390/chemistry3010007 ; WOS: 000708214700007. Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADM Ohlasy: 1. [1] SHAH, Saima Ahmad - HUSAIN, Mudasser - RAHMAN, Nasir - SOHAIL, Mohammad - KHAN, Rajwali - KHAN, Abid Ali - ULLAH, Asad - ABDELMOHSEN, Shaimaa A. M. - ABDELBACKI, Ashraf M. M. - EL-SABROUT, Ahmed M. - ELANSARY, Hosam O. - KHAN, Aurangzeb. Insight into the exemplary structural, elastic, electronic and optical nature of GaBeCl₃ and InBeCl₃: a DFT study. In <i>RSC ADVANCES</i>, 2022, vol. 12, no. 13, pp. 8172-8177., Registrované v: WOS, CC Ohlas: zahraničný 2. [1] KHAN, Hukam - SOHAIL, Mohammad - KHAN, Rajwali - RAMAN, Nasir - ULLAH, Asad - KHAN, Aurangzeb - ALATAWAY, Abed - DEWIDAR, Ahmed Z. - ELANSARY, Hosam O. - YESSOUFOU, Kowiyou. Theoretical Investigations into the Different Properties of Al-Based Fluoroperovskite AIMF₃ (M = Cr, B) Compounds by the TB-MBJ Potential Method. In: <i>MATERIALS</i>, 2022, vol. 15, no. 17, pp., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 3. [1] KHAN, Hukam - SOHAIL, Mohammad - RAHMAN, Nasir - KHAN, Rajwali - ULLAH, Asad - HUSSAIN, Mudassir - KHAN, Aurangzeb - HEGAZY, H. H. Theoretical study of different aspects of Al-based fluoroperovskite AIMF₃/supinf3/inf3(M = Cu, Mn) compounds using TB-MBJ potential approximation method for generation of energy. In: <i>Results in Physics</i>, 2022-11-01, 42, pp., Registrované v: SCOPUS Ohlas: zahraničný</p>
V3_11	<p>KURZYDŁOWSKI, Dominik - DERZSI, Mariana - BARONE, Paolo - GRZELAK, Adam - STRUZHKIN, Viktor - LORENZANA, Jose - GROCHALA, Wojciech. Dramatic enhancement of spin-spin coupling and quenching of magnetic dimensionality in compressed silver difluoride. In <i>Chemical Communications</i>. Vol. 54, iss. 73 (2018), s. 10252-10255. ISSN 1359-7345 (2018: 6.164 - IF, Q1 - JCR Best Q, 2.177 - SJR, Q1 - SJR Best Q). V databáze: WOS: 000444242900037 ; CC: 000444242900037 ; SCOPUS: 2-s2.0-85053287198 ; MLJ ; DOI: DOI: 10.1039/C8CC05002C. Kategória publikácie do 2021: ADC Ohlasy: 1. [1] MILLER, Clark - BOTANA, Antia Sanchez. Cupratelike electronic and magnetic properties of layered transition-metal difluorides from first-principles calculations. In <i>PHYSICAL REVIEW B</i>, 2020, vol. 101, no. 19, pp. ISSN 2469-9950., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný</p>
V3_12	<p>KURZYDŁOWSKI, Dominik - DERZSI, Mariana - ZUREK, Eva - GROCHALA, Wojciech. Fluorides of Silver Under Large Compression**. In <i>Chemistry - A European Journal</i>. Vol. 27, iss. 17 (2021), s. 5536-5545. ISSN 0947-6539 (2021: 5.020 - IF, Q2 - JCR Best Q, 1.343 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1002/chem.202100028 ; SCOPUS: 2-s2.0-85101656218 ; WOS: 000621374100001 ; CC: 000631691600022. Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC Ohlasy: 1. [1] ZHANG, Shoutao - YANG, Qiuping - ZHANG, Xiaohua - ZHAO, Kaixuan - YU, Hong - ZHU, Li - LIU, Hanyu. Crystal structures and superconductivity of lithium and fluorine implanted gold hydrides under high pressures. In <i>Physical Chemistry Chemical Physics</i>, 2021, 23, 38, pp. 21544-21553. ISSN 14639076., Registrované v: SCOPUS, WOS,</p>

CC

Ohlas: zahraničný

- V3_13 PIEKARZ, Przemyslaw - WIŚNIEWSKI, Pawel - DERZSI, Mariana. Structural and electronic properties of Fe monolayer on BaTiO₃(001). In *Journal of Physics: Condensed Matter*. Vol. 30, iss. 36, (2018), s. 1-10. ISSN 0953-8984 (2018: 2.711 - IF, Q2 - JCR Best Q, 0.943 - SJR, Q1 - SJR Best Q). V databáze: WOS: 000442016500001 ; CC: 000442016500001 ; SCOPUS: 2-s2.0-85052725561.
Kategória publikácie do 2021: ADC
- V3_14 PIOMBO, Riccardo - JEZERSKI, Daniel - MARTINS PERIN, Henrique - JARON, Tomasz - GASTIASORO, Maria N. - BARONE, Paolo - TOKÁR, Kamil - PIEKARZ, Przemyslaw - DERZSI, Mariana - MAZEJ, Zoran - ABBATE, Miguel - GROCHALA, Wojciech - LORENZANA, Jose. Strength of correlations in a silver-based cuprate analog. In *Physical Review B*. Vol. 106, iss. 3 (2022), s. 1-12. ISSN 2469-9950 (2021: 3.908 - IF, Q2 - JCR Best Q, 1.537 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1103/PhysRevB.106.035142 ; SCOPUS: 2-s2.0-85135726994 ; WOS: 000834358500003 ; CC: 000834358500003.
Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC
- V3_15 TOKÁR, Kamil - DERZSI, Mariana - GROCHALA, Wojciech. Comparative computational study of antiferromagnetic and mixed-valent diamagnetic phase of AgF₂: Crystal, electronic and phonon structure and p-T phase diagram. In *Computational Materials Science*. Vol. 188, (2021), s.1-10. ISSN 0927-0256 (2021: 3.572 - IF, Q3 - JCR Best Q, 0.777 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1016/j.commatsci.2020.110250 ; SCOPUS: 2-s2.0-85098118677 ; WOS: 000621030500001 ; CC: 000621030500001.
Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC
Ohlasy:
1. [1] LIU, Xiaoqiang - PANDEY, Shishir K. - FENG, Ji. Silver(II) route to unconventional superconductivity. In *Physical Review B*, 2022-04-01, 105, 13, pp. ISSN 24699950., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- V3_16 WEGNER, W. - TOKÁR, Kamil - LORENZANA, Jose - DERZSI, Mariana - GROCHALA, Wojciech. Gigantic work function in layered AgF₂. In *Physical Chemistry Chemical Physics*. Vol. 22, iss. 38 (2020), s. 21809-21815. ISSN 1463-9076 (2020: 3.676 - IF, Q1 - JCR Best Q, 1.053 - SJR, Q1 - SJR Best Q). V databáze: WOS: 000576194400018 ; CC: 000576194400018 ; DOI: 10.1039/d0cp03706k ; SCOPUS: 2-s2.0-85092681891.
Kategória publikácie do 2021: ADC
Ohlasy:
1. [1] SANCHEZ-MOVELLAN, Ines - MORENO-CEBALLOS, Jorge - GARCIA-FERNANDEZ, Pablo - ARAMBURU, Jose Antonio - MORENO, Miguel. New Ideas for Understanding the Structure and Magnetism in AgF₂: Prediction of Ferroelasticity. In *CHEMISTRY-A EUROPEAN JOURNAL*, 2021, vol. 27, no. 54, pp. 13582-13590. ISSN 0947-6539., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
2. [1] DAVYDOV, S. Yu. On the Properties of Two-Dimensional Compounds AgX₂ (X = F, Cl, Br, I). In *Physics of the Solid State*, 2021-11-01, 63, 11, pp. 1633-1637. ISSN 10637834., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
3. [1] PROSNIKOV, M. A. Magnons in AgF₂, AgCuF₄, and AgNiF₄. In *Journal of Magnetism and Magnetic Materials*, 2022-09-01, 557, pp. ISSN 03048853., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný

O2 Odborný výstup publikačnej činnosti ako časť knižnej publikácie alebo zborníka

- O2_01 TOKÁR, Kamil - DERZSI, Mariana - PIEKARZ, Przemyslaw - GROCHALA, Wojciech. Description of charge ordering mechanism in silver difluoride using DFT calculations. In *PSI-K 2022 Conference : 6th general conference for the worldwide PSI-K community, 22-25 August 2022, Lausanne, Switzerland*. 1. vyd, 2022, S. 276.
Typ výstupu: abstrakt z podujatia; Výstup: zahraničný; Kategória publikácie do 2021: BFA

O3 Odborný výstup publikačnej činnosti z časopisu

- O3_01 DERZSI, Mariana. Prekročí nový kandidát rekordne vysoké teploty supravodivosti keramických supravodičov? In *Spektrum*. Roč. 25, č. 5 (2019), s. 3. ISSN 1336-2593.
Kategória publikácie do 2021: BDF
- O3_02 DERZSI, Mariana. Výskumná skupina počítačového modelovania a materiálov na ATRI MTF STU v Trnave. In *HPC FOCUS*. Vol. 2022, (2022), s. 41-57. ISSN 2729-9090 (online).
Typ výstupu: článok; Výstup: domáci; Kategória publikácie do 2021: BDF

I2 Iný výstup publikačnej činnosti ako časť publikácie alebo zborníka

- I2_01 BUJDÁK, Radovan - GAŠPÁRKOVÁ, Michaela - TOKÁR, Kamil - DERZSI, Mariana. Exploring new phases in Ni-O binary system from ab initio. In *2022 Workshop on Recent Developments in Electronic Structure (ES22) : May 31 - June 3, 2022 at Columbia University in the City of New York*. 1. vyd. New York : Columbia University, 2022, S. 1.
Typ výstupu: poster z podujatia; Výstup: zahraničný; Kategória publikácie do 2021: AFK
- I2_02 FABUŠOVÁ, Diana - TOKÁR, Kamil - DERZSI, Mariana. Ab Initio Study of Impact of Pressure and Temperature on Stability and Polymorphism of PdO₂. In *2022 Workshop on Recent Developments in Electronic Structure (ES22) : May 31 - June 3, 2022 at Columbia University in the City of New York*. 1. vyd. New York : Columbia University, 2022, S. 1.
Typ výstupu: poster z podujatia; Výstup: zahraničný; Kategória publikácie do 2021: AFK

- I2_03 FERENČÍK, Filip - HALANDA, Juraj - VAŇA, Dušan - DERZSI, Mariana - NOGA, Pavol. Ion beam synthesis of high oxidation state palladium and copper oxides. In *IBMM 22 : 22th International Conference on ION Beam Modification of Materials, Lisbon, 10-15 July 2022*. 1. vyd. Lisbon : Universidade de Lisboa, 2022, S. 184.
Typ výstupu: časti, ktoré nemožno zaradiť do kategórie V, O, P, U alebo D; Výstup: zahraničný; Kategória publikácie do 2021: AFK
- I2_04 TOKÁR, Kamil - DERZSI, Mariana - PIEKARZ, Przemyslaw - GROCHALA, Wojciech. Charge ordering mechanism in silver difluoride from first principles. In *2022 Workshop on Recent Developments in Electronic Structure (ES22) : May 31 - June 3, 2022 at Columbia University in the City of New York*. 1. vyd. New York : Columbia University, 2022, S. 1.
Typ výstupu: poster z podujatia; Výstup: zahraničný; Kategória publikácie do 2021: AFK
- XXX XXX
_01 ANZOLINI, C. - ANGEL, R. J. - MERLINI, M. - DERZSI, Mariana - TOKÁR, Kamil - MILANI, S. - KREBS, M. Y. - BRENKER, F. E. - NESTOLA, F. - HARRIS, J. W. Depth of formation of CaSiO₃-walsstromite included in super-deep diamonds. In *LITHOS*. Vol. 265, no. (2016), pp. 138-147. V databáze: WOS: 000389283300012 ; DOI: 10.1016/j.lithos2016.09.025.
Ohlasy:
1. [1] GU, Tingting - WANG, Wuyi. Optical defects in milky type IaB diamonds. In *DIAMOND AND RELATED MATERIALS*, 2018, vol. 89, no., pp. 322-329. ISSN 0925-9635., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
2. [1] LIAN, Dongyang - YANG, Jingsui - WIEDENBECK, Michael - DILEK, Yildirim - ROCHOLL, Alexander - WU, Weiwei. Carbon and nitrogen isotope, and mineral inclusion studies on the diamonds from the Pozanti-Karsanti chromitite, Turkey. In *CONTRIBUTIONS TO MINERALOGY AND PETROLOGY*, 2018, vol. 173, no. 9, pp. ISSN 0010-7999., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
3. [1] BULATOV, V. K. - GIRNIS, A. V. - BREY, G. P. - WOODLAND, A. B. - HÖFER, H. E. Ferropicliase crystallization under upper mantle conditions. In *Contributions to Mineralogy and Petrology*, 2019, 174, 5, pp. ISSN 00107999., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
4. [1] MOORE, Andy E. - HELMSTAEDT, Herwart. Evidence for two blue (type IIb) diamond populations. In *Nature*, 2019, 570, 7760, pp. E26-E27. ISSN 00280836., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
5. [1] LIAN, Dongyang - YANG, Jingsui. Ophiolite-Hosted Diamond: A New Window for Probing Carbon Cycling in the Deep Mantle. In *ENGINEERING*, 2019, vol. 5, no. 3, pp. 406-420. ISSN 2095-8099., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
6. [1] LIAN, Dongyang - YANG, Jingsui - LIU, Fei - WU, Weiwei. Diamond Classification, Compositional Characteristics, and Research Progress: A Review. In *Diqiu Kexue Zhongguo Dizhi Daxue Xuebao/Earth Science Journal of China University of Geosciences*, 2019, 44, 10, pp. 3409-3453. ISSN 10002383., Registrované v: SCOPUS
Ohlas: zahraničný
7. [1] TSCHAUNER, Oliver. High-pressure minerals. In *AMERICAN MINERALOGIST*, 2019, vol. 104, no. 12, pp. 1701-1731. ISSN 0003-004X., Registrované v: WOS, SCOPUS, CC
Ohlas: zahraničný
8. [1] FEDORAEVA, Anastasia S. - SHATSKIY, Anton - LITASOV, Konstantin D. The join CaCO₃-CaSiO₃ at 6 GPa with implication to Ca-rich lithologies trapped by kimberlitic diamonds. In *High Pressure Research*, 2019, 39, 4, pp. 547-560. ISSN 08957959., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
9. [1] DE PAUW, Ella - TACK, Pieter - LINDNER, Miles - ASHAUER, Antonia - GARREVOET, Jan - VEKEMANS, Bart - FALKENBERG, Gerald - BRENKER, Frank E. - VINCZE, Laszlo. Highly Sensitive Nondestructive Rare Earth Element Detection by Means of Wavelength-Dispersive X-ray Fluorescence Spectroscopy Enabled by an Energy Dispersive pn-Charge-Coupled-Device Detector. In *ANALYTICAL CHEMISTRY*, 2020, vol. 92, no. 1, pp. 1106-1113. ISSN 0003-2700., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
10. [1] VON DER HEYDEN, Bjorn P. Shedding light on ore deposits: A review of synchrotron X-ray radiation use in ore geology research. In *Ore Geology Reviews*, 2020, 117, pp. ISSN 01691368., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
11. [1] WOODLAND, Alan B. - GIRNIS, Andrei V. - BULATOV, Vadim K. - BREY, Gerhard P. - HÖFER, Heidi E. Breyite inclusions in diamond: Experimental evidence for possible dual origin. In *European Journal of Mineralogy*, 2020, 32, 1, pp. 171-185. ISSN 09351221., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
12. [1] KRZAȚAŁA, Arkadiusz - KRÜGER, Biljana - GALUSKINA, Irina - VAPNIK, Yevgeny - GALUSKIN, Evgeny. Walsstromite, bca₂(Si₃O₉), from rankinite paralava within gehlenite hornfels of the hatrurim basin, negev desert, Israel. In *Minerals*, 2020, 10, 5, pp., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
13. [1] SAGATOVA, Dinara - SHATSKIY, Anton - SAGATOV, Nursultan - GAVRYUSHKIN, Pavel N. - LITASOV, Konstantin D. Calcium orthocarbonate, Ca₂CO₄-Pnma: A potential host for subducting carbon in the transition zone and lower mantle. In *Lithos*, 2020, 370-371, pp. ISSN 00244937., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
14. [1] ZEDGENIZOV, Dmitry - KAGI, Hirioyuki - OHTANI, Eiji - TSUJIMORI, Tatsuki - KOMATSU, Kazuki. Retrograde phases of former bridgmanite inclusions in superdeep diamonds. In *LITHOS*, 2020, vol. 370, no., pp. ISSN 0024-4937., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný

15. [1] TAPPE, Sebastian - STRACKE, Andreas - VAN ACKEN, David - STRAUSS, Harald - LUGUET, Ambre. Origins of kimberlites and carbonatites during continental collision Insights beyond decoupled Nd-Hf isotopes. In *EARTH-SCIENCE REVIEWS*, 2020, vol. 208, no., pp. ISSN 0012-8252., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
16. [1] SOKOLOVA, T. S. - DOROGOKUPETS, P. I. Equations of state for CaSiO₃ phases based on the Helmholtz free energy. In *Journal of Physics: Conference Series*, 2021, 1787, 1, pp. ISSN 17426588., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
17. [1] HOLTSTAM, Dan - CÁMARA, Fernando - KARLSSON, Andreas. Instalment of the margarosane group, and data on walstromite-margarosane solid solutions from the Jakobsberg Mn-Fe deposit, Värmland, Sweden. In *Mineralogical Magazine*, 2021, 85, 2, pp. 224-232. ISSN 0026461X., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
18. [1] YANG, Jingsui - WU, Weiwei - LIAN, Dongyang - RUI, Huichao. Peridotites, chromitites and diamonds in ophiolites. In *NATURE REVIEWS EARTH & ENVIRONMENT*, 2021, vol. 2, no. 3, pp. 198-212., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
19. [1] WANG, Sea Fue - LAI, Bo Cheng - HSU, Yung Fu - LU, Chun An. Dielectric properties of CaO-B₂O₃-SiO₂ glass-ceramic systems in the millimeter-wave frequency range of 20–60 GHz. In *Ceramics International*, 2021, 47, 16, pp. 22627-22635. ISSN 02728842., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
20. [1] SAGATOVA, D. N. - SHATSKIY, A. F. - SAGATOV, N. E. - LITASOV, K. D. Phase Relations in CaSiO₃ System up to 100 GPa and 2500 K. In *GEOCHEMISTRY INTERNATIONAL*, 2021, vol. 59, no. 8, pp. 791-800. ISSN 0016-7029., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
21. [1] LI, Jie - ZHU, Feng - LIU, Jiachao - DONG, Junjie. Reactive Preservation of Carbonate in Earth's Mantle Transition Zone. In *CARBON IN EARTH'S INTERIOR*, 2020, vol. 249, no., pp. 167-177. ISSN 0065-8448., Registrované v: WOS
Ohlas: zahraničný
22. [1] KRIVOVICHEV, S. V. High-pressure silicates: Crystal chemistry and systematics. In *Zapiski Rossiiskogo Mineralogicheskogo Obshchestva*, 2021, 150, 5, pp. 1-78. ISSN 08696055., Registrované v: SCOPUS
Ohlas: zahraničný
23. [1] WANG, Wenzhong - TSCHAUNER, Oliver - HUANG, Shichun - WU, Zhongqing - MENG, Yufei - BECHTEL, Hans - MAO, Ho Kwang. Coupled deep-mantle carbon-water cycle: Evidence from lower-mantle diamonds. In *The Innovation*, 2021-05-28, 2, 2, pp., Registrované v: SCOPUS, WOS
Ohlas: zahraničný
24. [1] DAVER, Lucille - BUREAU, Hélène - BOULARD, Églantine - GAILLOU, Éloïse - CARTIGNY, Pierre - PINTI, Daniele L. - BELHADJ, Oulfa - GUIGNOT, Nicolas - FOY, Eddy - ESTÈVE, Imène - BAPTISTE, Benoit. From the lithosphere to the lower mantle: An aqueous-rich metal-bearing growth environment to form type IIb blue diamonds. In: *Chemical Geology*, 2022-12-20, 613, pp. ISSN 00092541., Registrované v: SCOPUS
Ohlas: zahraničný

- _02 BANDARU, Subrahmanyam - DERZSI, Mariana - LORENZANA, Jose - GROCHALA, Wojciech. Fate of charge carriers in AgF₂. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 233.
Kategória publikácie do 2021: BFA
- _03 BANDARU, Subrahmanyam - DERZSI, Mariana - LORENZANA, Jose - GROCHALA, Wojciech. Polaron formation tendency in AgF₂ with charge carrier doping. In *62. zjazd naukowy polskiego towarzystwa chemicznego : Warszawa, 2-6 september 2019*. 1. vyd, 2019, S. 02-31.
Kategória publikácie do 2021: BFA
- _04 BANDARU, Subrahmanyam - DERZSI, Mariana - LORENZANA, Jose - GROCHALA, Wojciech. Polan formation tendency in AgF₂ with charge carrier doping. In *Online-Vortragstagung für Anorganische Chemie der Fachgruppen Wöhler-Vereinigung und Festkörperchemie und Materialforschung : 29-30. september 2020*. 1. vyd. Frankfurt nad Mohanom, Nemecko : Gesellschaft Deutscher Chemiker, 2020, S. 1.
Kategória publikácie do 2021: GII
- _05 BUDZIANOWSKI, Armand - DERZSI, Mariana - LESZCZYSKI, Piotr J. - CYRASKI, Micha K. - GROCHALA, Wojciech. Structural polymorphism of pyrazinium hydrogen sulfate: Extending chemistry of the pyrazinium salts with small anions. In *Acta Crystallographica Section B: Structural Science*. 66, 4 (2010-07-27), pp. 451-457. V databáze: SCOPUS: 2-s2.0-77954824026 ; DOI: 10.1107/S0108768110019580 ; SCOPUS_INTID.
Ohlasy:
1. [1] BAZARGAN, Maryam - MIRZAEI, Masoud - AKBARI, Mahmood. Substantiation to structure-property of pyrazine-based compounds by undeniable impress of its different connectivities. In *Journal of Molecular Structure*, 2019, 1188, pp. 129-141. ISSN 00222860., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
2. [1] MAZUREK, Anna Helena - SZELESZCZUK, Łukasz - PISKLAK, Dariusz Maciej. Periodic DFT calculations—Review of applications in the pharmaceutical sciences. In *Pharmaceutics*, 2020, 12, 5, pp., Registrované v: SCOPUS, WOS
Ohlas: zahraničný

- _06 DERZSI, Mariana - PIEKARZ, Przemyslaw - JOCHYM, Pawel T. - LAZEWSKI, Jan - STERNIK, Malgorzata - OLES, Andrzej M. - PARLINSKI, Krzysztof. Effects of Coulomb interaction on the electronic structure and lattice dynamics of the Mott insulator Fe₂SiO₄ spinel. In *PHYSICAL REVIEW B*. Vol. 79, no. 20 (2009), pp. V databáze: WOS: 000266501500032 ; DOI: 10.1103/PhysRevB.79.205105.
Ohlasy:
1. [1] XIAO, Lingping - LI, Xiaobin - YANG, Xue. Electronic and optical properties of Fe₂SiO₄ under pressure effect: ab initio study. In *EUROPEAN PHYSICAL JOURNAL B*, 2018, vol. 91, no. 5, pp. ISSN 1434-6028., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
2. [1] BAIMA, Jacopo - GONIAKOWSKI, Jacek - NOGUERA, Claudine - KOLTSOV, Alexey - MATAIGNE, Jean-Michel. Surface thermodynamics of silicate compounds: the case of Zn₂SiO₄(001) surfaces and thin films. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, 2019, vol. 21, no. 24, pp. 13287-13295. ISSN 1463-9076., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
3. [1] LUO, Zigui - FAN, Xi'an - HU, Wentao - LUO, Fan - LI, Guangqiang - LI, Yawei - WANG, Jian - LIU, Xin. Effect of sintering temperature on microstructure and magnetic properties for Fe-Si soft magnetic composites prepared by water oxidation combined with spark plasma sintering. In *Journal of Magnetism and Magnetic Materials*, 2019, 491, pp. ISSN 03048853., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
4. [1] LUO, Zigui - FAN, Xi'an - HU, Wentao - LUO, Fan - WANG, Jian - WU, Zhaoyang - LIU, Xin - LI, Guangqiang - LI, Yawei. Properties of Fe₂SiO₄/SiO₂ coated Fe-Si soft magnetic composites prepared by sintering Fe-6.5wt%Si/Fe₃O₄ composite particles. In *Journal of Magnetism and Magnetic Materials*, 2020, 499, pp. ISSN 03048853., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
5. [1] RAM, Mahesh - SAXENA, Atul - ALY, Abeer E. - SHANKAR, Amit. Half-metallicity in new Heusler alloys Mn₂ScZ (Z = Si, Ge, Sn). In *RSC Advances*, 2020, 10, 13, pp. 7661-7670., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
6. [1] KAUR, Harleen - SINHA, M. M. Phonon dispersion and density of States of Fe₂SiO₄ in spinel phase. In *AIP Conference Proceedings*, 2021, 2352, pp. ISSN 0094243X., Registrované v: SCOPUS
Ohlas: zahraničný
7. [1] ASSADI, M. Hussein N. - FRONZI, Marco - HANAOR, Dorian A.H. Unusual ferrimagnetic ground state in rhenium ferrite. In *European Physical Journal Plus*, 2022-01-01, 137, 1, pp., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- _07 DERZSI, Mariana - PIEKARZ, Przemyslaw - TOKÁR, Kamil - JOCHYM, Pawel T. - LAZEWSKI, Jan - STERNIK, Malgorzata - PARLINSKI, Krzysztof. Comparative ab initio study of lattice dynamics and thermodynamics of Fe₂SiO₄- and Mg₂SiO₄- spinels. In *JOURNAL OF PHYSICS-CONDENSED MATTER*. Vol. 23, no. 10 (2011), pp. V databáze: WOS: 000287968700010 ; DOI: 10.1088/0953-8984/23/10/105401.
Ohlasy:
1. [1] PERVERSI, Giuditta - AREVALO-LOPEZ, Angel M. - RITTER, Clemens - ATTFIELD, J. Paul. Frustration wave order in iron(II) oxide spinels. In *COMMUNICATIONS PHYSICS*, 2018, vol. 1, no., pp. ISSN 2399-3650., Registrované v: WOS, SCOPUS
Ohlas: zahraničný
2. [1] KUSHWAHA, A. K. - MA, C.G. - BRIK, M. G. - AKBUDAK, S. Vibrational and elastic properties of silicate spinels A₂(SiO₄) (A = Mg, Fe, Ni, and Co). In *JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS*, 2018, vol. 117, no., pp. 167-172. ISSN 0022-3697., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
3. [1] CHANDRAKALA, Ch - REDDY, A. Siva Sessa - JEDRYKA, J. - KUMAR, Valluri Ravi - RAJU, G. Naga - VENKATRAMAIAH, N. - KUMAR, V. Ravi - LAKSHMINARAYANA, G. - VEERAAIAH, N. Third-order nonlinear optical features of zirconia-added lead silicate glass ceramics embedded with Pb₂Fe₂O₅ perovskite crystal phases and role of Fe ions. In *Applied Physics A: Materials Science and Processing*, 2020, 126, 6, pp. ISSN 09478396., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
4. [1] KOSTRZEWA, M. - REDDY, A. Siva Sessa - INGRAM, A. - SMIRNOV, Anton - KUMAR, V. Ravi - VEERAAIAH, N. Exploration of nano sized defects in Fe₂O₃ doped lead zirconium silicate glass ceramics by using positron annihilation lifetime spectroscopy. In *CERAMICS INTERNATIONAL*, 2021, vol. 47, no. 15, pp. 21785-21790. ISSN 0272-8842., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
5. [1] KAUR, Harleen - SINHA, M. M. Phonon dispersion and density of States of Fe₂SiO₄ in spinel phase. In *AIP Conference Proceedings*, 2021, 2352, pp. ISSN 0094243X., Registrované v: SCOPUS
Ohlas: zahraničný
6. [1] CHANDRAKALA, Ch - SIVA SESSA REDDY, A. - KOSTRZEWA, M. - PURNACHAND, N. - VENKATRAMAIAH, N. - NAGA RAJU, G. - RAVI KUMAR, V. - VEERAAIAH, Nalluri. Dielectric Relaxation Dynamics and Polaronic Tunneling Conduction Mechanism of Electrical Conductivity of Fe²⁺/Fe³⁺-Doped PbO-ZrO₂-SiO₂ Glass Ceramics. In *Physica Status Solidi (A) Applications and Materials Science*, 2021, 218, 16, pp. ISSN 18626300., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- _08 DERZSI, Mariana - PIEKARZ, Przemyslaw - GROCHALA, Wojciech. Structures of Late Transition Metal Monoxides from Jahn-Teller Instabilities in the Rock Salt Lattice. In *PHYSICAL REVIEW LETTERS*. Vol. 113, no. 2 (2014), pp. V databáze: WOS: 000339171300021 ; DOI: 10.1103/PhysRevLett.113.025505.

Ohlasy:

1. [1] HE, Bingling - WANG, Jinlong - MA, Dongwei - TIAN, Zhixue - JIANG, Lijuan - XU, Yan - CHENG, Sujun. Interaction of Pd single atoms with different CeO₂ crystal planes: A first-principles study. In *APPLIED SURFACE SCIENCE*, 2018, vol. 433, no., pp. 1036-1048. ISSN 0169-4332., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

2. [1] VAN DEN BOSSCHE, Maxime - GRONBECK, Henrik - HAMMER, Bjork. Tight-Binding Approximation-Enhanced Global Optimization. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, 2018, vol. 14, no. 5, pp. 2797-2807. ISSN 1549-9618., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

3. [1] BOTANA, A. S. - NORMAN, M. R. Layered palladates and their relation to nickelates and cuprates. In *PHYSICAL REVIEW MATERIALS*, 2018, vol. 2, no. 10, pp. ISSN 2475-9953., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

4. [1] LIU, Jinjia - YANG, Tao - XU, Aiju - MARTIN, Richard L. - YANG, Yong - JIAO, Haijun - LI, Yongwang - WEN, Xiao Dong. Predication of screened hybrid functional on transition metal monoxides: From Mott insulator to charge transfer insulator. In *Journal of Alloys and Compounds*, 2019, 808, pp. ISSN 09258388., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

5. [1] HILLEKE, Katerina P. - BI, Tiange - ZUREK, Eva. Materials under high pressure: a chemical perspective. In *APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING*, 2022, vol. 128, no. 5, pp. ISSN 0947-8396., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

_09 DERZSI, Mariana - GRZELAK, Adam - KONDRATIUK, P. - TOKÁR, Kamil - GROCHALA, Wojciech. Quest for compounds at the verge of charge transfer instabilities in halides: the case of elusive silver(II) chloride. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 335. Kategória publikácie do 2021: BFA

_10 DERZSI, Mariana - GROCHALA, Wojciech. Exploring crystal chemistry of silver(II) with DFT modelling. In *CESTC 2019 : 17th Central European Symposium on Theoretical Chemistry, 9. - 12. 9. 2019, Burg Schlaining, Austria*. 1. vyd. Wien : Universität Wien, 2019, S. 22. Kategória publikácie do 2021: BFA

_11 DERZSI, Mariana - COLOGNESI, Daniele. Inelastic neutron scattering and DFT study of potassium hydrogen phthalate. In *JOURNAL OF MOLECULAR STRUCTURE*. Vol. 967, no. 1-3 (2010), pp. 89-93. V databáze: WOS: 000276114400013 ; DOI: 10.1016/j.molstruc.2009.12.044.

Ohlasy:

1. [1] PETRENKO, Arsen - NOVIKOVA, Nataliya - BLAGOV, Alexander - KULIKOV, Anton - PISAREVSKII, Yury - VERIN, Igor - KOVALCHUK, Michail. Lateral deformations of a crystal of potassium acid phthalate in an external electric field. In *JOURNAL OF APPLIED CRYSTALLOGRAPHY*, 2021, vol. 54, no., pp. 1317-1326., Registrované v: WOS, CC

Ohlas: zahraničný

_12 DERZSI, Mariana - DYMKOWSKI, Krzysztof - GROCHALA, Wojciech. The Theoretical Quest for Sulfate of Ag²⁺: Genuine Ag(II)SO₄, Diamagnetic Ag(I)(2)S₂O₈, or Rather Mixed-Valence Ag(I)[Ag(III)(SO₄)₂]? In *Inorganic Chemistry*. Vol. 49, iss. 6 (2010), s. 2735-2742. ISSN 0020-1669 (2010: 4.601 - IF, Q1 - JCR Best Q, 2.006 - SJR, Q1 - SJR Best Q).

Typ výstupu: článok

Ohlasy:

1. [1] ZHOU, Dan - CHEN, Yi-Xiang - YUAN, Xiao-Yu - CHAI, Zhuang-Lei - LIU, Jin-Ku. Gradient Design of Vacancies and Their Positive Correlation with Electrochemical Anticorrosion Protection br. In *INORGANIC CHEMISTRY*, 2022, vol. 61, no. 20, pp. 8053-8065. ISSN 0020-1669., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

_13 DERZSI, Mariana - STASIEWICZ, Juliusz - GROCHALA, Wojciech. *Crystal and electronic structures and high-pressure behavior of AgSO₄, a unique narrow band gap antiferromagnetic semiconductor: LDA(+U) picture*. NEW YORK SPRINGER 2011. ISSN 1610-2940. V databáze: WOS: 000294735900016 ; DOI: 10.1007/s00894-010-0950-y.

Ohlasy:

1. [1] JERABEK, Paul - SANTHOSH, Archa - SCHWERDTFEGER, Peter. Relativistic Effects Stabilize Unusual Gold(II) Sulfate Structure via Aurophilic Interactions. In: *INORGANIC CHEMISTRY*, 2022, vol. 61, no. 33, pp. 13077-13084. ISSN 0020-1669., Registrované v: WOS, CC

Ohlas: zahraničný

_14 DERZSI, Mariana - BUDZIANOWSKI, Armand - STRUZHNIKIN, Viktor V. - MALINOWSKI, Przemyslaw J. - LESZCZYNSKI, Piotr J. - MAZEJ, Zoran - GROCHALA, Wojciech. *Redetermination of crystal structure of Ag(II)SO₄ and its high-pressure behavior up to 30 GPa*. CAMBRIDGE ROYAL SOC CHEMISTRY 2013. ISSN 1466-8033. V databáze: WOS: 000311826400023 ; DOI: 10.1039/c2ce26282g.

Ohlasy:

1. [1] JERABEK, Paul - SANTHOSH, Archa - SCHWERDTFEGER, Peter. Relativistic Effects Stabilize Unusual Gold(II) Sulfate Structure via Aurophilic Interactions. In: *INORGANIC CHEMISTRY*, 2022, vol. 61, no. 33, pp. 13077-13084. ISSN 0020-1669., Registrované v: WOS, CC

Ohlas: zahraničný

- _15 DOMANSKI, M. - DERZSI, Mariana - GROCHALA, Wojciech. High-pressure DFT+U modelling of ternary fluoride AgCuF₄. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 351.
Kategória publikácie do 2021: BFA
- _16 DOMANSKI, M. - DERZSI, Mariana - GROCHALA, Wojciech. Towards copper and silver ternary fluoride system. In *Online-Vortragstagung für Anorganische Chemie der Fachgruppen Wöhler-Vereinigung und Festkörperchemie und Materialforschung : 29-30. september 2020*. 1. vyd. Frankfurt nad Mohanom, Nemecko : Gesellschaft Deutscher Chemiker, 2020, S. 1.
Kategória publikácie do 2021: GII
- _17 DOMANSKI, M. - DERZSI, Mariana - GROCHALA, Wojciech. Towards copper and silver ternary fluoride system. In *Online conference "Pierwsza Wirtualna Konferencja Naukowa Kampusu Ochota (WKNKO-1)" : Ochota Campus of the University of Warsaw, June 30 - July 1, 2020*. Varšava : University of Warsaw, 2020, S. 1.
Kategória publikácie do 2021: GII
- _18 DOMANSKI, M. - DERZSI, Mariana - GROCHALA, Wojciech. Theoretical quest for novel ternary silver fluorides: study of AgMF₄ (M=Co, Ni, Cu) formation at pressures up to 20 GPa. In *58th European High Pressure Research Group International Conference (EHPRG 2020) : 6-11 September 2020, Puerto de la Cruz Tenerife, Spain, 2020*, S.1-2.
Kategória publikácie do 2021: BFA
- _19 FABUŠOVÁ, Diana. *Návrh atomistických modelov málo známeho oxidu paládia PdO₂(2)*. 2020. Dostupné na internete: <http://is.stuba.sk/zp/portal_zp.pl?podrobnosti=141352>.
- _20 FABUŠOVÁ, Diana. *Modelovanie fázových premien PdO₂ pod vysokým tlakom*. 2022. Dostupné na internete: <http://is.stuba.sk/zp/portal_zp.pl?podrobnosti=164196>.
- _21 FIJALKOWSKI, Karol J. - GENOVA, Radostina V. - FILINCHUK, Yaroslav - BUDZIANOWSKI, Armand - DERZSI, Mariana - JARON, Tomasz - LESZCZYNSKI, Piotr J. - GROCHALA, Wojciech. Na[Li(NH₂BH₃)(₂)] the first mixed-cation amidoborane with unusual crystal structure. In *DALTON TRANSACTIONS*. Vol. 40, no. 17 (2011), pp. 4407-4413. V databáze: WOS: 000289686600009 ; DOI: 10.1039/c0dt01491e.
Ohlasy:
1. [1] JORGENSEN, Mathias - LEE, Young-Su - BJERRING, Morten - JEPSEN, Lars H. - AKBEY, Umit - CHO, Young Whan - JENSEN, Torben R. Disorder induced polymorphic transitions in the high hydrogen density compound Sr(BH₄)₂(NH₃BH₃)₂₊. In *DALTON TRANSACTIONS*, 2018, vol. 47, no. 46, pp. 16737-16746. ISSN 1477-9226., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
2. [1] LUO, Junhong - WANG, Jinchuan - FENG, Xingwen - CAI, Jinguang - YAO, Weizhi - SONG, Jiangfeng - CHEN, Changan - LUO, Deli. Mechanistic insight into the promoting effect of magnesium nickel hydride on the dehydrogenation of ammonia borane. In *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*, 2018, vol. 43, no. 3, pp. 1681-1690. ISSN 0360-3199., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
3. [1] DIAZ, Laura Bravo - HANLON, James M. - BIELEWSKI, Marek - MILEWSKA, Aleksandra - GREGORY, Duncan H. Ammonia Borane Based Nanocomposites as Solid-State Hydrogen Stores for Portable Power Applications. In *ENERGY TECHNOLOGY*, 2018, vol. 6, no. 3, pp. 583-594. ISSN 2194-4288., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
4. [1] WANG, Kun - PAN, Zuxiong - YU, Xuebin. Metal B-N-H hydrogen-storage compound: Development and perspectives. In *Journal of Alloys and Compounds*, 2019, 794, pp. 303-324. ISSN 09258388., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
5. [1] LAI, Qiwen - SUN, Yahui - WANG, Ting - MODI, Poojan - CAZORLA, Claudio - DEMIRCI, Umit B. - ARES FERNANDEZ, Jose Ramon - LEARDINI, Fabrice - AGUEY-ZINSOU, Kondo François. How to Design Hydrogen Storage Materials? Fundamentals, Synthesis, and Storage Tanks. In *Advanced Sustainable Systems*, 2019, 3, 9, pp., Registrované v: SCOPUS, WOS
Ohlas: zahraničný
6. [1] LIU, Xiaoran - WU, Yuanfang - WANG, Shumao - LI, Zhinian - GUO, Xiumei - YE, Jianhua - JIANG, Lijun. Current progress and research trends on lithium amidoborane for hydrogen storage. In *Journal of Materials Science*, 2020, 55, 7, pp. 2645-2660. ISSN 00222461., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
7. [1] CASTILLA-MARTINEZ, Carlos A. - MOURY, Romain - DEMIRCI, Umit B. Amidoboranes and hydrazinidoboranes: State of the art, potential for hydrogen storage, and other prospects. In *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*, 2020, vol. 45, no. 55, pp. 30731-30755. ISSN 0360-3199., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
8. [1] MILANOVIC, Igor - BILISKOV, Nikola - UZAREVIC, Krunoslav - LUKIN, Stipe - ETTER, Martin - HALASZ, Ivan. Mechanochemical Synthesis and Thermal Dehydrogenation of Novel Calcium-Containing Bimetallic Amidoboranes. In *ACS SUSTAINABLE CHEMISTRY & ENGINEERING*, 2021, vol. 9, no. 5, pp. 2089-2099. ISSN 2168-0485., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
9. [1] HASSAN, I. A. - RAMADAN, Haitham S. - SALEH, Mohamed A. - HISSEL, Daniel. Hydrogen storage technologies for stationary and mobile applications: Review, analysis and perspectives. In *Renewable and Sustainable*

Energy Reviews, 2021, 149, pp. ISSN 13640321., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

10. [1] GUAN, Rongfeng - WANG, Pan - SONG, Yang - STAROVEROV, Viktor N. Pressure-Induced Polymorphic Transformations of Ethylenediamine Bisborane. In JOURNAL OF PHYSICAL CHEMISTRY C, 2021, vol. 125, no. 34, pp. 18614-18622. ISSN 1932-7447., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

- _22 GAŠPÁRKOVÁ, Michaela. *Modelovanie kryštálovej štruktúry a termodynamickej stability nového oxidu niklu Ni₂O₃*. 2020. Dostupné na internete: <http://is.stuba.sk/zp/portal_zp.pl?podrobnosti=151371>.
- _23 GAWRACZYNSKI, Jakub - TOKÁR, Kamil - MAZEJ, Zoran - DERZSI, Mariana - LORENZANA, Jose - GROCHALA, Wojciech. Excitons in AgF₂, a layered 2D antiferromagnet. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 336.
Kategória publikácie do 2021: BFA
- _24 GAWRACZYNSKI, Jakub - TOKÁR, Kamil - MAZEJ, Zoran - DERZSI, Mariana - LORENZANA, Jose - GROCHALA, Wojciech. Excitons in AgF₂ and KAgF₃. In *62. zjazd naukowy polskiego towarzystwa chemicznego : Warszawa, 2-6 september 2019*. 1. vyd, 2019, S. 02-24.
Kategória publikácie do 2021: BFA
- _25 GILEWSKI, Tomasz E. - GAWRACZYNSKI, Jakub - DERZSI, Mariana - JAGLICIC, Zvonko - MAZEJ, Zoran - POLCZYNSKI, Piotr - JURCZAKOWSKI, Rafal - LESZCZYNSKI, Piotr J. - GROCHALA, Wojciech. [Ag(OH)₂]₂[Ag(SO₄)₂]: A Hydrate of a Silver(II) Salt. In *CHEMISTRY-A EUROPEAN JOURNAL*. Vol. 23, no. 8 (2017), pp. 1805-1813. V databáze: WOS: 000395754800013 ; DOI: 10.1002/chem.201604179.
Ohlasy:
1. [1] WALTERS, Lauren N. - ZHANG, Chi - DRAVID, Vinayak P. - POEPELMEIER, Kenneth R. - RONDINELLI, James M. First-Principles Hydrothermal Synthesis Design to Optimize Conditions and Increase the Yield of Quaternary Heteroanionic Oxychalcogenides. In *CHEMISTRY OF MATERIALS*, 2021, vol. 33, no. 8, pp. 2726-2741. ISSN 0897-4756., Registrované v: WOS, SCOPUS
Ohlas: zahraničný
- _26 GROCHALA, Wojciech - CYRANSKI, Michal Ksawery - DERZSI, Mariana - MICHALOWSKI, Tomasz - MALINOWSKI, Przemyslaw J. - MAZEJ, Zoran - KURZYDLOWSKI, Dominik - KOZMINSKI, Wiktor - BUDZIANOWSKI, Armand - LESZCZYNSKI, Piotr J. Crystal and electronic structure, lattice dynamics and thermal properties of Ag(I)(SO₃R) (R = F, CF₃) Lewis acids in the solid state. In *DALTON TRANSACTIONS*. Vol. 41, no. 7 (2012), pp. 2034-2047. V databáze: WOS: 000299505100015 ; DOI: 10.1039/c1dt11747e.
Ohlasy:
1. [1] GARDINIER, James R. - MEISE, Kristin J. - JAHAN, Fathiya - LINDEMAN, Sergey V. Reaction Chemistry of Silver(I) Trifluoromethanesulfonate Complexes of Nitrogen-Confused C-Scorpionates. In *INORGANIC CHEMISTRY*, 2018, vol. 57, no. 3, pp. 1572-1589. ISSN 0020-1669., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
2. [1] SEOW, Celestine - BIN ISMAIL, Muhammad Luthfi - XI, Hong-Wei - LI, Yongxin - LIM, Kok Hwa - SO, Cheuk-Wai. A Bis(germyliumylidene)silver(I) Complex Dication. In *ORGANOMETALLICS*, 2018, vol. 37, no. 9, pp. 1368-1372. ISSN 0276-7333., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
3. [1] KUMAR, Shanish - JANA, Oishi - SUBRAMANIYAN, Vasudevan - MANI, Ganesan. The 'reverse transmetalation' reaction of the pyrrole-based PNP pincer Ni(II) complexes: X-ray structures of binuclear silver(I) and thiocyanate nickel(II) complexes. In *INORGANICA CHIMICA ACTA*, 2018, vol. 480, no., pp. 113-119. ISSN 0020-1693., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
4. [1] ZHANG, Huang - LIU, Xu - LI, Huihua - QIN, Bingsheng - PASSERINI, Stefano. High-Voltage Operation of a V₂O₅ Cathode in a Concentrated Gel Polymer Electrolyte for High-Energy Aqueous Zinc Batteries. In *ACS APPLIED MATERIALS & INTERFACES*, 2020, vol. 12, no. 13, pp. 15305-15312. ISSN 1944-8244., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
5. [1] ANSMANN, Nils - HARTMANN, Deborah - SAILER, Sonja - ERDMANN, Philipp - MASKEY, Rezisha - SCHORPP, Marcel - GREB, Lutz. Synthesis and Characterization of Hypercoordinated Silicon Anions: Catching Intermediates of Lewis Base Catalysis. In: *Angewandte Chemie International Edition*, 2022-07-04, 61, 27, pp. ISSN 14337851., Registrované v: SCOPUS
Ohlas: zahraničný
- _27 GROCHALA, Wojciech - GRZELAK, Adam - GAWRACZYNSKI, Jakub - KURZYDLOWSKI, Dominik - MAZEJ, Zoran - PRAKAPENKA, Vitali - DERZSI, Mariana - STRUZHKIN, Viktor - BARONE, Paolo. Tuning magnetic and electronic properties in exotic Silver(II) fluorides using pressure. In *APS March Meeting 2020 : Vol. 65, Number 1, March 2-6, 2020 Denver, Colorado*. Denver : American Physical Society, 2020, S. 1.
Kategória publikácie do 2021: BFA
- _28 GRZELAK, Adam - GAWRACZYNSKI, Jakub - JARON, Tomasz - SOMAYAZULU, Maddury - DERZSI, Mariana - STRUZHKIN, Viktor - GROCHALA, Wojciech. Persistence of Mixed and Non-intermediate Valence in the High-Pressure Structure of Silver(I, III) Oxide, AgO: A Combined Raman, X-ray Diffraction (XRD), and Density Functional Theory (DFT) Study. In

INORGANIC CHEMISTRY. Vol. 56, no. 10 (2017), pp. 5804-5812. V databáze: WOS: 000401593800037 ; DOI: 10.1021/acs.inorgchem.7b00405.

Ohlasy:

1. [1] TANG, Meng - ZHANG, Yanmei - LI, Siya - WU, Xi - JIA, Yan - YANG, Guochun. Mixed-valence Compounds: AuO₂ and AuS. In *CHEMPHYSICHEM*, 2018, vol. 19, no. 22, pp. 2989-2994. ISSN 1439-4235., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

2. [1] SHEN, Wenning - WANG, Xu - GE, Yanfeng - FENG, Hui - FENG, Lajun. Synthesis and characterization of AgO/g-C₃N₄ hybrids with enhanced visible-light photocatalytic activity for Rhodamine B degradation and bactericidal inactivation. In *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2019, 575, pp. 102-110. ISSN 09277757., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

3. [1] SCHVVAL, Ana B. - JUAN, Alfredo - CABEZA, Gabriela F. Theoretical study of the role of the interface of Ag-4 nanoclusters deposited on TiO₂(110) and TiO₂(101). In *APPLIED SURFACE SCIENCE*, 2019, vol. 490, no., pp. 343-351. ISSN 0169-4332., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

4. [1] BIAN, Haiqin - ZHANG, Zhengmei - XU, Xiaoli - GAO, Yang - WANG, Tao. Photocatalytic activity of Ag/ZnO /AgO/TiO₂ composite. In *Physica E: Low-Dimensional Systems and Nanostructures*, 2020, 124, pp. ISSN 13869477., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

5. [1] WANG, R. Y. - CHEN, Z. J. - HUANG, Z. Q. - XIA, B. W. - XU, H. Classification and materials realization of topologically robust nodal ring phonons. In *PHYSICAL REVIEW MATERIALS*, 2021, vol. 5, no. 8, pp. ISSN 2475-9953., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

6. [1] GHOSH, Rajarshi. Chemistry of silver(III) and some of its compounds: A review. In *Journal of the Indian Chemical Society*, 2021, 98, 12, pp. ISSN 00194522., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

7. [1] ZWAWI, M. - ATTAR, A. - AL-HOSSAINY, A. F. - ABDEL-AZIZ, M. H. - ZOROMBA, M. Sh. Polypyrrole/functionalized multi-walled carbon nanotube composite for optoelectronic device application. In *Chemical Papers*, 2021, 75, 12, pp. 6575-6589. ISSN 03666352., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

8. [1] KISHIMURA, Hiroaki - SHIMONO, Seiya - ABE, Hiroshi. Effect of dynamic high-pressure loading on decomposition reaction and negative thermal expansion of silver oxide. In *Japanese Journal of Applied Physics*, 2022-04-01, 61, 4, pp. ISSN 00214922., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

_29

GRZELAK, Adam - GAWRACZYNSKI, Jakub - JARON, Tomasz - KURZYDŁOWSKI, Dominik - BUDZIANOWSKI, Armand - MAZEJ, Zoran - LESZCZYNSKI, Piotr J. - PRAKAPENKA, Vitali B. - DERZSI, Mariana - STRUZHKIN, Viktor V. - GROCHALA, Wojciech. High-Pressure Behavior of Silver Fluorides up to 40 GPa. In *INORGANIC CHEMISTRY*. Vol. 56, no. 23 (2017), pp. 14651-14661. V databáze: WOS: 000417342200029 ; DOI: 10.1021/acs.inorgchem.7b02528.

Ohlasy:

1. [1] LIN, Jianyan - ZHANG, Shoutao - GUAN, Wei - YANG, Guochun - MA, Yanming. Gold with +4 and +6 Oxidation States in AuF₄ and AuF₆. In *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*, 2018, vol. 140, no. 30, pp. 9545-9550. ISSN 0002-7863., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

2. [1] ANTONIO ARAMBURU, Jose - MORENO, Miguel. Understanding the Structure and Ground State of the Prototype CuF₂ Compound Not Due to the Jahn-Teller Effect. In *INORGANIC CHEMISTRY*, 2019, vol. 58, no. 7, pp. 4609-4618. ISSN 0020-1669., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

3. [1] LIN, Jianyan - DU, Xin - RAHM, Martin - YU, Hong - XU, Haiyang - YANG, Guochun. Exploring the Limits of Transition-Metal Fluorination at High Pressures. In *Angewandte Chemie International Edition*, 2020, 59, 23, pp. 9155-9162. ISSN 14337851., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

4. [1] ROSTAMI, Samare - GHASEMI, S. Alireza - GOEDECKER, Stefan. Novel polymorphs and polytypes of lithium chloride from structure predictions based on charge equilibration via neural network technique. In *Physical Review Materials*, 2021, 5, 12, pp., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

5. [1] SANCHEZ-MOVELLAN, Ines - MORENO-CEBALLOS, Jorge - GARCIA-FERNANDEZ, Pablo - ARAMBURU, Jose Antonio - MORENO, Miguel. New Ideas for Understanding the Structure and Magnetism in AgF₂: Prediction of Ferroelasticity. In *CHEMISTRY-A EUROPEAN JOURNAL*, 2021, vol. 27, no. 54, pp. 13582-13590. ISSN 0947-6539., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

_30

GRZELAK, Adam - DERZSI, Mariana - LORENZANA, Jose - GROCHALA, Wojciech. Charge doping of silver(II) fluoride via fluorine depletion - a computational (DFT) study. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 254.

Kategória publikácie do 2021: BFA

_31

GRZELAK, Adam - DERZSI, Mariana - GROCHALA, Wojciech. Hole doping to silver(II) fluoride - a DFT study. In *62. zjazd naukowy polskiego towarzystwa chemicznego : Warszawa, 2-6 september 2019*. 1. vyd, 2019, S. 02-39.

Kategória publikácie do 2021: BFA

- _32 GRZELAK, Adam - DERZSI, Mariana - GROCHALA, Wojciech. Exploring the phases diagram of Ag/Cl₂ system by means of DFT and hybrid DFT calculations. In *58th European High Pressure Research Group International Conference (EHPRG 2020): 6-11 September 2020, Puerto de la Cruz Tenerife, Spain, 2020, S.1.*
Kategoria publikácie do 2021: BFA
- _33 GRZELAK, A. - GAWRACZYŃSKI, J. - JAROŃ, T. - KURZYDŁOWSKI, D. - MAZEJ, Z. - LESZCZYŃSKI, P. J. - PRAKAPENKA, V. B. - DERZSI, Mariana - STRUZHKIN, V. V. - GROCHALA, W. Metal fluoride nanotubes featuring square-planar building blocks in a high-pressure polymorph of AgFinF₂/inf. In *Dalton Transactions*. 46, 43 (2017-01-01), pp. 14742-14745. V databáze: SCOPUS: 2-s2.0-85033238163 ; DOI: 10.1039/c7dt03178e ; SCOPUS_INTID.
Ohlasy:
1. [1] KUANG, Minquan - LI, Tingzhou - CHENG, Zhenxiang - KHACHAI, Houari - KHENATA, R. - YANG, Tie - LIN, Tingting - WANG, Xiaotian. Perovskite R3C phase AgCuF₃: Multiple dirac cones, 100% spin polarization and its thermodynamic properties. In *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, 2019, 75, pp. 354-360. ISSN 20525192., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
2. [1] SANCHEZ-MOVELLAN, Ines - MORENO-CEBALLOS, Jorge - GARCIA-FERNANDEZ, Pablo - ARAMBURU, Jose Antonio - MORENO, Miguel. New Ideas for Understanding the Structure and Magnetism in AgF₂: Prediction of Ferroelasticity. In *CHEMISTRY-A EUROPEAN JOURNAL*, 2021, vol. 27, no. 54, pp. 13582-13590. ISSN 0947-6539., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
- _34 HERMANN, Andreas - DERZSI, Mariana - GROCHALA, Wojciech - HOFFMANN, Roald. AuO: Evolving from Dis- to Comproportionation and Back Again. In *INORGANIC CHEMISTRY*. Vol. 55, no. 3 (2016), pp. 1278-1286. V databáze: WOS: 000369356800034 ; DOI: 10.1021/acs.inorgchem.5b02528.
Ohlasy:
1. [1] TANG, Meng - ZHANG, Yanmei - LI, Siya - WU, Xi - JIA, Yan - YANG, Guochun. Mixed-valence Compounds: AuO₂ and AuS. In *CHEMPHYSICHEM*, 2018, vol. 19, no. 22, pp. 2989-2994. ISSN 1439-4235., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
2. [1] ZUREK, Eva - BI, Tiange. High-temperature superconductivity in alkaline and rare earth polyhydrides at high pressure: A theoretical perspective. In *Journal of Chemical Physics*, 2019, 150, 5, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
3. [1] LI, Pingping - WANG, Jinshu - ZU, Guannan - JIAO, Peng - LIU, Shaojing - YANG, Yunfei - CHEN, Shuqun - LI, Hongyi. Synergetic catalytic properties of gold nanoparticles planted on transparent titanium dioxide nanotube array bed. In *MATERIALS CHEMISTRY AND PHYSICS*, 2018, vol. 217, no., pp. 437-444. ISSN 0254-0584., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
4. [1] WAN, Wei - YIN, Jun - WU, Yaping - ZHENG, Xuanli - YANG, Weihuang - WANG, Hao - ZHOU, Jiangpeng - CHEN, Jiajun - WU, Zhiming - LI, Xu - KANG, Junyong. Polarization-Controllable Plasmonic Enhancement on the Optical Response of Two-Dimensional GaSe Layers. In *ACS Applied Materials and Interfaces*, 2019, 11, 21, pp. 19631-19637. ISSN 19448244., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
5. [1] LIU, Guangtao - FENG, Xiaolei - WANG, Linyan - REDFERN, Simon A.T. - YONG, Xue - GAO, Guoying - LIU, Hanyu. Theoretical investigation of the valence states in Au via the Au-F compounds under high pressure. In *Physical Chemistry Chemical Physics*, 2019, 21, 32, pp. 17621-17627. ISSN 14639076., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
6. [1] ZHANG, Jurong - FENG, Xiaolei - LIU, Guangtao - REDFERN, Simon A. T. - LIU, Hanyu. Computational prediction of a+4 oxidation state in Au via compressed AuO₂ compound. In *JOURNAL OF PHYSICS-CONDENSED MATTER*, 2020, vol. 32, no. 1, pp. ISSN 0953-8984., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
7. [1] EKLUND, Kim - KUKLIN, Mikhail S. - KRAUS, Florian - KARTTUNEN, Antti J. Evolutionary Algorithm-based Crystal Structure Prediction for Gold(I) Fluoride. In *CHEMPHYSICHEM*, 2020, vol. 21, no. 8, pp. 802-808. ISSN 1439-4235., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
8. [1] KURZYDŁOWSKI, Dominik - KOBYAKOV, Serhiy - MAZEJ, Zoran - PILLAI, Sharad Babu - CHAKRABORTY, Brahmananda - JHA, Prafulla K. Unexpected persistence of cis-bridged chains in compressed AuF₃. In *Chemical Communications*, 2020, 56, 36, pp. 4902-4905. ISSN 13597345., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
9. [1] HILLEKE, Katerina P. - ZUREK, Eva. Tuning chemical precompression: Theoretical design and crystal chemistry of novel hydrides in the quest for warm and light superconductivity at ambient pressures. In *JOURNAL OF APPLIED PHYSICS*, 2022, vol. 131, no. 7, pp. ISSN 0021-8979., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
- _35 CHURCHARD, Andrew J. - DERZSI, Mariana - JAGLICIC, Zvonko - REMHOF, Arndt - GROCHALA, Wojciech. Chemo-switched chromatic, magnetic and structural changes with retention of molecular crystallinity, Ni(12anes(4))(BF₄)(2). In *DALTON TRANSACTIONS*. Vol. 41, no. 17 (2012), pp. 5172-5176. V databáze: WOS: 000302364000009 ; DOI: 10.1039/c2dt12468h.
Ohlasy:
1. [1] LACROIX, Matthew R. - BUKOVSKY, Eric V. - LOZINSEK, Matic - FOLSOM, Travis C. - NEWELL, Brian S. - LIU, Yong - PERYSHKOV, Dmitry V. - STRAUSS, Steven H. Manifestations of Weak O-H ... F Hydrogen Bonding in

M(H₂O)(n)(B12F12) Salt Hydrates: Unusually Sharp Fourier Transform Infrared ν(OH) Bands and Latent Porosity (M = Mg-Ba, Co, Ni, Zn). In *INORGANIC CHEMISTRY*, 2018, vol. 57, no. 23, pp. 14983-15000. ISSN 0020-1669., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

2. [1] CHEU, Elizabeth L.S. - HUXHAM, Lynsey A. - PATRICK, Brian O. - EZHOVA, Maria B. - JAMES, Brian R. Aqueous chemistry of ruthenium(II) complexes containing dimethylsulfoxide, and a chelated disulfoxide ligand or a cyclotetraethia ligand. In *Inorganica Chimica Acta*, 2020, 512, pp. ISSN 00201693., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

3. [1] FINK, Daniel - ORTH, Nicole - LINSEIS, Michael - IVANOVIC-BURMAZOVIC, Ivana - WINTER, Rainer F. Structural Versatility and Supramolecular Isomerism in Redox-Active Tetra- and Hexaruthenium Macrocycles. In *EUROPEAN JOURNAL OF INORGANIC CHEMISTRY*, 2020, vol. 2020, no. 29, pp. 2816-2829. ISSN 1434-1948., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

_36 KOTERAS, Kacper - DOMANSKI, M. - WITKOWSKI, M. - GRZELAK, Adam - DERZSI, Mariana - SU, Haibin - GROCHALA, Wojciech. Chemical and physical doping to AgF₂. In *62. zjazd naukowy polskiego towarzystwa chemicznego : Warszawa, 2-6 september 2019*. 1. vyd, 2019, S. 02-43.

Kategória publikácie do 2021: BFA

_37 KOTERAS, Kacper - DERZSI, Mariana - GROCHALA, Wojciech. Modelling of nickel-doped silver(II) fluoride. In *Online-Vortragstagung für Anorganische Chemie der Fachgruppen Wöhler-Vereinigung und Festkörperchemie und Materialforschung : 29-30. september 2020*. 1. vyd. Frankfurt nad Mohanom, Nemecko : Gesellschaft Deutscher Chemiker, 2020, S. 1.

Kategória publikácie do 2021: GII

_38 KOTERAS, Kacper - DERZSI, Mariana - GAWRACZYNSKI, Jakub - GROCHALA, Wojciech. Modelling of KAgF₃ phonom structure. In *Online-Vortragstagung für Anorganische Chemie der Fachgruppen Wöhler-Vereinigung und Festkörperchemie und Materialforschung : 29-30. september 2020*. 1. vyd. Frankfurt nad Mohanom, Nemecko : Gesellschaft Deutscher Chemiker, 2020, S. 1.

Kategória publikácie do 2021: GII

_39 KOTERAS, Kacper - DERZSI, Mariana - GROCHALA, Wojciech. Modelling of nickel-doped silver(II) fluoride. In *Online conference "Pierwsza Wirtualna Konferencja Naukowa Kampusu Ochota (WKNKO-1)" : Ochota Campus of the University of Warsaw, June 30 - July 1, 2020*. Varšava : Univerzity of Warsaw, 2020, S. 1.

Kategória publikácie do 2021: GII

_40 KOTERAS, Kacper - DERZSI, Mariana - GAWRACZYNSKI, Jakub - GROCHALA, Wojciech. Modelling of KAgF₃ phonom structure. In *Online conference "Pierwsza Wirtualna Konferencja Naukowa Kampusu Ochota (WKNKO-1)" : Ochota Campus of the University of Warsaw, June 30 - July 1, 2020*. Varšava : Univerzity of Warsaw, 2020, S. 1.

Kategória publikácie do 2021: GII

_41 KURZYDŁOWSKI, Dominik - DERZSI, Mariana - MAZEJ, Zoran - GROCHALA, Wojciech. Crystal, electronic, and magnetic structures of M₂AgF₄ (M = Na-Cs) phases as viewed from the DFT plus U method. In *DALTON TRANSACTIONS*. Vol. 45, no. 41 (2016), pp. 16255-16261. V databáze: WOS: 000386221300027 ; DOI: 10.1039/c6dt03125k.

Ohlasy:

1. [1] ARAMBURU, J. A. - GARCÍA-FERNÁNDEZ, P. - MATHIESEN, N. R. - GARCIA-LASTRA, J. M. - MORENO, M. Changing the Usual Interpretation of the Structure and Ground State of Cu₂-Layered Perovskites. In *Journal of Physical Chemistry C*, 2018, 122, 9, pp. 5071-5082. ISSN 19327447., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

2. [1] BERGESON-KELLER, Anyka M. - SANDERS, Michael D. - O'HAYRE, Ryan P. Reduction Thermodynamics of Sr_{1-x}Ce_xMnO₃ and CexSr_{2-x}MnO₄ Perovskites for Solar Thermochemical Hydrogen Production. In *Energy Technology*, 2022-01-01, 10, 1, pp. ISSN 21944288., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

_42 KURZYDŁOWSKI, Dominik - DERZSI, Mariana - ZUREK, E. - GROCHALA, Wojciech. Mixed-valent fluorides of silver stabilized at high pressure. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 310.

Kategória publikácie do 2021: BFA

_43 KURZYDŁOWSKI, Dominik - DERZSI, Mariana - BUDZIANOWSKI, Armand - JAGLICIC, Zvonko - KOZMINSKI, Wiktor - MAZEJ, Zoran - GROCHALA, Wojciech. Polymorphism of Fluoroargentates(II): Facile Collapse of a Layered Network of alpha-K₂AgF₄ Due to the Insufficient Size of the Potassium Cation. In *EUROPEAN JOURNAL OF INORGANIC CHEMISTRY*. Vol. , no. 19 (2010), pp. 2919-2925. V databáze: WOS: 000280211800005 ; DOI: 10.1002/ejic.201000124.

Ohlasy:

1. [1] LIU, Huimin - WU, Ping - LI, Haitao - CHEN, Zibin - WANG, Lizhuo - ZENG, Xin - ZHU, Yuxiang - JIANG, Yijiao - LIAO, Xiaozhou - HAYNES, Brian S. - YE, Jinhua - STAMPFL, Catherine - HUANG, Jun. Unravelling the effects of layered supports on Ru nanoparticles for enhancing N₂ reduction in photocatalytic ammonia synthesis. In *APPLIED CATALYSIS B-ENVIRONMENTAL*, 2019, vol. 259, no., pp. ISSN 0926-3373., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

- _44 LESZCZYNSKI, Piotr J. - BUDZIANOWSKI, Armand - DOBRZYCKI, Lukasz - CYRANSKI, Michal K. - DERZSI, Mariana - GROCHALA, Wojciech. Thermal and chemical decomposition of di(pyrazine)silver(II) peroxydisulfate and unusual crystal structure of a Ag(I) by-product. In *DALTON TRANSACTIONS*. Vol. 41, no. 2 (2012), pp. 396-402. V databáze: WOS: 000298000000013 ; DOI: 10.1039/c1dt10744e.
Ohlasy:
1. [1] HONG, Boseok - AGANDA, Kim Christopher C. - LEE, Anna. Oxidative C-S Bond Cleavage of Benzyl Thiols Enabled by Visible-Light-Mediated Silver(II) Complexes. In *Organic Letters*, 2020, 22, 11, pp. 4395-4399. ISSN 15237060., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
2. [1] BEHERA, Prafulla K. - KISAN, Hemanta K. - ISAB, Anvarhusein A. - DINDA, Joydev. Novel synthesis, structural characterization, DFT and TDDFT investigation of 'Butterfly' like Ag(I)- complex supported by 3-pyrazinyl [1-methyl]imidazolium hexafluorophosphate. In *Journal of Molecular Structure*, 2021, 1235, pp. ISSN 00222860., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- _45 LORENZANA, Jose - GAWRACZYNSKI, Jakub - KURZYDŁOWSKI, Dominik - EWINGS, Russel A. - GADOMSKI, Wojciech - BANDARU, Subrahmanyam - MAZEJ, Zoran - RUANI, Giampiero - BERGENTI, Ilaria - TOKÁR, Kamil - DERZSI, Mariana - BARONE, Paolo - GROCHALA, Wojciech. Silver(II) fluoride as a strong analogue of parent superconducting cuprates. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 102.
Kategória publikácie do 2021: BFA
- _46 MALINOWSKI, Przemyslaw Jan - DERZSI, Mariana - BUDZIANOWSKI, Armand - LESZCZYNSKI, Piotr J. - GAWEL, Bartłomiej - MAZEJ, Zoran - GROCHALA, Wojciech. Unusual Thermal Decomposition of (AgSO₄)-S-II Yielding (Ag₂S₂O₇)-S-I: Bending Hammond's Rule. In *CHEMISTRY-A EUROPEAN JOURNAL*. Vol. 17, no. 38 (2011), pp. 10524-10527. V databáze: WOS: 000295880300005 ; DOI: 10.1002/chem.201101952.
Ohlasy:
1. [1] NETZSCH, Philip - HOEPPE, Henning A. Ag[B(S₂O₇)](2): The First Transition Metal Borosulfate Featuring Disulfate Groups. In *EUROPEAN JOURNAL OF INORGANIC CHEMISTRY*, 2021, vol. 2021, no. 11, pp. 1065-1070. ISSN 1434-1948., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
- _47 MALINOWSKI, Przemyslaw J. - MAZEJ, Zoran - DERZSI, Mariana - JAGLICIC, Zvonko - SZYDŁOWSKA, Jadwiga - GILEWSKI, Tomasz - GROCHALA, Wojciech. Silver(II) triflate with one-dimensional [Ag(II)(SO₃CF₃)(4/2)](infinity) chains hosting antiferromagnetism. In *CRYSTENGCOMM*. Vol. 13, no. 22 (2011), pp. 6871-6879. V databáze: WOS: 000296160000042 ; DOI: 10.1039/c1ce05712j.
Ohlasy:
1. [1] DIXON, Sebastian C. - MANZI, Joe A. - POWELL, Michael J. - CARMALT, Claire J. - PARKIN, Ivan P. Reflective Silver Thin Film Electrodes from Commercial Silver(I) Triflate via Aerosol-Assisted Chemical Vapor Deposition. In *ACS APPLIED NANO MATERIALS*, 2018, vol. 1, no. 7, pp. 3724-3732. ISSN 2574-0970., Registrované v: WOS
Ohlas: zahraničný
2. [1] RUSU, Aura - IMRE, Silvia - MARE, Anca Delia - LUNGU, Ioana Andreea - PASCU, Georgiana Andreea - UIVAROSI, Valentina. Synthesis, characterization and antibacterial activity of a new derivative of levofloxacin. In *Journal of the Chilean Chemical Society*, 2020, 65, 3, pp. 4857-4860. ISSN 07179324., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
3. [1] KUMAR, A. Madhan - EHSAN, Muhammad Ali - SULEIMAN, Rami K. - HAKEEM, Abbas Saeed. Fabrication and Characterization of Nanostructured AACVD Thin Films on 316L SS as Surface Protective Layers in Simulated Body Fluid. In *METALLURGICAL AND MATERIALS TRANSACTIONS A-PHYSICAL METALLURGY AND MATERIALS SCIENCE*, 2020, vol. 51, no. 8, pp. 4301-4312. ISSN 1073-5623., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
- _48 MALINOWSKI, Przemyslaw J. - DERZSI, Mariana - MAZEJ, Zoran - JAGLICIC, Zvonko - GAWEL, Bartłomiej - LASOCHA, Wieslaw - GROCHALA, Wojciech. Ag₂SO₄: A Genuine Sulfate of Divalent Silver with Anomalously Strong One-Dimensional Antiferromagnetic Interactions. In *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*. Vol. 49, no. 9 (2010), pp. 1683-1686. V databáze: WOS: 000275234800031 ; DOI: 10.1002/anie.200906863.
Ohlasy:
1. [1] ARCHIREL, Pierre - LÉONARD, Céline - LE QUÉRÉ, Frédéric - ADJEI, Daniel - DENISOV, Sergey A. - MOSTAFAVI, Mehran. Oxidation of silver cyanide Ag(CN)₂ By the OH radical- By ab initio calculation to molecular simulation and to experiment. In *Journal of Physical Chemistry A*, 2020, 124, 51, pp. 10787-10798. ISSN 10895639., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
2. [1] NETZSCH, Philip - HOEPPE, Henning A. Ag[B(S₂O₇)](2): The First Transition Metal Borosulfate Featuring Disulfate Groups. In *EUROPEAN JOURNAL OF INORGANIC CHEMISTRY*, 2021, vol. 2021, no. 11, pp. 1065-1070. ISSN 1434-1948., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
3. [1] WALTERS, Lauren N. - ZHANG, Chi - DRAVID, Vinayak P. - POEPELMEIER, Kenneth R. - RONDINELLI, James M. First-Principles Hydrothermal Synthesis Design to Optimize Conditions and Increase the Yield of Quaternary Heteroanionic Oxychalcogenides. In *CHEMISTRY OF MATERIALS*, 2021, vol. 33, no. 8, pp. 2726-2741. ISSN 0897-4756., Registrované v: WOS, SCOPUS

Ohlas: zahraničný

4. [1] XIANG, Danlei - IÑIGUEZ, Jesus A. - DENG, Jiao - GUAN, Xun - MARTINEZ, Antonio - LIU, Chong. Agli-Mediated Electrocatalytic Ambient CH₄ Functionalization Inspired by HSAB Theory. In *Angewandte Chemie International Edition*, 2021, 60, 33, pp. 18152-18161. ISSN 14337851., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

5. [1] JERABEK, Paul - SANTHOSH, Archa - SCHWERDTFEGGER, Peter. Relativistic Effects Stabilize Unusual Gold(II) Sulfate Structure via Auophilic Interactions. In: *INORGANIC CHEMISTRY*, 2022, vol. 61, no. 33, pp. 13077-13084. ISSN 0020-1669., Registrované v: WOS, CC

Ohlas: zahraničný

_49

MAZEJ, Zoran - GILEWSKI, Tomasz - GORESHNIK, Evgeny A. - JAGLIČIĆ, Zvonko - DERZSI, Mariana - GROCHALA, Wojciech. Canted Antiferromagnetism in Two-Dimensional Silver(II) Bis[pentafluoridooxidotungstate(VI)]. In *Inorganic Chemistry*, 56, 1 (2017-01-03), pp. 224-233. V databáze: SCOPUS: 2-s2.0-85008883045 ; DOI: 10.1021/acs.inorgchem.6b02034 ; SCOPUS_INTID.

Ohlasy:

1. [1] TURNBULL, Douglas - WETMORE, Stacey D. - GERKEN, Michael. Synthesis, Characterization, and Lewis Acid Behavior of [W(NC 6 F 5)F 4] x and Computational Study of W(NR)F 4 (R = H, F, CH 3 , CF 3 , C 6 H 5). In *Inorganic Chemistry*, 2019, 58, 9, pp. 6363-6375. ISSN 00201669., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

2. [1] LI, Zhong Yi - WANG, Wen Jing - WU, Dong Qing - ZHANG, Chi - ZHANG, Fu Li - ZHAI, Bin - ZHANG, Jian Jun. Two 1D carboxylate-bridged magnets displaying solvent-dependent canted antiferromagnetic ordering. In *CrystEngComm*, 2019, 21, 27, pp. 4098-4103., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

3. [1] DORN, Katharina, V - HARTENBACH, Ingo. Press to Success: Gd₅FW₃O₁₆-The First Gadolinium(III) Fluoride Oxidotungstate(VI). In *CRYSTALS*, 2019, vol. 9, no. 8, pp. ISSN 2073-4352., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

4. [1] STOLL, Christiane - HEYMANN, Gunter - SEIBALD, Markus - BAUMANN, Dominik - HUPPERTZ, Hubert. K₃WO₇:Mn⁴⁺ A red oxyfluoride phosphor. In *JOURNAL OF FLUORINE CHEMISTRY*, 2019, vol. 226, no., pp. ISSN 0022-1139., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

5. [1] GOETTEL, James T. - BORTOLUS, Mark R. - STUART, Daniel G. - MERCIER, Helene P. A. - SCHROBILGEN, Gary J. Chromium Oxide Tetrafluoride and Its Reactions with Xenon Hexafluoride; the [XeF₅](+) and [Xe₂F₁₁](+) Salts of the [(CrOF₅)-O-VI](-), [(CrOF₅)-O-V](2-), [(Cr₂O₂F₈)-O-V](2-), and [(CrF₆)-F-IV](2-) Anions. In *CHEMISTRY-A EUROPEAN JOURNAL*, 2019, vol. 25, no. 69, pp. 15815-15829. ISSN 0947-6539., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

6. [1] BORTOLUS, Mark R. - MERCIER, Helene P. A. - SCHROBILGEN, Gary J. Group 6 Oxyfluoro-Anion Salts of [XeF₅](+)and [Xe₂F₁₁](+): Syntheses and Structures of [XeF₅][M₂O₂F₉] (M=Mo, W), [Xe₂F₁₁][M' OF₅] (M '=Cr, Mo, W), [XeF₅][HF₂].CrOF₄, and [XeF₅][WOF₅].XeOF₄. In *CHEMISTRY-A EUROPEAN JOURNAL*, 2020, vol. 26, no. 41, pp. 8935-8950. ISSN 0947-6539., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

7. [1] TURNBULL, Douglas - GERKEN, Michael. Crystal structure of an ordered [WOF₅]- salt: (1,10-phen-H)[WOF₅] (1,10-phen = 1,10-phenanthroline). In *Acta Crystallographica Section E: Crystallographic Communications*, 2020, 76, pp. 1345-1348., Registrované v: SCOPUS, WOS

Ohlas: zahraničný

8. [1] STOLL, Christiane - SEIBALD, Markus - BAUMANN, Dominik - HUPPERTZ, Hubert. K₂SnOF₄ and K₂WO₃F₂ different but similar. In *ZEITSCHRIFT FÜR NATURFORSCHUNG SECTION B-A JOURNAL OF CHEMICAL SCIENCES*, 2020, vol. 75, no. 9-10, pp. 833-841. ISSN 0932-0776., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

_50

MILANI, Sula - ANGEL, Ross J. - SCANDOLO, Lorenzo - MAZZUCHELLI, Mattia L. - BALLARAN, Tiziana Boffa - KLEMME, Stephan - DOMENEGHETTI, Maria C. - MILETICH, Ronald - SCHEIDL, Katharina S. - DERZSI, Mariana - TOKÁR, Kamil - PRENCIPE, Mauro - ALVARO, Matteo - NESTOLA, Fabrizio. Thermo-elastic behavior of grossular garnet at high pressures and temperatures. In *AMERICAN MINERALOGIST*. Vol. 102, no. 4 (2017), pp. 851-859. V databáze: WOS: 000401108600015 ; DOI: 10.2138/am-2017-5855.

Ohlasy:

1. [1] MIOZZI, F. - MORARD, G. - ANTONANGELI, D. - CLARK, A. N. - MEZOUAR, M. - DORN, C. - ROZEL, A. - FIQUET, G. Equation of State of SiC at Extreme Conditions: New Insight Into the Interior of Carbon-Rich Exoplanets. In *Journal of Geophysical Research: Planets*, 2018, 123, 9, pp. 2295-2309. ISSN 21699097., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

2. [1] BARKOFF, Drew W. - ASHLEY, Kyle T. - GUIMARAES DA SILVA, Raquel - MAZDAB, Frank K. - STEELE-MACINNIS, Matthew. THERMOBAROMETRY OF THREE SKARNS IN THE LUDWIG AREA, NEVADA, BASED ON RAMAN SPECTROSCOPY AND ELASTIC MODELING OF MINERAL INCLUSIONS IN GARNET. In *CANADIAN MINERALOGIST*, 2019, vol. 57, no. 1, pp. 25-45. ISSN 0008-4476., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

3. [1] KROLL, Herbert - SCHMID-BEURMANN, Peter - SELL, Alexander - BUESCHER, Julia - DOHR, Robin - KIRFEL, Armin. Thermal expansion and thermal pressure in Co and Ni olivines: A comparison with Mn and Fe olivines. In *EUROPEAN JOURNAL OF MINERALOGY*, 2019, vol. 31, no. 2, pp. 313-324. ISSN 0935-1221., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

4. [1] CISNEROS, M. - BEFUS, K. S. Applications and Limitations of Elastic Thermobarometry: Insights From

- Elastic Modeling of Inclusion-Host Pairs and Example Case Studies. In *Geochemistry, Geophysics, Geosystems*, 2020, 21, 10, pp., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
5. [1] YE, Zhilin - FAN, Dawei - TANG, Qizhe - XU, Jingui - ZHANG, Dongzhou - ZHOU, Wenge. Constraining the density evolution during destruction of the lithospheric mantle in the eastern North China Craton. In *Gondwana Research*, 2021, 91, pp. 18-30. ISSN 1342937X., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
6. [1] SU, Chang - LIU, Yonggang. Thermal expansion, heat capacity and Gruneisen parameter of grossular at high temperature and high pressure. In *HIGH TEMPERATURES-HIGH PRESSURES*, 2021, vol. 50, no. 2, pp. 105-119. ISSN 0018-1544., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
7. [1] MULLIGAN, Suzanne R. - STAVROU, Elissaios - CHARITON, Stella - TSCHAUNER, Oliver - SALAMAT, Ashkan - WELLS, Michael L. - SMITH, Alexander G. - HOISCH, Thomas D. - PRAKAPENKA, Vitali. Equation of state for natural almandine, spessartine, pyrope garnet: Implications for Quartz-in-Garnet elastic geobarometry. In *Minerals*, 2021, 11, 5, pp., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
8. [1] WEI, Wei - MAO, Zhu - SUN, Ningyu - SUN, Daoyuan - TKACHEV, Sergey N. High Pressure-Temperature Single-Crystal Elasticity of Grossular: Implications for the Low-Velocity Layer in the Bottom Transition Zone. In *Geophysical Research Letters*, 2021, 48, 9, pp. ISSN 00948276., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
9. [1] CISNEROS, Miguel - BARNES, Jaime D. - BEHR, Whitney M. - KOTOWSKI, Alissa J. - STOCKLI, Daniel F. - SOUKIS, Konstantinos. Insights from elastic thermobarometry into exhumation of high-pressure metamorphic rocks from Syros, Greece. In *SOLID EARTH*, 2021, vol. 12, no. 6, pp. 1335-1355. ISSN 1869-9510., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
10. [1] SCHOENIG, Jan - VON EYNATTEN, Hilmar - MEINHOLD, Guido - LUENSDORF, N. Keno. Life-cycle analysis of coesite-bearing garnet. In *GEOLOGICAL MAGAZINE*, 2021, vol. 158, no. 8, pp. 1421-1440. ISSN 0016-7568., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
11. [1] ZHONG, Xin - PETLEY-RAGAN, Arianne J. - INCCEL, Sarah H.M. - DABROWSKI, Marcin - ANDERSEN, Niels H. - JAMTVEIT, Bjørn. Lower crustal earthquake associated with highly pressurized frictional melts. In *Nature Geoscience*, 2021, 14, 7, pp. 519-525. ISSN 17520894., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
12. [1] CISNEROS, Miguel - BEHR, Whitney M. - PLATT, John P. - ANCZKIEWICZ, Robert. Quartz-in-garnet barometry constraints on formation pressures of eclogites from the Franciscan Complex, California. In *Contributions to Mineralogy and Petrology*, 2022-01-01, 177, 1, pp. ISSN 00107999., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
13. [1] LI, Bo - JIANG, Junjie - XU, Jingui - TKACHEV, Sergey N. - YE, Zhilin - HUANG, Shijie - GUO, Weihua - ZENG, Yongjun - PRAKAPENKA, Vitali B. - FAN, Dawei - ZHOU, Wenge. Effect of Thermoelastic Properties of the Pyrope-Almandine Solid Solutions on the Entrapment Pressure of Garnet-Related Elastic Geobarometer. In *FRONTIERS IN EARTH SCIENCE*, 2022, vol. 9, no., pp., Registrované v: WOS, CC
Ohlas: zahraničný
14. [1] SU, Chang - LIU, Yonggang - FAN, Dawei - SONG, Wei - YANG, Guang. Self-consistent thermodynamic parameters of pyrope and almandine at high-temperature and high-pressure conditions: Implication on the adiabatic temperature gradient. In *Physics of the Earth and Planetary Interiors*, 2022-01-01, 322, pp. ISSN 00319201., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
15. [1] YE, Zhilin - FAN, Dawei - LI, Bo - TANG, Qizhe - XU, Jingui - ZHANG, Dongzhou - ZHOU, Wenge. Thermal equation of state of the main minerals of eclogite: Constraining the density evolution of eclogite during the delamination process in Tibet. In *Solid Earth*, 2022-03-30, 13, 3, pp. 745-759. ISSN 18699510., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
16. [1] ULIAN, Gianfranco - VALDRÈ, Giovanni. QUANTAS: a Python software for the analysis of thermodynamics and elastic behavior of solids from ab initio quantum mechanical simulations and experimental data. In *Journal of Applied Crystallography*, 2022-04-01, 55, pp. 386-396. ISSN 00218898., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
17. [1] MULLIGAN, Suzanne R. - WELLS, Michael L. - HOISCH, Thomas D. - SALAMAT, Ashkan - CHILDS, Christian - TSCHAUNER, Oliver - CRADDOCK AFFINATI, Suzanne - WILLS, Marci A. - SMITH, G. Alexander. Deviation between quartz-in-garnet elastic geobarometry and equilibrium-based pressure-temperature modelling in Barrovian metamorphic rocks. In: *Journal of Metamorphic Geology*, 2022-08-01, 40, 6, pp. 1067-1086. ISSN 02634929., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
18. [1] XU, Jingui - FAN, Dawei - LI, Bo - TKACHEV, Sergey N. - PRAKAPENKA, Vitali B. - ZHANG, Dongzhou - YANG, Guangzhong - ZHOU, Yi - ZHOU, Wenge. High-Pressure and High-Temperature Single-Crystal Elasticity of Cr-Pyrope: Implications for the Density and Seismic Velocity of Subcontinental Lithospheric Mantle. In: *Geochemistry, Geophysics, Geosystems*, 2022-08-01, 23, 8, pp., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
19. [1] HU, Yancheng - WANG, Qingbo - YE, Yu - CHEN, Huawei - SMYTH, Joseph R. - ZHU, Xi - LIU, Dan - MIAO, Yunfan - CHEN, Guangchen. Thermal expansivity and Raman spectra of natural cordierite: A potential cordierite-garnet elastic thermometer. In: *Physics of the Earth and Planetary Interiors*, 2022-11-01, 332, pp. ISSN 00319201.,

Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

- _51 POLCZYNSKI, Piotr - GILEWSKI, Tomasz E. - GAWRACZYNSKI, Jakub - DERZSI, Mariana - LESZCZYNSKI, Piotr Jerzy - GADOMSKI, Wojciech - MAZEJ, Zoran - JURCZAKOWSKI, Rafal - GROCHALA, Wojciech. Efficient Electrosynthesis of (AgSO₄)-S-II: A Powerful Oxidizer and Narrow Band Gap Semiconductor. In *EUROPEAN JOURNAL OF INORGANIC CHEMISTRY*. Vol. , no. 35 (2016), pp. 5401-5404. V databáze: WOS: 000390348800001 ; DOI: 10.1002/ejic.201601183.
Ohlasy:
1. [1] WALTERS, Lauren N. - ZHANG, Chi - DRAVID, Vinayak P. - POEPELMEIER, Kenneth R. - RONDINELLI, James M. First-Principles Hydrothermal Synthesis Design to Optimize Conditions and Increase the Yield of Quaternary Heteroanionic Oxychalcogenides. In *CHEMISTRY OF MATERIALS*, 2021, vol. 33, no. 8, pp. 2726-2741. ISSN 0897-4756., Registrované v: WOS, SCOPUS
Ohlas: zahraničný
2. [1] XIANG, Danlei - IÑIGUEZ, Jesus A. - DENG, Jiao - GUAN, Xun - MARTINEZ, Antonio - LIU, Chong. AgII-Mediated Electrocatalytic Ambient CH₄ Functionalization Inspired by HSAB Theory. In *Angewandte Chemie International Edition*, 2021, 60, 33, pp. 18152-18161. ISSN 14337851., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
3. [1] JERABEK, Paul - SANTHOSH, Archa - SCHWERDTFEGER, Peter. Relativistic Effects Stabilize Unusual Gold(II) Sulfate Structure via Auophilic Interactions. In: *INORGANIC CHEMISTRY*, 2022, vol. 61, no. 33, pp. 13077-13084. ISSN 0020-1669., Registrované v: WOS, CC
Ohlas: zahraničný
- _52 TOKÁR, Kamil - DERZSI, Mariana - GROCHALA, Wojciech. Response of valence ordering in AgF₂ to B₂gAg-F stretching phonon. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 260.
Kategória publikácie do 2021: BFA
- _53 TOKÁR, Kamil - DERZSI, Mariana - MAZEJ, Zoran - GROCHALA, Wojciech. Lattice dynamics and thermodynamic stability of two polymorphic forms of AgF₂. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 327.
Kategória publikácie do 2021: BFA
- _54 TOKÁR, Kamil - PIEKARZ, Przemyslaw - DERZSI, Mariana - JOCHYM, Pawel T. - LAZEWSKI, Jan - STERNIK, Malgorzata - OLES, Andrzej M. - PARLINSKI, Krzysztof. Electronic and optical properties of the Mg_{2-x}FexSiO₄ spinel: From band insulator to Mott insulator. In *PHYSICAL REVIEW B*. Vol. 82, no. 19 (2010), pp. V databáze: WOS: 000284090600003 ; DOI: 10.1103/PhysRevB.82.195116.
Ohlasy:
1. [1] MA, Xing-Yu - ZHU, Yan-Yan - YAN, Qing-Bo - YOU, Jing-Yang - SU, Gang. Towards understanding physical origin of 2175 angstrom extinction bump in interstellar medium. In *MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY*, 2020, vol. 497, no. 2, pp. 2190-2200. ISSN 0035-8711., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
2. [1] MONTOYA-BAUTISTA, Claudia Victoria - ACEVEDO-PEÑA, Próspero - ZANELLA, Rodolfo - RAMÍREZ-ZAMORA, Rosa María. Characterization and Evaluation of Copper Slag as a Bifunctional Photocatalyst for Alcohols Degradation and Hydrogen Production. In *Topics in Catalysis*, 2021, 64, 1-2, pp. 131-141. ISSN 10225528., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- _55 UHLIAR, Matej. *Modelling of chlorine enriched crystal lattice of silver*. 2019. Dostupné na internete: <http://is.stuba.sk/zp/portal_zp.pl?podrobnosti=134264>.
- _56 UHLIAR, Matej. *Modelling of novel crystalline binary silver chloride phases with evolutionary algorithms*. 2021. Dostupné na internete: <http://is.stuba.sk/zp/portal_zp.pl?podrobnosti=157938>.
- _57 UHLIAR, M. - DERZSI, Mariana. Towards new binary silver halides: from fluorine to chlorine. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 328.
Kategória publikácie do 2021: BFA
- _58 WEGNER, W. - TOKÁR, Kamil - DERZSI, Mariana - GROCHALA, Wojciech. Theoretical estimation of the work function of AgF₂. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 229.
Kategória publikácie do 2021: BFA
- _59 WITKOWSKI, M. - DERZSI, Mariana - GROCHALA, Wojciech. 1/3 Ni-doped AgF₂? DFT+U study of as yet unknown Ag₂NiF₆. In *19th European Symposium on Fluorine Chemistry : 19th ESFC, 25. - 31. 8. 2019, Warsaw, Poland*. 1. vyd. Varšava : University of Warsaw, 2019, S. 331.
Kategória publikácie do 2021: BFA

I2	I2	4
O2	O2	1
O3	O3	2
V2	V2	2
V3	V3	16
XXX	Nezaradené	59
Súčet		84
Štatistika: kategória ohlasov		
1	Citácie v zahraničných publikáciách, registrované v citačných indexoch Web of Science a databáze SCOPUS	127
Súčet		127