

Publikácie / Publications

Institute: SAVANOCH - Ústav anorganickej chémie SAV
Year of publication 2016~2021

Statistics publication category

ABA	Monographic studies in journals and proceedings published abroad	2
ABC	Chapters in scientific monographs published abroad	9
ADCA	Scientific papers in foreign journals registered in Current Contents Connect with IF (impacted)	358
ADDA	Scientific papers in domestic journals registered in Current Contents Connect with IF (impacted)	2
ADMA	Scientific papers in foreign impacted journals registered in Web of Sciences or Scopus	10
ADMB	Scientific papers in foreign non-impacted journals registered in Web of Sciences or Scopus	16
ADNB	Scientific papers in domestic non-impacted journals registered in Web of Sciences or Scopus	5
AFA	Published invited papers from foreign scientific conferences	2
AFC	Published papers from foreign scientific conferences	20
AFD	Published papers from domestic scientific conferences	55
AFE	Abstracts of invited papers from foreign conferences	7
AFF	Abstracts of invited papers from domestic conferences	6
AFG	Abstracts of papers from foreign conferences	87
AFH	Abstracts of papers from domestic conferences	190
BCB	Textbooks for primary and secondary schools	1
BDE	Professional papers in other foreign journals (not registered in CCC)	2
BEE	Professional papers in foreign proceedings (conference/non-conference; peer-reviewed/non-peer-reviewed)	1
BEF	Professional papers in domestic proceedings (conference/non-conference; peer-reviewed/non-peer-reviewed)	16
FAI	Editorial work on book publications (bibliographies, encyclopedias, catalogues, dictionaries, collective publications/proceedings, atlases ...)	6
GII	Other publications and documents which is not possible to categorize into classes/categories mentioned above	148
Count		943

ABA Monographic studies in journals and proceedings published abroad

ABA01 BUJDÁK, Juraj. Hybrids with functional dyes : Chapter 18. In *Inorganic nanosheets and nanosheet-based materials : Fundamentals and applications of two-dimensional systems*. - Tokyo, Japan : Springer Japan, 2017, p. 419-465. ISBN

978-4-431-56494-2. ISSN 1571-5744. Dostupné na:
https://doi.org/10.1007/978-4-431-56496-6_18

- ABA02 BUJDÁK, Juraj. Resonance energy transfer in hybrid systems of photoactive dye molecules and layered inorganics. In *Dyes and Photoactive Molecules in Microporous Systems : Structure and Bonding*. - Švajčiarsko : Springer, 2020, 2020, vol. 183, p. 205-250. ISBN 978-3-030-56633-3. Dostupné na:
https://doi.org/10.1007/430_2020_55

ABC Chapters in scientific monographs published abroad

- ABC01 GALUSKOVÁ, Dagmar - GALUSEK, Dušan. Corrosion and degradation of glass. In *Encyclopedia of Materials: Technical ceramics and glasses*. - Oxford : Elsevier, 2021, 2021, vol. 1, p. 932-940. ISBN 978-0-12-818542-1. Dostupné na:
<https://doi.org/10.1016/B978-0-12-818542-1.00069-2>
- ABC02 GATES, W.P. - PETIT, Sabine - MADEJOVÁ, Jana. Applications of NIR/MIR to determine site occupancy in smectites : Chapter 7. In *Infrared and Raman spectroscopies of clay minerals*. - Netherlands : Elsevier, 2017, p. 200-221. ISBN 978-0-08-100355-8. ISSN 1572-4352. Dostupné na:
<https://doi.org/10.1016/B978-0-08-100355-8.00007-2>
- ABC03 MADEJOVÁ, Jana - GATES, W.P. - PETIT, Sabine. IR spectra of clay minerals : Chapter 5. In *Infrared and Raman spectroscopies of clay minerals*. - Netherlands : Elsevier, 2017, p. 107-149. ISBN 978-0-08-100355-8. ISSN 1572-4352. Dostupné na: <https://doi.org/10.1016/B978-0-08-100355-8.00005-9>
- ABC04 MADEJOVÁ, Jana - PÁLKOVÁ, Helena. NIR contribution to the study of modified clay minerals. In *Infrared and Raman spectroscopies of clay minerals*. - Netherlands : Elsevier, 2017, p. 447-481. ISBN 978-0-08-100355-8. ISSN 1572-4352. Dostupné na: <https://doi.org/10.1016/B978-0-08-100355-8.00013-8>
- ABC05 MACHÁČEK, Jan - CHROMČÍKOVÁ, Mária - LIŠKA, Marek. Parameterization and validation of thermochemical models of glass by advanced statistical analysis of spectral data : Chapter 12. In *Thermal physics and thermal analysis : From macro to micro, highlighting thermodynamics, kinetics and nanomaterials*. - Switzerland : Springer International Publishing AG, 2017, p. 257-278. ISBN 978-3-319-45897-7. ISSN 1571-3105. Dostupné na:
https://doi.org/10.1007/978-3-319-45899-1_12
- ABC06 PROTSENKO, V.** - KITYK, Anna - DANILOV, F.I. - PAVLÍK, Viliam - BOČA, Miroslav. Electropolishing of metals and alloys using electrochemical systems based on environmentally safe deep eutectic solvents. In *Environmentally friendly technologies : Advances in research and future directions*. - New York, USA : Nova Science Publishers, Inc., 2020, p. 101-131. ISBN 978-1-53678-400-6.
- ABC07 RIAZ, Ufana - ASHRAF, S. M. - BUJDÁK, Juraj. Recent advances in nano photodynamic therapy : Chapter 6. In *Recent advances in analytical techniques*. - UAE, Sharjah : Bentham Science Publishers, 2017, vol. 1, p. 200-223. ISBN 978-1-68108-448-0.

ABC08 SCHOLTZOVÁ, Eva**. Computational modeling of nanoclays. In *Micro & Nano Technologies Series : Clay Nanoparticles. Properties and Applications*. - Netherlands : Elsevier, 2020, p. 139-166. ISBN 978-0-12-816783-0.

ABC09 TATARKOVÁ, Monika - TATARKO, Peter - ŠAJGALÍK, Pavol. Si₃N₄ ceramics, structure and properties. In *Encyclopedia of Materials: Technical ceramics and glasses*. - Oxford : Elsevier, 2021, 2021, vol. 2, p. 109-118. ISBN 978-0-12-818542-1. Dostupné na: <https://doi.org/10.1016/B978-0-12-818542-1.00021-7>

ADCA Scientific papers in foreign journals registered in Current Contents Connect with IF (impacted)

ADCA01 AFSHARIMANI, Nasima** - DURÁN, Alicia - GALUSEK, Dušan - CASTRO, Yolanda. Hybrid sol-gel silica coatings containing graphene nanosheets for improving the corrosion protection of AA2024-T3. In *Nanomaterials-Basel*, 2020, vol.10, no. 6, p. 1050-1-1050-13. (2019: 4.324 - IF, Q2 - JCR, 0.858 - SJR, Q1 - SJR, Current Contents - CCC). (2020 - Current Contents, WOS, SCOPUS). ISSN 2079-4991. Dostupné na: <https://doi.org/10.3390/nano10061050>

ADCA02 AKUSEVICH, A. - PARCHOVIANSKÁ, I. - PARCHOVIANSKÝ, Milan - PRNOVÁ, Anna - LOFAJ, František - VOJTKO, Marek - KLEMENT, Róbert**. Glass-ceramic Ce³⁺-doped YAG-Al₂O₃ composites prepared by sintering of glass microspheres. In *International Journal of Applied Glass Science*, 2021, vol. 12, no. 4, p. 497-508. (2020: 2.029 - IF, Q2 - JCR, 0.383 - SJR, Q3 - SJR, Current Contents - CCC). (2021 - Current Contents). ISSN 2041-1286. Dostupné na: <https://doi.org/10.1111/ijag.16174>

ADCA03 ALDERMAN, Oliver - LIŠKA, Marek - MACHÁČEK, Jan - BENMORE, C.J. - LIN, A. - TAMALONIS, A. - WEBER, J.K.R. Temperature-driven structural transitions in molten sodium borates Na₂O-B₂O₃: X-ray diffraction, thermodynamic modeling, and implications for topological constraint theory. In *Journal of Physical Chemistry C*, 2016, vol. 120, no. 1, p. 553-560. (2015: 4.509 - IF, Q1 - JCR, 1.886 - SJR, Q1 - SJR, Current Contents - CCC). (2016 - Current Contents). ISSN 1932-7447. Dostupné na: <https://doi.org/10.1021/acs.jpcc.5b10277>

ADCA04 AMSLER, Jonas** - PLESSOW, Philipp N. - STUDT, Felix - BUČKO, Tomáš**. Anharmonic correction to adsorption free energy from DFT-based MD using thermodynamic integration. In *Journal of Chemical Theory and Computation*, 2021, vol. 17, no. 2, p. 1155-1169. (2020: 6.006 - IF, Q1 - JCR, 2.001 - SJR, Q1 - SJR, Current Contents - CCC). (2021 - Current Contents). ISSN 1549-9618. Dostupné na: <https://doi.org/10.1021/acs.jctc.0c01022>

ADCA05 ASHER, James Richard**. An animated visualization of orbital angular momentum and spin-orbit coupling. In *International Journal of Quantum Chemistry*, 2018, vol. 118, no. 18, art. no. e25683, p. 1-7. (2017: 2.568 - IF, Q1 - JCR, 1.003 - SJR, Q1 - SJR, Current Contents - CCC). (2018 - Current Contents). ISSN 0020-7608. Dostupné na: <https://doi.org/10.1002/qua.25683>

ADCA06 AZZI, Andrezza de Almeida** - UHLÍK, Peter - OSACKÝ, Marek - ZANARDO, Antenor - PÁLKOVÁ, Helena. Changes in technological properties

and microstructure of clayey raw materials from the Corumbataí Formation upon drying: Relevance to dry route tilemaking process. In *Applied Clay Science*, 2018, vol. 157, p. 92-101. (2017: 3.641 - IF, Q1 - JCR, 0.992 - SJR, Q1 - SJR, Current Contents - CCC). (2018 - Current Contents). ISSN 0169-1317. Dostupné na: <https://doi.org/10.1016/j.clay.2018.02.033>

- ADCA07 AZZI, Andrezza de Almeida - OSACKÝ, Marek - UHLÍK, Peter - ČAPLOVIČOVÁ, Mária - ZANARDO, Antenor - MADEJOVÁ, Jana. Characterization of clays from the Corumbataí formation used as raw material for ceramic industry in the Santa Gertrudes district, Sao Paulo, Brazil. In *Applied Clay Science*, 2016, vol. 132-133, p. 232-242. (2015: 2.586 - IF, Q1 - JCR, 0.806 - SJR, Q2 - SJR, Current Contents - CCC). (2016 - Current Contents). ISSN 0169-1317. Dostupné na: <https://doi.org/10.1016/j.clay.2016.06.009>
- ADCA08 BABU, Singarapu** - GALUSEK, Dušan - DURÁN, Alicia - PASCUAL, María Jesús**. Glass-ceramics processed by spark plasma sintering (SPS) for optical applications. In *Applied Sciences-Basel*, 2020, vol. 10, no. 8, p. 2791-1-2791-21. (2019: 2.474 - IF, Q2 - JCR, 0.418 - SJR, Q1 - SJR, Current Contents - CCC). (2020 - Current Contents). ISSN 2076-3417. Dostupné na: <https://doi.org/10.3390/APP10082791>
- ADCA09 BAČÍK, Peter** - FRIDRICHOVÁ, Jana - UHER, Pavel - VACULOVÍČ, T. - KUREKOVÁ, Valéria - ŠKODA, Radek - DEKAN, Július - MIGLIERINI, Marcel - MALÍČKOVÁ, Iveta. Beryl crystal chemistry and trace elements: Indicators of pegmatite development and fractionation (Damara Belt, Namibia). In *Lithos*, 2021, vol. 404-405, p. 106441-1-106441-16. (2020: 4.004 - IF, Q1 - JCR, 1.899 - SJR, Q1 - SJR, Current Contents - CCC). (2021 - Current Contents). ISSN 0024-4937. Dostupné na: <https://doi.org/10.1016/j.lithos.2021.106441>
- ADCA10 BAČÍK, Peter** - FRIDRICHOVÁ, Jana - UHER, Pavel - RYBÁR, S. - KUREKOVÁ, Valéria - LUPTÁKOVÁ, Jarmila - VRABLÍKOVÁ, Dana - PUKANČÍK, Libor - VACULOVÍČ, T. Octahedral substitution in beryl from weakly fractionated intragranitic pegmatite Predne Solisko, Tatry Mountains (Slovakia): the indicator of genetic conditions. In *Journal of Geosciences*, 2019, vol. 64, no. 1, p. 59-72. (2018: 1.275 - IF, Q3 - JCR, 0.559 - SJR, Q2 - SJR, Current Contents - CCC). (2019 - Current Contents). ISSN 1802-6222. Dostupné na: <https://doi.org/10.3190/jgeosci.272>
- ADCA11 BAČÍK, Peter** - FRIDRICHOVÁ, Jana - ŠTUBŇA, Ján - BANCÍK, T. - ILLÁŠOVÁ, Ľudmila - PÁLKOVÁ, Helena - ŠKODA, Radek - MIKUŠ, Tomáš - MILOVSKÁ, Stanislava - VACULOVÍČ, T. - SEČKÁR, Peter. The REE-induced absorption and luminescence in yellow gem-quality Durango-type hydroxylapatite from Muránska Dlhá Lúka, Slovakia. In *MINERALS-BASEL*, 2020, vol. 10, no. 11, p. 1001-1-1001-21. (2019: 2.380 - IF, Q2 - JCR, 0.494 - SJR, Q2 - SJR, Current Contents - CCC). (2020 - Current Contents). ISSN 2075-163X. Dostupné na: <https://doi.org/10.3390/min10111001>
- ADCA12 BALÁZSI, Csaba - FOGARASSY, Zsolt - TAPASZTÓ, Orsolya - KAILER, Andreas - SCHRÖDER, Christian - PARCHOVIANSKÝ, Milan - GALUSEK, Dušan - DUSZA, Ján - BALAZSI, K. Si₃N₄/graphene nanocomposites for

tribological application in aqueous environments prepared by attritor milling and hot pressing. In *Journal of the European Ceramic Society*, 2017, vol. 37, no. 12, p. 3797-3804. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, Current Contents - CCC). (2017 - Current Contents). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2017.03.022>

ADCA13 BALESTRAT, Maxime - ACOSTA, Emanuelle Diz - HANZEL, Ondrej - TESSIER-DOYEN, Nicolas - MACHADO, Ricardo - ŠAJGALÍK, Pavol - LENČEŠ, Zoltán - BERNARD, Samuel**. Additive-free low temperature sintering of amorphous Si-B-C powders derived from boron-modified polycarbosilanes: Toward the design of SiC with tunable mechanical, electrical and thermal properties. In *Journal of the European Ceramic Society*, 2020, vol. 40, no. 7, p. 2604-2612. (2019: 4.495 - IF, Q1 - JCR, 1.164 - SJR, Q1 - SJR, Current Contents - CCC). (2020 - Current Contents). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2019.12.037>

ADCA14 BALTRUSAITIS, Jonas - BUČKO, Tomáš - MICHAELS, W. - MAKKEE, M. - MUL, G. Catalytic methyl mercaptan coupling to ethylene in chabazite: DFT study of the first C-C bond formation. In *Applied Catalysis B: Environmental*, 2016, vol. 187, p. 195-203. (2015: 8.328 - IF, Q1 - JCR, 2.326 - SJR, Q1 - SJR, Current Contents - CCC). (2016 - Current Contents). ISSN 0926-3373. Dostupné na: <https://doi.org/10.1016/j.apcatb.2016.01.021>

ADCA15 BARLOG, Martin** - PÁLKOVÁ, Helena - BUJDÁK, Juraj. Luminescence of a laser dye in organically-modified layered silicate pigments. In *Dyes and Pigments*, 2021, vol. 191, p. 109380-1-109380-11. (2020: 4.889 - IF, Q1 - JCR, 0.827 - SJR, Q1 - SJR, Current Contents - CCC). (2021 - Current Contents). ISSN 0143-7208. Dostupné na: <https://doi.org/10.1016/j.dyepig.2021.109380>

ADCA16 BELUŠÁKOVÁ, Silvia - SOLA-LLANO, R. - LOPEZ ARBELOA, I. - MARTÍNEZ-MARTÍNEZ, V.* - BUJDÁK, Juraj**. Resonance energy transfer between dye molecules in hybrid films of a layered silicate, including the effect of dye concentration thereon. In *Applied Clay Science*, 2018, vol. 155, p. 57-64. (2017: 3.641 - IF, Q1 - JCR, 0.992 - SJR, Q1 - SJR, Current Contents - CCC). (2018 - Current Contents). ISSN 0169-1317. Dostupné na: <https://doi.org/10.1016/j.clay.2018.01.001>

ADCA17 BELUŠÁKOVÁ, Silvia - MARTÍNEZ-MARTÍNEZ, V. - LOPEZ ARBELOA, I. - BUJDÁK, Juraj. Resonance energy transfer between dye molecules in colloids of a layered silicate. The effect of dye surface concentration. In *Journal of Physical Chemistry C*, 2017, vol. 121, p. 8300-8309. (2016: 4.536 - IF, Q1 - JCR, 1.964 - SJR, Q1 - SJR, Current Contents - CCC). (2017 - Current Contents). ISSN 1932-7447. Dostupné na: <https://doi.org/10.1021/acs.jpcc.7b00947>

ADCA18 BERTOLLA, Luca** - CHLUP, Zdeněk - TATARKO, Peter - HANZEL, Ondrej - ŠEVEČEK, Oldřich - ROUPCOVÁ, Pavla - DLOUHÝ, Ivo. Preparation and characterization of novel environmentally friendly Al₂O₃/SiO₂/CaO ceramic foams. In *Ceramics International*, 2018, vol. 44, p. 19063-19069. (2017: 3.057 - IF, Q1 - JCR, 0.784 - SJR, Q1 - SJR, Current Contents - CCC). (2018 - Current

Contents). ISSN 0272-8842. Dostupné na:
<https://doi.org/10.1016/j.ceramint.2018.07.107>

- ADCA19 BERTOLLA, Luca - DLOUHÝ, Ivo - TATARKO, Peter - VIANI, Alberto - MAHAJAN, Amit - CHLUP, Zdeněk - REECE, Michael J. - BOCCACCINI, Aldo. Pressureless spark plasma-sintered Bioglass® 45S5 with enhanced mechanical properties and stress-induced new phase formation. In *Journal of the European Ceramic Society*, 2017, vol. 37, no. 7, p. 2727-2736. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, Current Contents - CCC). (2017 - Current Contents). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2017.02.003>
- ADCA20 BOČA, Miroslav** - NETRIOVÁ, Zuzana - RAKHMATULLIN, Aydar - VASKOVÁ, Zuzana - HADZIMOVÁ, Eva - SMRČOK, Ľubomír - HANZEL, Ondrej - KUBÍKOVÁ, Blanka. The differing responses of various techniques in measuring the phase transformations of K₂ZrF₆. In *Journal of Molecular Liquids*, 2019, vol. 287, p. 110969-1-110969-10. (2018: 4.561 - IF, Q1 - JCR, 0.862 - SJR, Q1 - SJR, Current Contents - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0167-7322. Dostupné na: <https://doi.org/10.1016/j.molliq.2019.110969>
- ADCA21 BOČA, Miroslav** - MOLOKEEV, Maxim - RAKHMATULLIN, Aydar - KUBÍKOVÁ, Blanka - NETRIOVÁ, Zuzana. The structure of the metastable K₁₈Ta₅Zr₅F₆₃ phase. In *New Journal of Chemistry*, 2020, vol. 44, no. 22, p. 9264-9270. (2019: 3.288 - IF, Q2 - JCR, 0.712 - SJR, Q1 - SJR, Current Contents - CCC). (2020 - Current Contents). ISSN 1144-0546. Dostupné na: <https://doi.org/10.1039/d0nj02428g>
- ADCA22 BODIŠOVÁ, Katarína - KLEMENT, Róbert - GALUSEK, Dušan - POUCHLÝ, Václav - DRDLÍK, Daniel - MACA, Karel. Luminescent rare-earth-doped transparent alumina ceramics. In *Journal of the European Ceramic Society*, 2016, vol. 36, no. 12, p. 2975-2980. (2015: 2.933 - IF, Q1 - JCR, 1.135 - SJR, Q1 - SJR, Current Contents - CCC). (2016 - Current Contents). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2015.12.032>
- ADCA23 BOHÁČ, Peter - CZÍMEROVÁ, Adriana - BUJDÁK, Juraj. Enhanced luminescence of 3,3'-diethyl-2,2'-thiacyanine cations adsorbed on saponite particles. In *Applied Clay Science*, 2016, vol. 127-128, p. 64-69. (2015: 2.586 - IF, Q1 - JCR, 0.806 - SJR, Q2 - SJR, Current Contents - CCC). (2016 - Current Contents). ISSN 0169-1317. Dostupné na: <https://doi.org/10.1016/j.clay.2016.04.008>
- ADCA24 BOHÁČ, Peter** - CZÍMEROVÁ, Adriana - SASAI, Ryo - BUJDÁK, Juraj. Luminescence and resonance energy transfer in the colloids of cyanine dyes and saponite modified with cationic surfactants. In *Applied Clay Science*, 2020, vol. 189, p. 105536-1-105536-9. (2019: 4.605 - IF, Q1 - JCR, 1.069 - SJR, Q1 - SJR, Current Contents - CCC). (2020 - Current Contents). ISSN 0169-1317. Dostupné na: <https://doi.org/10.1016/j.clay.2020.105536>
- ADCA25 BOHÁČ, Peter** - SASAI, Ryo - SOONTORNCHAIYAKUL, W. - CZÍMEROVÁ, Adriana - BUJDÁK, Juraj. Resonance energy transfer between cyanine dyes in hybrid films of layered silicate prepared by layer-by-layer method. In *Applied Clay Science*, 2021, vol. 202, p. 105985-1-105985-9. (2020: 5.467 - IF,

Q1 - JCR, 1.062 - SJR, Q1 - SJR, Current Contents - CCC). (2021 - Current Contents). ISSN 0169-1317. Dostupné na:
<https://doi.org/10.1016/j.clay.2021.105985>

ADCA26 BOHÁČ, Peter** - BUJDÁK, Juraj. Tuning the photophysical properties of cyanine dyes with clay minerals. In *Clays and Clay Minerals*, 2018, vol. 66, no. 2, p. 127-137. (2017: 1.825 - IF, Q2 - JCR, 0.532 - SJR, Q2 - SJR, Current Contents - CCC). (2018 - Current Contents). ISSN 0009-8604. Dostupné na:
<https://doi.org/10.1346/CCMN.2018.064090>

ADCA27 BOJE, Astrid - TAIFAN, William E. - STRÖM, Henrik - BUČKO, Tomáš - BALTRUSAITIS, Jonas - HELLMAN, Anders**. First-principles-informed energy span and microkinetic analysis of ethanol catalytic conversion to 1,3-butadiene on MgO. In *Catalysis Science and Technology*, 2021, vol. 11, no. 20, p. 6682-6694. (2020: 6.119 - IF, Q2 - JCR, 1.635 - SJR, Q1 - SJR, Current Contents - CCC). (2021 - Current Contents). ISSN 2044-4753. Dostupné na:
<https://doi.org/10.1039/d1cy00419k>

ADCA28 BORA, Pankaj L. - NOVOTNÝ, Jan - RUUD, Kenneth - KOMOROVSKÝ, Stanislav - MAREK, Radek**. Electron-spin structure and metal-ligand bonding in open-shell systems from relativistic EPR and NMR: A case study of square-planar iridium catalysts. In *Journal of Chemical Theory and Computation*, 2019, vol. 15, no. 1, p. 201-214. (2018: 5.313 - IF, Q1 - JCR, 2.236 - SJR, Q1 - SJR, Current Contents - CCC). (2019 - Current Contents). ISSN 1549-9618. Dostupné na:
<https://doi.org/10.1021/acs.jctc.8b00914>

ADCA29 BRANDOVÁ, Daniela - SVOBODA, Roman - LIŠKA, Marek - MÁLEK, Jiří. Thermal characterization of (As₂Se₃)_{0.5}(As₂Te₃)_{0.5} infrared glass. In *Journal of Non-Crystalline Solids*, 2017, vol. 475, p. 121-128. (2016: 2.124 - IF, Q1 - JCR, 0.685 - SJR, Q1 - SJR, Current Contents - CCC). (2017 - Current Contents, WOS, SCOPUS). ISSN 0022-3093. Dostupné na:
<https://doi.org/10.1016/j.jnoncrysol.2017.09.011>

ADCA30 BROCLAWIK, Ewa - GÓRA-MAREK, Kinga - RADOŃ, Mariusz - BUČKO, Tomáš - STEPNIIEWSKI, Adam. The dependence on ammonia pretreatment of N-O activation by Co(II) sites in zeolites: a DFT and ab initio molecular dynamics study. In *Journal of molecular modeling*, 2017, vol. 23, no. 5, p. 160-1-160-13. (2016: 1.425 - IF, Q3 - JCR, 0.466 - SJR, Q2 - SJR, Current Contents - CCC). (2017 - Current Contents). ISSN 1610-2940. Dostupné na:
<https://doi.org/10.1007/s00894-017-3322-z>

ADCA31 BUČKO, Tomáš** - GEŠVANDTNEROVÁ, Monika - ROCCA, Dario**. Ab initio calculations of free energy of activation at multiple electronic structure levels made affordable: An effective combination of perturbation theory and machine learning. In *Journal of Chemical Theory and Computation*, 2020, vol. 16, no. 10, p. 6049-6060. (2019: 5.011 - IF, Q1 - JCR, 1.759 - SJR, Q1 - SJR, Current Contents - CCC). (2020 - Current Contents). ISSN 1549-9618. Dostupné na:
<https://doi.org/10.1021/acs.jctc.0c00486>

- ADCA32 BUČKO, Tomáš - CHIBANI, Siwar - PAUL, Jean-François - CANTREL, Laurent - BADAWI, Michael. Dissociative iodomethane adsorption on Ag-MOR and the formation of AgI clusters: an ab initio molecular dynamics study. In *Physical Chemistry Chemical Physics*, 2017, vol. 19, no. 40, p. 27530-27543. (2016: 4.123 - IF, Q1 - JCR, 1.685 - SJR, Q1 - SJR, Current Contents - CCC). (2017 - Current Contents). ISSN 1463-9076. Dostupné na: <https://doi.org/10.1039/c7cp05562e>
- ADCA33 BUČKO, Tomáš** - ŠIMKO, František**. Effect of alkaline metal cations on the ionic structure of cryolite melts: Ab-initio NpT MD study. In *Journal of Chemical Physics*, 2018, vol. 148, no. 6, art. no. 064501. (2017: 2.843 - IF, Q2 - JCR, 1.252 - SJR, Q1 - SJR, Current Contents - CCC). (2018 - Current Contents). ISSN 0021-9606. Dostupné na: <https://doi.org/10.1063/1.5017106>
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