



## Projekta Izp-2018/1-0147 rezultāti

### Jaunu materiālu teorētiskā prognozēšana vidēju temperatūru keramiskām kurināmā šūnām

Oriģināli zinātniskie raksti, kas publicēti zinātniskos žurnālos, rakstu krājumos vai konferenču rakstu krājumos, kuri ir indeksēti datu bāzēs Web of Science Core Collection, SCOPUS vai ERIH PLUS

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2. Chesnokov, A.; Gryaznov, D.; Kotomin, E. First principles calculations on CeO<sub>2</sub> doped with Tb<sup>3+</sup> ions. – Opt. Mater., 2019, 90, 76-83, <https://doi.org/10.1016/j.optmat.2019.02.016>
3. Evarestov, R. A.; Senocrate, A.; Kotomin, E. A.; Maier, J. First-principles calculations of iodine-related point defects in CsPbI<sub>3</sub>. - Phys. Chem. Chem. Phys., 2019, 21 (15), 7841-7846, <https://doi.org/10.1039/c9cp00414a>
4. Heifets, E.; Kotomin, E. A.; Bagaturyants, A. A.; Maier, J. Thermodynamic stability of non-stoichiometric SrFeO<sub>3-δ</sub>: A hybrid DFT study. - Phys. Chem. Chem. Phys., 2019, 21 (7), 3918-3931, <https://doi.org/10.1039/c8cp07117a>
5. Zvejnieks, G.; Rusevich, L. L.; Gryaznov, D.; Kotomin, E. A. Interface-induced enhancement of piezoelectricity in the (SrTiO<sub>3</sub>): M/(BaTiO<sub>3</sub>)M - M superlattice for energy harvesting applications. - Phys. Chem. Chem. Phys., 2019, 21 (42), 23541-23551, <https://doi.org/10.1039/c9cp04086b>
6. Zvejnieks, G.; Zavickis, D.; Kotomin, E. A.; Gryaznov, D. BaCoO<sub>3</sub>monoclinic structure and chemical bonding analysis: Hybrid DFT calculations. - Phys. Chem. Chem. Phys., 2021, 23 (32), 17493-17501, <https://doi.org/10.1039/d1cp01900g>
7. Lushchik, A.; Kuzovkov, V. N.; Kotomin, E. A.; Prieditis, G.; Seeman, V.; Shablonin, E.; Vasil'chenko, E.; Popov, A. I. Evidence for the formation of two types of oxygen interstitials in neutron-irradiated α-Al<sub>2</sub>O<sub>3</sub> single crystals. - Sci. Rep., 2021, 11 (1), <https://doi.org/10.1038/s41598-021-00336-0>



8. Zavickis, D.; Zvejnieks, G.; Chesnokov, A.; Gryaznov, D. Single oxygen vacancy in BaCoO<sub>3</sub>: Hybrid DFT calculations and local site symmetry approach. - Solid State Ionics, 2022, 375, <https://doi.org/10.1016/j.ssi.2021.115835>