



## Projekta Izp-2020/2-0009 rezultāti

### Jaunu uzlaboto perovskītu skaitļošanas izpēte pielietojumiem enerģētikā

*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*

1. Eglitis, R. I.; Purans, J.; Popov, A. I.; Jia, R. Tendencies in abo3 perovskite and srf2, baf2 and caf2 bulk and surface f-center ab initio computations at high symmetry cubic structure. – Symmetry, 2021, 13 (10), <https://doi.org/10.3390/sym13101920>
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4. Eglitis, R. I.; Kotomin, E. A.; Popov, A. I.; Kruchinin, S. P.; Jia, R. Comparative ab initio calculations of SrTiO<sub>3</sub>, BaTiO<sub>3</sub>, PbTiO<sub>3</sub>, and SrZrO<sub>3</sub> (001) and (111) surfaces as well as oxygen vacancies. – Fiz. Nizk. Temp., 2022, 48 (1), 87-96, <https://doi.org/10.1063/10.0008968>