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FUNDAMENTĀLO UN LIETIŠĶO PĒTĪJUMU PROJEKTI

Projekta Izp-2018/2-0353 rezultāti

Metālu hidrīdu rentgena absorbcijas pētījumi ekstrēma spiediena apstākļos

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. Nataf, L.; Baudelet, F.; Polian, A.; Jonane, I.; Anspoks, A.; Kuzmin, A.; Irifune, T. Recent progress in high pressure X-ray absorption spectroscopy studies at the ODE beamline. - High. Pressure. Res., 2020, 40 (1), 82-87, https://doi.org/10.1080/08957959.2019.1700979

2. Kuzmin, A.; Timoshenko, J.; Kalinko, A.; Jonane, I.; Anspoks, A. Treatment of disorder effects in X-ray absorption spectra beyond the conventional approach. - Radiat. Phys. Chem., 2020, 175, https://doi.org/10.1016/j.radphyschem.2018.12.032

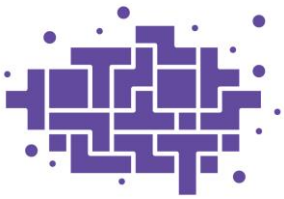
3. Kuzmin, A. First-principles LCAO study of the low- and room-temperature phases of CdPS3. - Low Temp. Phys., 2020, 46 (12), 1217-1222, https://doi.org/10.1063/10.0002477

4. Kuzmin, A. First-principles LCAO study of the low- and room-temperature phases of CdPS3. – Fiz. Nizk. Temp., 2020, 46 (12), 1430-1436.

5. Evarestov, R. A.; Kuzmin, A. Origin of pressure-induced insulator-to-metal transition in the van der Waals compound FePS3 from first-principles calculations. - J. Comput. Chem., 2020, 41 (14), 1337-1344, https://doi.org/10.1002/jcc.26178

6. Evarestov, R. A.; Kuzmin, A. Topological analysis of chemical bonding in the layered FePSe3 upon pressure-induced phase transitions. - J. Comput. Chem., 2020, 41 (31), 2610-2623, https://doi.org/10.1002/jcc.26416

7. Bocharov, D.; Krack, M.; Rafalskij, Y.; Kuzmin, A.; Purans, J. Ab initio molecular dynamics simulations of negative thermal expansion in ScF3: The effect of the supercell size. – Comput. Mater. Sci., 2020, 171, https://doi.org/10.1016/j.commatsci.2019.109198



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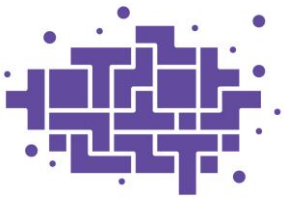

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