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DFT-Based Computational Prediction of Hypothetical Cubic C1b SrMgSi and SrMgSn Half-Heusler Phases

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Abstract

The search for new functional materials with suitable electronic, optical, and thermoelectric properties is of great interest for future energy and optoelectronic technologies. In this context, a first-principles computational investigation is carried out on the hypothetical cubic C1b Half-Heusler compounds SrMgSi and SrMgSn.

Using density functional theory (DFT), the study examines their structural, electronic, optical, mechanical, and thermoelectric properties. The electronic structure is analyzed within both PBE-GGA and mBJ-GGA approximations, and the thermoelectric properties are evaluated using the BoltzTraP code. The main objective is to assess the potential of these materials for optoelectronic and thermoelectric applications.

Keywords: DFT, C1b half-Heusler phases, SrMgSi, SrMgSn, thermoelectric properties.