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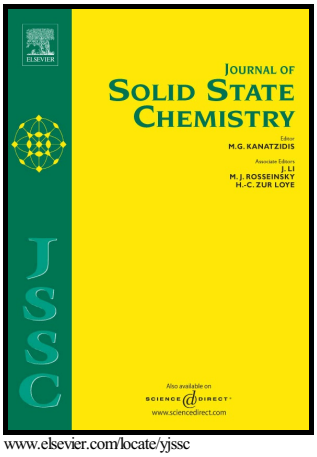

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Ab-initio study of thermodynamic stability, thermoelectric and optical properties of perovskites$ATiO_3$ (A=Pb, Sn)

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Abstract

The physical behavior of perovskites $ATiO_3$ (A=Pb, Sn) has been explored by using density functional theory based full-potential linearized-augmented-plane-wave plus local-orbital (FP-LAPW+lo) method. The lattice parameters calculated from the optimized structures by using Murnaghan equation of state and Chapin's method have been found in good agreement with the available literature that ensures the reliability of the adopted methodology. Moreover, the optoelectronic and thermoelectric properties have been elaborated by using modified Becke-Johnson exchange potential. The optical behavior has been explored in terms the dielectric constants, refractive indices, absorption spectra and optical loss factors. The absorption spectra of these materials reveal a large absorption in the visible and low ultraviolet part of incident light. The thermoelectric properties of $ATiO_3$ are explained in terms of electrical conductivities, thermal conductivities, power factors, and the specific heat capacities. The$ATiO_3$family of pervoskites has been found to exhibit the bandgaps falling in the visible region of solar spectrum