First-principles Study of Structural, Electronic, Elastic and Thermal Properties of $XBPd_3$ (X = Ca, Mg)

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ABSTRACT

We report results obtained from first principle calculations of $XBPd_3$ (X = Ca, Mg) compounds with antiperovskite structure. The estimated equilibrium lattice parameters are in agreement with the experimental ones. Elastic constants Cij for single crystal are calculated, then polycrystalline elastic moduli (bulk, shear and Young moduli, Poisson ration, anisotropy factor) are presented. Based on Debye model, Debye temperature Θ_D is calculated from the sound velocities V_l, V_t and V_m. Band structure results show that the compounds under study are electrical conductors and the conduction mechanism is assured by Pd-d electrons. Bonding nature and bonds strength are discussed based on the partial densities of states, population analysis and the electronic charge distribution.

Keywords: Intermetallic compounds, Ab initio calculations, Elastic properties

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