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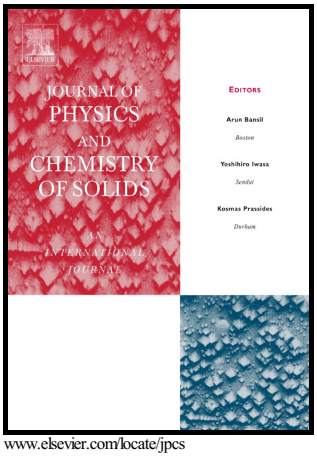

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Topological phase, structural, electronic, thermodynamic and optical properties of XPtSb (X=Lu, Sc) compounds

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Abstract

The electronic, thermodynamic and optical properties of XPtSb (X=Lu, Sc) half Heusler compounds are studied based on density functional theory. The calculations are carried out in the presence of spin orbit interaction. The exchange correlation part of total energy is calculated within local density approximation, generalized gradient approximation, Engel-Vosco generalized gradient approximation and modified Becke and Johnson exchange potential with the correlation potential of the generalized gradient approximation. The effect of pressure on the electron density of states and linear coefficient of the electronic specific heat is studied. Using the band structure calculations at different pressures, the band inversion strength and topological phase transition of these compounds are investigated. Some thermodynamic properties of XPtSb compounds by different thermal models using the non-equilibrium Gibbs function are studied and compared with experiment. Furthermore the effect of pressure on dielectric function of XPtSb (X=Lu, Sc) compounds is investigated.

Keywords: XPtSb, Density functional theory, Topological phase, Thermodynamic, Optical properties

1. Introduction

The topological insulators and metals are the novel class of quantum materials with the protected helical conducting states on their surfaces (or edges in two dimensions) [1-3]. These surface states sit on a massless Dirac cone (a relativistic dispersion of energy-momentum in reciprocal space) [1]. The topological insulators and metals have the spintronic and quantum computing applications and individual properties [4]. The topological phase transition in these materials can be determined by band inversion between the Γ_6 (s-type orbital with 2-fold degeneracy) and Γ_8 (p-type orbital with 4-fold degeneracy) in the Brillouin zone and Z_2 topological invariant [2-4]. In topologically nontrivial insulators and metals the Γ_6 state is located below the Γ_8 state, so the band inversion occurs and the wave function parity changes