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Emergence of thermoelectricity in Half Heusler topological semimetals with strain

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ABSTRACT

The band structure and thermoelectric properties of Half Heusler topological materials XPtBi (X = Sc,Y, Lu) have been investigated using density functional theory and semi-classical Boltzmann equations. At 5% strain, the band gap opens in all the materials but maximum band opens in LuPtBi and acts as thermoelectric materials. We have calculated the Seebeck coefficient, electrical conductivity, electronic thermal conductivity and lattice thermal conductivity of these materials. Thermoelectric properties at high temperature and lattice thermal conductivity of these materials are studied first time in this work. The thermoelectric performance of LuPtBi is high because of low lattice thermal conductivity as compared to ScPtBi and YPtBi.

1. Introduction

The recent discovery of topological insulators has created a great interest in the fields of material science and condensed matter physics. Topological insulator (TI) materials are a new state of quantum matter with a full insulating gap inside the bulk but their surface contains the conducting states [1]. According to the band structure calculations [2,3], ternary half Heusler [THH] compounds are topologically nontrivial. Their band structures are similar to the well known topological material HgTe with zinc blende structure. The topology of electronic band structures of these materials can be characterized by band inversion between Γ_6 and Γ_8 energy levels at the Γ high symmetry point. The band inversion strength (BIS) is defined as the energy difference between the two states ($\Delta = E_{\Gamma_8} - E_{\Gamma_6}$). The half Heusler compounds are topologically nontrivial when Δ value is positive and topologically trivial when Δ value is negative. The basic criterion to assert whether a crystalline material is topological is by its Z_2 topological invariants [4]. A topological insulator is characterized by 4 Z_2 invariants ($\nu_0, \nu_1, \nu_2, \nu_3$). The most important invariant is ν_0, the value of $\nu_0 = 1$ is for strong topological insulators and $\nu_0 = 0$ for trivial insulator (a weak TI when at least one of the other ν_i's is 1). These materials have similar properties like thermoelectric materials: narrow gap and heavy elements. These materials have narrow band gap and contain heavy elements which is primary requirement for material to be thermoelectric. These materials have a potential to act as thermoelectric materials [5]. Different studies on these materials have been reported. W. Al-Sawai et al. [6] have investigated the electronic properties of some Half Heusler topological insulators and G. Ding and co-workers [5] have elucidated that HH topological semimetals can act as better thermoelectric materials than Bi_2Te_3. Recently M. Meinert [7] has studied the electronic and phonon properties of some HH topological semimetal system using DFT. S. Chadov and his co-workers [3] have explained the quantum spin hall effect in half Heusler topological insulators. Half Heusler compounds are interesting due to some properties like superconductivity, thermoelectricity and half metallicity. It contains heavy elements and hence low lattice thermal conductivity. The thermoelectric properties of ScPtBi and YPtBi [5] have been well studied. To the best of our knowledge the thermoelectric performance at high temperature and lattice thermal conductivity of these materials have not been studied yet. The aim of this work is to give a compressive description of the electronic and thermoelectric properties of XPtBi(Sc, Y, Lu) under strain. In this work we have explored the effect of strain on electronic properties of XPtBi(Sc, Y, Lu). We have also evaluate the thermoelectric properties and the lattice thermal conductivity of XPtBi(Sc, Y, Lu) under 5% strain.

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The paper is organized as: In following section, computational approach is discussed. Thereafter, calculations for electronic and thermoelectric properties are given. Finally we summarize the results and conclude.

2. Computational details

The THH materials have face centred cubic structure (FCC) with space group F-43m (no. 216). The general chemical formula of these compounds is ABC, where A, B and C atoms occupy 4b, 4c and 4a Wyckoff atomic positions. In these materials, A and C atoms occupy the zinc blende structure and B atoms fill empty space in zinc blende structure together with C atoms. These compounds are characterized by an 18 valence electron configuration, where A atom contain ten *d* orbitals, two *s* orbitals and C atom contain six *p* orbitals.

The methodology used in this work has been discussed elsewhere [8]. The electronic structure calculations were carried out by using density functional theory (DFT) based on plane wave pseudopotential method as implemented in the Quantum Espresso package [9]. To calculate the thermoelectric transport properties, we have used BoltzTraP code [10], which is based on semi-classical Boltzmann theory. To calculate lattice thermal conductivity (k_l), ShengBTE code [11] based on phonon Boltzmann transport equation (pBTE) have been used. The Z_2 invariants were calculated with z2pack code [12].

3. Results and discussion

3.1. Electronic properties

The calculated lattice constant of XPtBi (X = Sc, Lu, Bi) systems is summarised in Table 1. The calculated band structures without strain and with strain are depicted in Figs. 1, 2. These band structures without strain are compared with the band structure of HgTe, which is a zero band gap semiconductor (topologically nontrivial semimetal). The valence and conduction bands touch at Γ high symmetry point [13]. The features of calculated band structures without strain are similar to the band structure of HgTe as reported by S. Chadov et al. [3]. In our calculations, ScPtBi and YPtBi materials show topologically nontrivial semimetal behaviour. But LuPtBi material is not a zero band gap semiconductor due to the finite band overlap at Γ point. The calculated band structures of ScPtBi, LuPtBi systems without strain have similar features as

Table 1
Calculated lattice constants, Z_2 invariant and band inversion strength (Δ).

System	Calculated lattice constant (Å) (this work)	Previous theoretical lattice constant (Å)	Calculated $\Delta = E_{\Gamma_8} - E_{\Gamma_6}$	Z_2
ScPtBi	6.53	6.56 [5]	0.72	1
LuPtBi	6.52	6.57 [5]	1.10	1
YPtBi	6.72	6.64 [5]	1.07	1

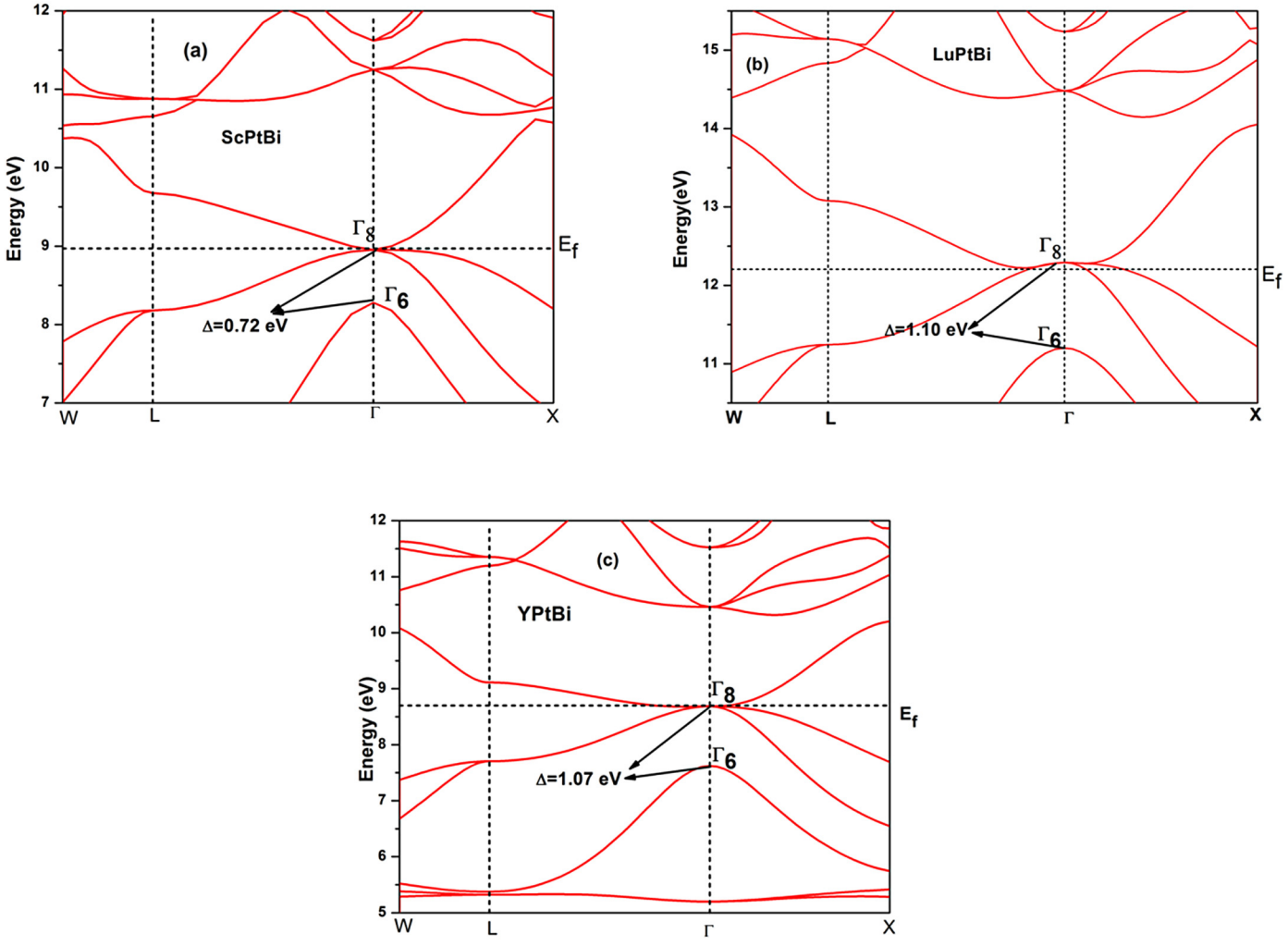

Fig. 1. Calculated Band Structures of XPtBi (X = Sc, Lu, Y) system without strain.