Computational Materials Science 91 (2014) 231–234

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Ab initio study of structural and electronic properties of ternary alkali-metal-based semimetal compounds

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ARTICLE INFO

Article history:
Received 29 July 2013
Received in revised form 24 February 2014
Accepted 20 April 2014
Available online 24 May 2014

Keywords:
Ab initio calculations
Energy band gap
Other inorganic semiconductors

ABSTRACT

Based on the *ab initio* calculations, we propose a new class of three dimensional (3D) topological insulators in alkali-metals-based ternary intermetallic compounds X_2YZ (X = alkali metals, Y = Ag, Z = Sb) with a highly ideal assumption that the X_2YZ compounds would crystallize in a cubic lattice. The band topology of X_2YZ is explored by using full-potential linear augmented plane wave method. The results reveal that the topological insulator state of X_2YZ can be realized by applying a uniaxial tensile strain of greater than 3% along the [001] direction and the electronic structure exhibits a distinct band-inversion feature. This new X_2YZ compounds provide an alternate platform for novel quantum phenomena and multifunctional topological devices.

1. Introduction

The new states of quantum matter, such as quantum spin Hall Effect and topological insulator have been investigated for both fundamental condensed-matter physics and material science in recent years [1–3]. Thus, searching new topological insulator material in real materials has become a crucial subject for both topological band theory and new topological devices [4]. Recently, this work has been extended to ternary compounds including the I-III-VI_2 and II-IV-V_2 chalcopyrite semiconductors, antiperovskite structure compounds, Tl-based III-V-VI_2 ternary chalcogenide series, half-Heusler compounds and full-Heusler compounds [5,6]. In particular, the Heusler compounds and their isoelectronic analogues have been extensively studied as 3D topological insulator materials [7] from theoretical to experimental point of view.

Heusler compounds with *C1b* structure are small band gap semiconductors or semimetals, which open wide possibilities for modulating the band gap and getting the desired band inversion by choosing compounds with appropriate hybridization strength, for example by varying the lattice parameter [8], and magnitude of spin–orbit coupling (SOC) [9,10]. A common feature of Heusler compounds is that the top of the valence band (VB) is located at the gamma (Γ) point and they are narrow band gap semiconductors or semimetals with very small electron and hole pockets around the Γ point. The topological state in these small band gap semiconductors or semimetals can be created by applying proper strain engineering or by designing an appropriate quantum well structure, as demonstrated in the case of HgTe [3].

In this work, we predict a new class of 3D topological insulators, the alkali metals-based ternary intermetallic compounds X_2YZ (X = alkali metals, Y = Ag, Z = Sb), away from the non-Heusler lithium-based ternary compounds. We made a highly ideal assumption that these hypothetical compounds would crystallize in a cubic lattice, and they only obtained with certain high constraints. Our argument is based on the observation of a distinct band-inversion feature similar with the known topologically nontrivial binary compound HgTe. The topological insulator state in X_2YZ is then confirmed by direct evaluation of the topological invariant (Z_2 number) [6]. Our calculations show that the topological insulating phase of X_2YZ can be realized by applying a uniaxial tensile strain of greater than 3% along the [001] direction. The rest of this article is organized as follows: The computational details are given in Section 2. In Section 3, we present the results and discussions. Finally, a brief summary is presented in Section 4.

2. Computational details

In order to explore the band topology [11], we perform the full-potential linear augmented plane-wave (FP-LAPW) method [12]

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http://dx.doi.org/10.1016/j.commatsci.2014.04.042
0927-0256/

using the program package WIEN2k [13] in the framework of density functional theory (DFT). The generalized gradient approximation (GGA) function using the latest improvement of the exchange functional by Perdew–Burke–Ernzerhof (PBE) [14] scheme has been used in this work. A converged ground state is obtained using over $21 \times 21 \times 21$ Monkhorst–Pack k-point grid (10000 k-points) in the first Brillouin zone. The valence wave functions inside the spheres are expanded up to $l_{max} = 10$ and the charge density is Fourier expanded up to $G_{max} = 14$ in the muffin-tins. The cut off parameter $R_{mt}K_{max}$ limiting the number of the plane waves is taken as 9.0, where K_{max} is the maximal value of the reciprocal lattice vector used in the plane wave expansion, and R_{mt} is the smallest atomic sphere radius in the surface cell. Spin–orbit coupling is also included by WIEN2k package using a basis of fully relativistic eigenfunctions, and the relativistic $p^{1/2}$ corrections are also considered for 5p and 6p orbits of Sb to improve the accuracy [15,16].

3. Results and discussion

Fig. 1 shows the crystal structure of X_2YZ (space group $F4\bar{3}m$). The X_2YZ compounds can be viewed as consisting of $[X_2]^{n+}$ ions 'stuffing' the zinc blende $[YZ]^{n-}$ sublattice, where the number of valence electrons associated with $[YZ]^{n-}$ are 18 ($d^{10}s^2p^6$). The eighteen electron compounds are closed-shell species and nonmagnetic. These factors suggest that X_2YZ could be candidates for 3D Z_2 topological insulators if some odd number of band inversions is realized.

We start our discussion with X = Li, or Li_2AgSb as a representative of the X_2YZ compounds for the case for topological insulators by making a direct comparison with the known 3D Z_2 topological insulator HgTe studied in the literature [3]. For Li_2AgSb, in order to eliminate the semi-metallic character, we apply a uniaxial tensile strain along the [001] direction with constant volume, resulting in a fully gapped topological insulator state. Consider the

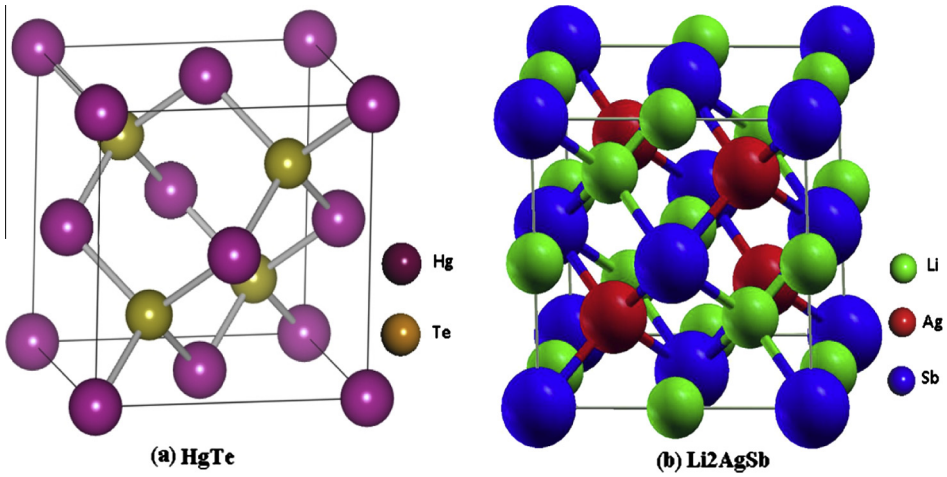

Fig. 1. Comparison of the zinc blende HgTe and Li_2AgSb crystal structure. (a) The zinc-blende compound HgTe and (b) the ternary compound Li_2AgSb.

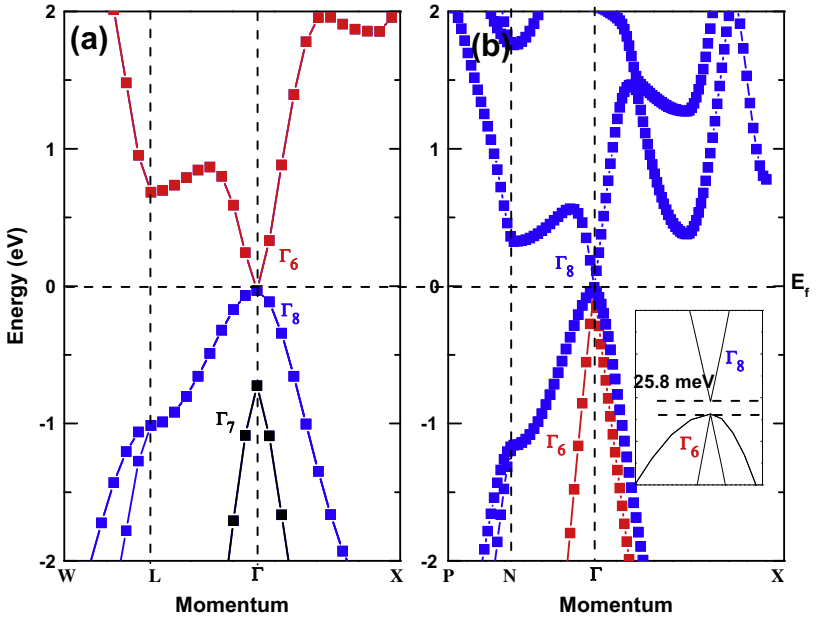

Fig. 2. (a) Band structure of HgTe and (b) band structure of Li_2AgSb under uniaxial strain with constant volume along [001] direction, with an increase in the c/a ratio by greater than 3%.