Prediction of topological insulating behavior in inverse Heusler compounds from first principles

X.M. Zhang a, E.K. Liu a, Z.Y. Liu b, G.D. Liu c, G.H. Wu a, W.H. Wang a,*

a Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, PR China
b State Key Laboratory of Metastable Material Sciences and Technology, Yanshan University of Technology, Qinhuangdao 066004, PR China
c School of Material Sciences and Engineering, Hebei University of Technology, Tianjin 300130, PR China

A R T I C L E   I N F O
Article history:
Received 23 October 2012
Received in revised form 4 December 2012
Accepted 5 December 2012
Available online 10 February 2013

Keywords:
Topological insulator
Heusler compound
Electronic structure

A B S T R A C T
The topological band structures of the X\(_2\)YZ inverse Heusler compounds have been investigated by the first-principle calculations. The results of this study clearly indicate that a large number of inverse Heusler compounds naturally exhibit an inverted band structure. We found that, similar to the half-Heusler family, these inverse Heusler compounds can realize the topological insulating state under hydrostatic or uniaxial lattice expansion. Importantly, most of these compounds possess a negative formation energy, which makes them more suitable in material growth and could easily achieve the topological insulating behavior by alloying or proper strain.

© 2012 Elsevier B.V. All rights reserved.

1. Introduction

Topological insulator (TI) is of a new class of materials, which has a full insulating gap in the bulk but contains topologically protected conducting states on edges or surfaces [1–4]. The surface states are chiral and inherently robust to external perturbations, which could be useful for future technological applications in spintronics and quantum computing as well [5,6]. Since the first two-dimensional (2D) TI with quantum spin-Hall effect was predicted in HgTe [7,8], a large number of three-dimensional (3D) TIs have also been proposed theoretically [9–20]. Very recently, the investigations on TIs have also gained great success experimentally: not only in binary compounds, but also the gapless half-Heusler TIs have been confirmed to possess metallic surface electronic state [21,22]. Most importantly, it was proposed that in the half-Heusler family the topological insulator allows the incorporation of superconductivity and/or magnetism [23].

In particular, the earlier computations [13,14] have proposed that the band structures near the Fermi level in the half-Heusler compounds exhibit almost the same behavior with those of CdTe and HgTe. They argue that the half-Heusler and zinc-blende lattice possess the same crystal symmetry with space group F\(_4\)\(_3\)m (No. 216). In full-Heusler compounds, however, there exists a family of materials called inverse Heusler possessing the F\(_4\)\(_3\)m crystal symmetry as well [24,25]. In Fig. 1, we show a comparison between inverse Heusler and zinc-blende structure. In general, the former can be considered as four interpenetrating face-centered-cubic (fcc) lattices, in which the X atoms occupy A(0,0,0) and B(1/4,1/4,1/4) sites, the Y, Z atoms site C(1/2,1/2,1/2) and D(3/4,3/4,3/4) respectively in Wyckoff coordinates. Similarly, the zinc-blende structure contains two inequivalent atoms, which occupy two nearest sites (C and D). We can make an analogous consideration with the previous studies [13,14], the inverse Heusler structure can thus be considered as two hybridized interpenetrating zinc-blendes (actually, a diamond and a zinc-blende structure), which are X–X and Y–Z. It is therefore very important to study whether the topologically nontrivial phase can be exploited in inverse Heusler compounds with 18 valence electrons.

In this work, by performing a systematic investigation on the band topology of some given inverse Heusler compounds, we will show that a large number of potential TIs are waiting for exploit in this rich inverse Heusler family. Our deduction and theoretical basis are mostly judged by making a comparison with the well-studied topologically nontrivial binary compound HgTe [7,8]. Similar to the half-Heusler TI, we also find that the topological insulating behavior in these inverse Heusler compounds is sensitive to the variation of lattice constant and also tetragonal uniaxial strain.

2. Computational details

The band-structure calculations were performed using full-potential linearized augmented plane-wave method [26], implemented in the package WIEN2K [27]. Experimental lattice constants are used when available, and others are obtained by minimizing the total energy using generalized gradient
approximation of Perdew–Burke–Ernzerhof 96 including SOC [28]. A converged ground state was obtained using 5000 k points in the first Brillouin zone and set $K_{\text{max}} \times R_{\text{MT}} = 8.0$, where $R_{\text{MT}}$ represents the muffin-tin radius and $K_{\text{max}}$ is the maximum size of the reciprocal-lattice vectors. The muffin-tin radius of different elements used in calculations are generated by the system. Moreover, wave functions and potentials inside the atomic sphere are expanded in spherical harmonics up to $l = 10$ and 4, respectively.

3. Results and discussions

In Fig. 2, we illustrate the calculated band structures of CdTe and HgTe with those of $Y_2RuPb$ and $Sc_2OsPb$. For clarity, we will divide into two groups for comparison: CdTe (Fig. 2a) and $Y_2RuPb$ (Fig. 2b), HgTe (Fig. 2c) and $Sc_2OsPb$ (Fig. 2d), respectively. The band structure of $Y_2RuPb$ is very similar to that of CdTe, which exhibits natural band ordering ($s$-like $\Gamma_6$ states (red lines) lie above the $p$-like $\Gamma_8$ states (blue lines)) and opens a direct gap at the $\Gamma$ point, indicating them just be trivial semiconductors. However, the band structures of HgTe and $Sc_2OsPb$ possess a inverted band order, in which the $\Gamma_6$ state sits below the $\Gamma_8$ state. Meanwhile, the valence and conduction bands away from the $\Gamma$ point are well separated without crossing each other. Such band inversion only occurs once throughout the Brillouin zone and therefore, HgTe and $Sc_2OsPb$ are both topologically nontrivial phases in their ground states.

We next perform a systematic investigation of the band topology of the $X_2YZ$ ($X = Sc, Y, La; Y = Ru, Re, Os; Z = Sb, Pb, Bi$) Fig. 1. Comparison of the inverse Heusler and zinc-blende crystal structures. The inverse Heusler ($X_2YZ$) and the zinc-blende ($YZ$) structures are shown in (a) and (b), respectively.

Fig. 2. Band structures of CdTe and HgTe compared with $Y_2RuPb$ and $Sc_2OsPb$ inverse Heusler compounds. The $\Gamma_6$ and $\Gamma_8$ states are denoted by red and blue lines, respectively. This comparison reveals obvious similarity between the two systems: both CdTe and $Y_2RuPb$ are only trivial semiconductors with $\Gamma_6$ situated above $\Gamma_8$. However, both HgTe and $Sc_2OsPb$ are topologically nontrivial with inverted band order.
compounds, which are all proposed to form the inverse Heusler structure. Here we define $\Delta E = E_{T8} - E_{T8}$ as topological band inversion strength, which would be positive for topologically trivial case and negative for topologically nontrivial phase. We have summarized the $\Delta E$ as a function of the lattice constant for these compounds in Fig. 3a. It can be found that most of them exhibit a negative $\Delta E$, indicating the TI candidate. While there are also some cases like Sc$_2$ReSb and La$_2$OsPb that the Fermi level visibly cuts the conduction or the valence bands, we can only call them topological insulators. For Y$_2$RuPb, Sc$_2$RuPb and La$_2$RuPb, they are just trivial semiconductors with a positive $\Delta E$. As mentioned before, the inverse Heusler structure can be considered as two hybridized interpenetrating zinc-blende sublattices: X–X and Y–Z. It is clear that the cubic symmetry and degenerate together at the $\Gamma$ point. However, the subbands with $C_8$ symmetry are protected by $C_8$ states is broken and forms a gable band gap at Fermi level. Interestingly, the system exhibits different responses upon the uniaxial compression and expansion: when introduced a compression (Fig. 4a), the conduction and valence bands are no longer overlapped and the system becomes an insulator with inverted band order retained, while upon expansion (Fig. 4b) it remains a semimetal as before. The result is well consistent with our previous calculations for half-Heusler compounds [29]. Indeed, a recent search model for possible TIs has suggested that the variational ‘descriptor’, namely ‘strain’ can be associated with the robustness or the feasibility of the TI state [30].

Fig. 3. (a) Energy difference between $\Gamma_8$ and $\Gamma_8$ bands ($\Delta E = E_{\Gamma_8} - E_{\Gamma_8}$) and (b) formation energy of the calculated inverse Heusler compounds as a function of the lattice constant. Here HgTe and CdTe binaries are shown for comparison.
4. Conclusion

We have shown by the first-principle calculations that a large number of inverse Heusler compounds exhibit an inverted band order naturally and are promising to realize the topological insulating order. We argue that the band structures near the Fermi level are determined by the X–X and Y–Z zinc-blende sublattices jointly, in which the Y–Z dominates the sign of topological band inversion strength $\Delta E$ and X–X just contributes as a fine tuning. We also found that the band topology is sensitive to the variation of lattice constant and uniaxial strain. Importantly, all of the inverse Heusler compounds possess a negative formation energy making them more suitable in material growth and could easily achieve the topological insulating behavior by proper strain. With the example of Sc$_2$OsPb, we show how the gapless system can be driven by uniaxial strain into a topological insulating state.
Acknowledgements

This work was supported by National Natural Science Foundation of China (Grant No. 51171207) and National Basic Research Program of China (973 Programs: 2012CB619405).

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.commatsci.2012.12.013.

References