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Topological electronic structure in half-Heusler topological insulators

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We have investigated band structures of a series of 28 ternary half-Heusler compounds $MM'X$ of MgAgAs type, where $M=(\mathrm{Lu},\mathrm{La},\mathrm{Sc},\mathrm{Y})$ and $M'X=(\mathrm{PtBi},\mathrm{AuPb},\mathrm{PdBi},\mathrm{PtSb},\mathrm{AuSn},\mathrm{NiBi},\mathrm{PdSb})$. Our results show that the Z_2 topological order is due to a single band inversion at the Γ point. In native states, these half-Heusler compounds are identified as being topologically nontrivial semimetals, or nontrivial metals, or trivial insulators, which can be turned into insulating thin films on suitable substrates. Our analysis reveals a straightforward relationship which connects the band inversion strength (extent of deviation from the critical point) to the atomic charge of constituents and the lattice parameter. Our findings suggest a general method for identifying Z_2 topological insulators in nonmagnetic ternary compounds.

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I. INTRODUCTION

Topological insulators (TI) are materials exhibiting a novel quantum state of matter involving conducting states on edges or surfaces.[1–14] While the first three-dimensional (3D) topological insulators to be discovered were binary compounds such as $\mathrm{Bi}_{1-x}\mathrm{Sb}_x$ (Ref. 7) and $\mathrm{Bi}_2\mathrm{Se}_3$,[9] the search for TI behavior has recently been extended to ternary compounds.[15–23] In particular, band computations[15,16] have predicted that many of the ternary half-Heusler (THH) compounds are topologically nontrivial with topological order $Z_2=-1$. Their electronic band structures have been shown to be similar to those of the well known topological material HgTe with zinc-blende structure. Here, we have investigated a series of 28 nonmagnetic THH compounds of the form $MM'X$ with $M=$Lu, La, Sc, and Y, $M'=$Pt, Pd, Au, and Ni, and $X=$Sb, Bi, and Sn. We find that the topology of the electronic band structures can be characterized by band inversion between the Γ_6 and Γ_8 energy levels at the Γ symmetry point in the Brillouin zone. We define the band inversion strength (BIS), Δ, as the energy difference between these two states, i.e., $\Delta=[E_{\Gamma_8}-E_{\Gamma_6}]$. The half-Heusler compounds with positive values of Δ are predicted to be topologically nontrivial, while those with negative Δ values are topologically trivial.

However, the earlier computations of Refs. 15 and 16 on the THHs suffer from the well known problem of underestimation of the band gap for semiconductors in the density-functional theory (DFT) using the local-density approximation (LDA) or the generalized gradient approximation (GGA), which results in a systematically larger estimate of the BIS value. An efficient way to correct this error is to utilize a semilocal exchange-correlation potential. With this motivation, in this study we use the modified Becke and Johnson potentials (MBJLDA) (Ref. 24) instead of the LDA or GGA. MBJLDA offers an improvement over LDA or GGA in describing band gaps of many materials, including semiconductors with the zinc-blende structure. We find similar improvements for BIS values. For example, in HgTe, LDA or GGA yields too low an energy for Γ_6, leading to a GGA-derived BIS value of 1.04 eV, which is considerably larger than the experimental value of 0.302 eV.[25] In contrast, the computed BIS value from MBJLDA of 0.415 eV is comparable to GW values of 0.37–0.57 eV,[26,27] representing a considerable improvement over the LDA or GGA. Our analysis also reveals a relatively simple relationship for predicting TI behavior in the present series of compounds by correlating the value of the BIS parameter with the lattice constants of the compounds and the atomic numbers of their constituent atoms.

An outline of this paper is as follows. The introductory remarks in Sec. I are followed in Sec. II by a description of the crystal structures and other computational details. Section III discusses our new GGA- and MBJLDA-based band structures of the THH compounds. Brief conclusions are presented in Sec. IV.

II. COMPUTATIONS

The THH compounds possess a face-centered-cubic (fcc) structure given by the space group $F\bar{4}3m$ (No 216). Crystalline compounds of this structure can be described by the chemical formula $MM'X$ where M, M', and X atoms occupy Wyckoff 4b, 4c and 4a atomic positions, respectively.[28] The M' and X positions when taken by themselves form a zinc-blende structure. M atoms fill empty spaces within the zinc-blende structure, and together with X atoms, yield a rocksalt arrangement. The present series of THH compounds are characterized by an 18 valence electron configuration, which consists of ten d orbitals of the M' atom, and two s orbitals, and six p orbitals of the X atom. In the ionic picture the stoichiometric THH compounds correspond to all three atoms having filled shells. Since all core electrons of the atomic and molecular orbitals in THH series have closed shell configuration, the total spin and angular momentum is zero, and the compounds are all nonmagnetic. Our electronic structure calculations are based on a full potential linearized augmented plane wave method with MBJLDA exchange-correlation potentials.[24] Experimental lattice constants are used when available, and in cases where compounds do not occur naturally, lattice constants are obtained by minimizing the total energy using GGA of Perdew, Burke, and Ernzerhof.[29] The WIEN2K package[30] has been employed to perform self-consistent band-structure calculations. Details of the 28 compounds studied, their crystal structures, and the computed Δ values obtained by using GGA and MBJLDA are summarized in Table I. Also shown for each compound is the value of the quantity t, which is introduced in Sec. III below.

III. RESULTS AND DISCUSSION

We have calculated the DFT-GGA as well as DFT-MBJLDA based band structures for the 28 THH compounds and HgTe as listed in Table I. The group of 28 compounds studied was obtained by combining $M=(\mathrm{Lu},\mathrm{Sc},\mathrm{La},\mathrm{Y})$ with $M'X=(\mathrm{PtBi},\mathrm{AuPb},\mathrm{PdBi},\mathrm{PtSb},\mathrm{AuSn},\mathrm{NiBi},\mathrm{PdSb})$, so that the seven resulting subgroups can be labeled by a particular binary $M'X$.[37–39] The crystal structures have been taken from the literature, except for the compounds labeled by a, b, or c in which case the compounds are artificial. These artificial compounds either do not exist naturally or have a different crystal structure as noted in the legend to Table I.

A comparison between the band structures of $\mathrm{Hg}_{1-x}\mathrm{Cd}_x\mathrm{Te}$ with the half-Heusler series simplifies the determination of possible presence of topological order in the half-Heusler compounds. $\mathrm{Hg}_{1-x}\mathrm{Cd}_x\mathrm{Te}$ is a family of 3D materials with strong spin-orbit coupling.[40] The topologically nontrivial HgTe (Ref. 5) and the trivial CdTe possess zinc-blende structure, and can be considered as being half-Heusler if one assigns a vacancy to the M site, i.e., these compounds can be written as []HgTe and []CdTe, where the symbol [] denotes a vacancy at the M site, $M'=(\mathrm{Hg},\mathrm{Cd})$, and $X=\mathrm{Te}$. Recall now that bulk HgTe is a zero gap semiconductor (topologically nontrivial semimetal) in which valence and conduction bands touch at the Γ point.[41] The Γ_8 states at the Fermi level have p-like symmetry with fourfold degeneracy ($j=3/2$), while the valence level Γ_6 has s-like symmetry. In contrast, the trivial bulk CdTe has a direct band gap at Γ between the s-like level Γ_6 and the fourfold ($j=3/2$) p-like Γ_8 level.[41] This difference between the ordering of the bands at Γ is shown schematically in Figs. 1(a) and 3(a). The size of the dots (red) indicates the degree of s-like occupancy with larger dots representing larger s-like occupancy. Since all topologically nontrivial compounds are characterized by a similar band inversion of Γ_8 and Γ_6 levels, we may define the quantity $\Delta=[E_{\Gamma_8}-E_{\Gamma_6}]$ as the BIS, which would be positive for topologically nontrivial cases and negative for topologically trivial systems. Δ values for the half-Heusler series are listed in Table I, and separate these compounds into topologically nontrivial semimetals/metals or trivial insulators.

TABLE I. Lattice constants, parameter $t=(Z_{M'}+Z_X)V$, and BIS, Δ, based on GGA and MBJLDA for the 28 THH compounds and HgTe in the fcc structure described in the text.

Compound	Lattice constant (Å)	Δ (GGA) (eV)	Δ (MBJLDA) (eV)	t (nm^3)
LuPtBi	6.57 (Ref. 31)	1.58	1.44	45.74
ScPtBi	6.56[a]	0.96	0.70	45.46
LaPtBi	6.83 (Ref. 31)	0.86	0.65	51.27
YPtBi	6.64 (Ref. 31)	1.10	0.87	47.13
LuAuPb	6.79[a]	1.17	1.11	50.05
ScAuPb	6.64[a]	0.06	−0.15	46.29
LaAuPb	7.11[b]	1.05	0.96	57.91
YAuPb	6.73 (Ref. 32)	0.70	0.54	49.05
LuPdBi	6.57 (Ref. 31)	0.72	0.47	36.52
ScPdBi	6.43 (Ref. 31)	−0.30	−0.74	34.34
LaPdBi	6.82 (Ref. 31)	−0.41	−0.76	41.01
YPdBi	6.64 (Ref. 31)	0.08	−0.29	37.76
LuPtSb	6.46 (Ref. 31)	0.23	−0.01	34.73
ScPtSb	6.31 (Ref. 33)	−0.74	−1.12	32.44
LaPtSb	6.88[c]	0.244	−0.03	41.96
YPtSb	6.53 (Ref. 33)	1.10	−0.45	34.73
LuAuSn	6.56 (Ref. 34)	−0.70	−0.89	36.05
ScAuSn	6.42 (Ref. 34)	−1.67	−1.98	34.12
LaAuSn	7.01[b]	−0.04	−0.11	44.41
YAuSn	6.74[c]	−0.58	−0.75	39.51
LuNiBi	6.34 (Ref. 31)	−0.17	−0.47	28.29
ScNiBi	6.19 (Ref. 31)	−1.20	−1.68	26.34
LaNiBi	6.72[b]	−0.47	−0.92	33.73
YNiBi	6.41 (Ref. 31)	−0.66	−1.11	29.25
LuPdSb	6.51[a]	−0.42	−0.76	26.72
ScPdSb	6.05 (Ref. 35)	−1.67	−2.17	24.39
LaPdSb	6.84[b]	−1.14	−1.44	31.09
YPdSb	6.53[a]	−1.18	−1.60	27.05
HgTe	6.46	1.04	0.41	35.58
YbPtBi	6.58 (Ref. 31)	2.13	2.06	45.87
GdPtBi	6.68 (Ref. 31)	1.86	1.04	47.99

[a] These compounds do not occur in nature. We have obtained the fcc lattice constants via a constrained minimization of the DFT-GGA total energy.

[b] Naturally occurring compound possesses hexagonal structure (Ref. 36).

[c] Naturally occurring compound possesses space group $P6_3/mmc$ (Ref. 31).

The nontrivial semimetal group along with HgTe is shown in Fig. 1, where the six half-Heusler compounds, namely, YPtBi, ScPtBi, LaPtBi, YAuPb, LaAuPb, and LuPdBi possess positive values of Δ. (Note that LaAuPb and ScPtBi here are artificial[36] compounds.) Band structures of these compounds are very similar to the band structure of HgTe shown in Fig. 1(b). In Figs. 1(b)–1(h) the fourfold degenerate states at Γ have p-type orbital symmetry with a total angular momentum eigenvalue of $j=3/2$, while the s-type state, labeled by red dots, lies below the p-type orbital. This inversion of the natural order of s- and p-type orbitals characterizes the topologically ordered material. The nontrivial metallic band structures of LuPtBi and LuAuPb are shown in Fig. 2. Here also band inversion occurs as it does in Fig. 1, but these compounds are not zero-gap semiconductors due to the presence of a finite band overlap, which leads to pockets

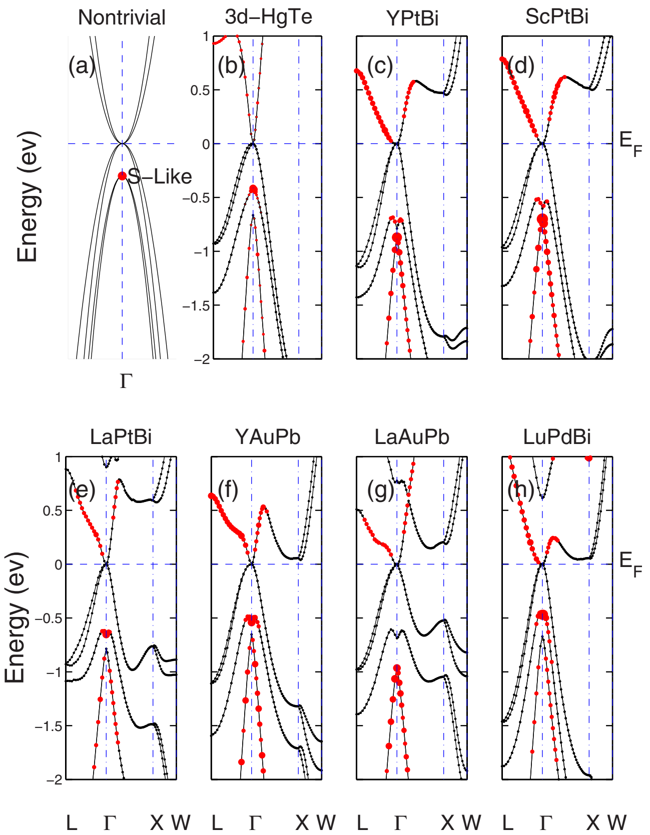

FIG. 1. (Color online) (a) Schematic band structure of a nontrivial THH compound near the Γ point. [(b)–(h)] MBJLDA band structures of seven nontrivial THH compounds with a zero gap at the Fermi level. Size of the dots (red) indicates the degree of s-like occupancy.

at either Γ or with a second band near X. We have also investigated the nonmagnetic electronic structures of YbPtBi and GdPtBi, and find that despite lowering of the E_F due to hole doping, the band inversion at Γ persists so that the band topology remains nontrivial.

Finally, Fig. 3 shows the 20 remaining compounds, which are all seen to be trivial insulators. Here the band structure is similar to that of CdTe with natural band ordering [s-type (red dots) band lies higher than the p-type band] and an open direct gap. Obviously, the s/p inversion which is responsible for topological order is absent in these compounds. Notably, LuPtSb is close to a topological critical point since the gap in LuPtSb is close to zero.

The cubic topologically nontrivial THH compounds in Figs. 1 and 2 are not naturally insulating because the positive- and negative-mass bands with Γ_8 symmetry are degenerate at the Γ point as a consequence of the high degree of crystal symmetry. This degeneracy can, however, be lifted by introducing a strain in the system. We demonstrate this with the example of LuPtBi in Fig. 4, where we have recomputed the band structure for a uniaxial strain along the [111] direction, which reduces the hexagonal lattice constant **a** by 3% and the lattice constant **c** by 4%. We now see in Fig. 4 that as a result of reduced crystal symmetry, the fourfold degeneracy of the Γ_8 states is broken. The conduction and valence bands no longer overlap and the system becomes an insulator. Note that the band structure still has the inversion out of the natural order of s- and p-type orbitals at the Γ point, which characterizes the topologically nontrivial phase.

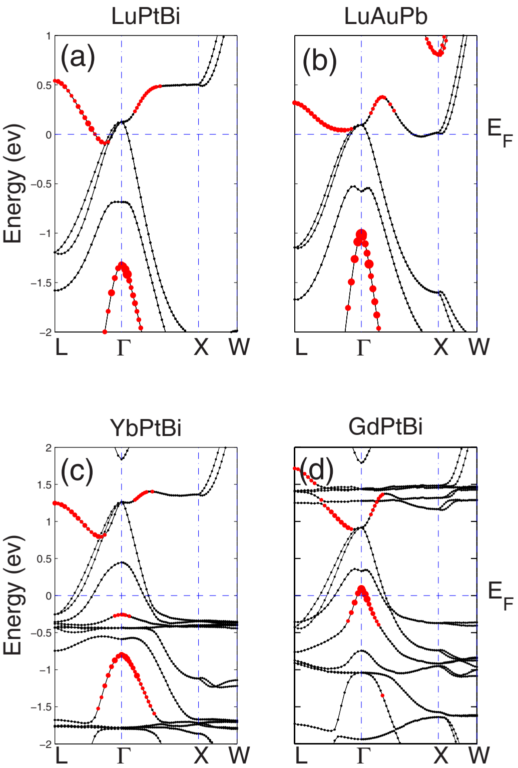

FIG. 2. (Color online) MBJLDA band structures of the nontrivial THH compounds which display a metallic band. The size of red dots indicates the degree of s-like occupancy as in Fig. 1.

Figure 5 summarizes the results of Table I and Figs. 1–3. It shows the relationship between Δ and the quantity $t=(Z_{M'}+Z_X)V$ for the entire group, where V is the unit cell volume, and $Z_{M'}$ and Z_X are the atomic numbers of the M' and X atoms in the binary $M'X$, respectively. The value of t captures the effects on Δ of the $M'X$ unit, which forms the backbone of the THH compounds, and also of the overall volume of the crystalline unit cell.[42] The critical line, $\Delta=0$, divides the figure into two parts: The compound is nontrivial for $\Delta>0$ and it is trivial for $\Delta<0$. The figure shows a systematic increase in Δ with increasing t values. Insight into the TI behavior of the 28 investigated THH compounds is gained by framing with a triangle the four compounds in each of the seven subgroups labeled by the same binary unit $M'X$. It is striking that for all seven subgroups, Sc, La, and Lu form the corners of the triangle while Y lies inside the triangle. In fact, the 'orientation' of all seven triangles is also the same in the sense that it runs counterclockwise going from La to Lu to Sc, where the element with the largest atomic mass, Lu, occupies the corner with highest Δ, except for MAuSn and MAuPb subgroups. Moreover, the volume of the compounds in each subgroup is ordered as Sc$M'X$ $<$Lu$M'X$$<YM'X$$<LaM'X$, except for MAuPb subgroup. The center of gravity for each triangle is seen to increase with t for all subgroups. All compounds, whether physically realized or artificial, follow the aforementioned trends independent of the sign of Δ. The preceding observations suggest

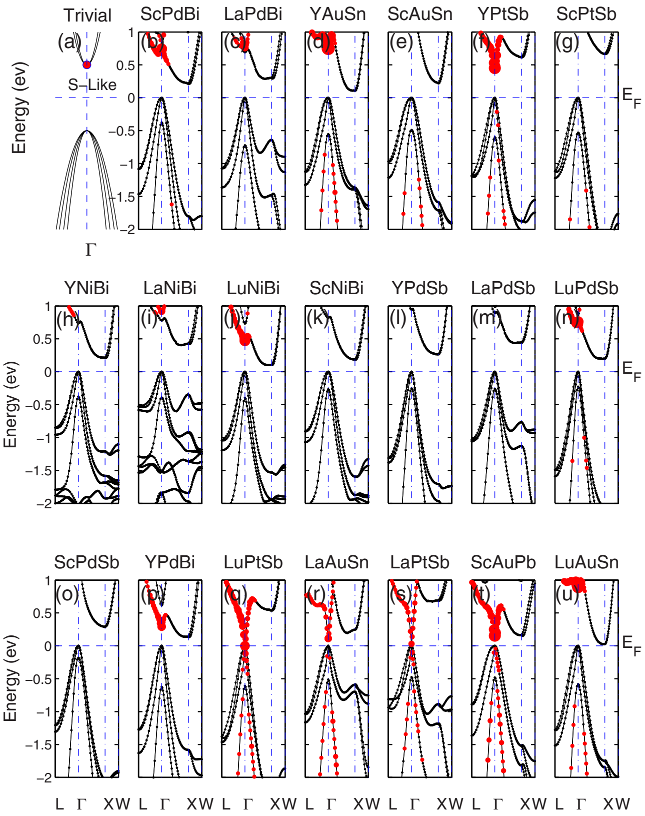

FIG. 3. (Color online) MBJLDA band structures of 20 trivial THH compounds which display a direct gap. Panel (a) shows the schematic band structure of this series of compounds.

that these relationships between Δ and t may be valid more generally and could be useful in ascertaining the nature of topological order and the value of the BIS in other nonmagnetic half-Heusler alloys.

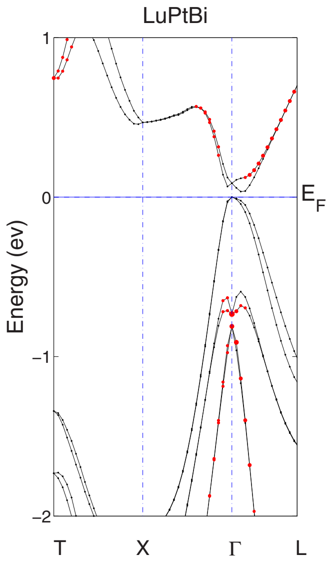

FIG. 4. (Color online) MBJLDA band structure of nontrivial THH LuPtBi under uniaxial strain along the [111]-direction. The distortion decreases the lattice constant a by 3% and c by 4%. A gap now opens up at the Fermi energy resulting in an insulating phase as a result of the distortion. The size of red dots indicates the degree of s-like occupancy as in Fig. 1.

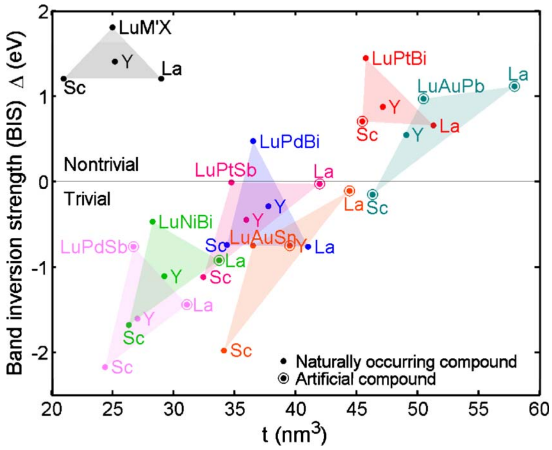

FIG. 5. (Color online) BIS, $\Delta=[\Gamma_8-\Gamma_6]$ for various THH compounds versus $t=(Z_{M'}+Z_X)V$, where $Z_{M'}$ and Z_X are atomic numbers M' and X atoms and V is the unit-cell volume. The 28 THH compounds investigated are divided into seven subgroups of four compounds each (marked by shaded triangles of different colors), where each subgroup corresponds to the same binary unit $M'X$. The schematic illustration of the components in each of the seven subgroups is given in the top left corner.

IV. CONCLUSION

We have investigated the band structures of 28 THH compounds listed in Table I using the GGA as well as MBJLDA exchange-correlation functional for the purpose of delineating their topologically interesting behavior. Six compounds of Fig. 1 are found to be topologically nontrivial with a zero band gap, two compounds of Fig. 2 are nontrivial with small electron pockets, and 20 compounds of Fig. 3 are trivial band insulators. With the example of LuPtBi, we show how the nontrivial system with small pockets can be driven by uniaxial strain along the [111] direction into a topological insulating state. We introduce the quantities BIS, Δ, and $t=(Z_{M'}+Z_X)V$, and show that the 28 THH compounds naturally divide into seven subgroups in terms of Δ and t, characterized by the binary unit $M'X$. Based on our analysis, we suggest that Δ and t may prove to be useful measures more generally for identifying other topologically interesting nonmagnetic half-Heusler compounds.

Note added. Recently, we became aware of a related work[22] that considers the present ternary half-Heusler compound.

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[42] In particular, Δ increases as V increases in the THH compounds, and the band gap decreases in the group III-V zinc-blende semiconductors with increasing atomic number.