Emergence of non-trivial $\mathbb{Z}_2$ topology in
-d-transition metal rich half-Heusler compounds

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Abstract

A 3D Topological Insulators (TI) is a material having a new state of matter exhibiting a gapless conducting surfaces over insulating bulk. Such exotic phase of matter has been tremendously studied in non-centrosymmetric ($C_{1b}$ type) cubic half-Heusler (HH) compounds due to their tuneable topological properties and versatile applications in the field of spintronics. Using ab initio investigation, we performed an in-depth analysis of nine $XX'O$ ($X = \text{Li, K, Rb} ; X' = \text{Cu, Ag, Au}$) HH compounds that were previously unreported for their topological signature. We observed SOC induced large non-trivial insulating gap of 0.11 eV, 0.18 eV, and 0.19 eV for LiAgO, KAuO, and RbAuO compounds respectively at their equilibrium lattice constant (other compounds exhibits $< 0.1$ eV energy gap). The cubic crystal symmetry and broken spatial inversion symmetry of HH compounds demonstrate a recognizable band inversion around $\Gamma$ point of Brillouin zone. The interplay between SOC and strong electronegativity further rises band inversion between $\Gamma_6$ and $\Gamma_7$ states. The band inversion is accompanied by a Mass-Darwin relativistic effect in which the $\Gamma_6$ state has been enforced by the compounds having larger -d orbital peculiarity to stay lower than $\Gamma_7$ and $\Gamma_8$ states. In addition, we also explore the effect of hydrostatic pressure (compressive and expansive) on the robust topological state to achieve large non-trivial energy gap. Finally, the strong TI nature was confirmed by computing $\mathbb{Z}_2$ indices as $(1, 000)$, surface states, Wannier charge centers (WCC), and slab band structure.

keywords: Topological Insulators, DFT, Mass-Darwin relativistic effect, half-Heusler
1 Introduction

A recent discovery of quantum insulating materials such as topological insulators (TIs)\textsuperscript{[1,2]} topological crystalline insulators\textsuperscript{[3,4]} and kondo insulators\textsuperscript{[5,6]} creates excitement in the research communities. Especially, TI is characterized by its insulating behavior in the D dimension and conductor in the D-1 dimension\textsuperscript{[7]}

The interconnected properties of TIs including robust surface/edge states (protected by time-reversal symmetry)\textsuperscript{[8]} high carrier mobility\textsuperscript{[9]} and giant magnetoresistance\textsuperscript{[10]} provide a potential root for reconnoitre TI. So far, a large number of TIs have been proposed theoretically and experimentally examined\textsuperscript{[11–14]}. In 3D TIs, Robust surface states initially were observed in tetradyntite compounds namely $Bi_{1-x}Sb_x$\textsuperscript{[15]} owing to their significant SOC strength was followed by other compounds belonging from the same rhombohedral structure having R3m space group such as $Bi_2Te_3$\textsuperscript{[16,17]} $Sb_2Te_3$\textsuperscript{[18]} and $Bi_2Se_3$\textsuperscript{[19,20]}. However, the non-trivial insulating nature was observed in cubic HgTe with inverted band orders (between s and p types bands).\textsuperscript{[19,20]} In particular, the non-trivial insulating phase in HgTe provoke community to explore other compounds of same crystal symmetry and band topology. This resulted into a new class of ternary materials with XYZ stochiometric composition called half-Heusler (HH) compounds.\textsuperscript{[21–23]} The crystal structure of HH arises due to the X substitution in a YZ zincblende sublattice.\textsuperscript{[21]} XYZ HH compounds can also exist in planar structure by dressing the honeycomb lattice. Zhang et al. predicted a large number of TIs (some of them are showing a very strong SOC effect) in the honeycomb HH family.\textsuperscript{[25]} Honeycomb structure is centrosymmetric, we can examine topological properties in terms of the parity of wave functions developed by Fu and Kane.\textsuperscript{[26]} However, Cubic HH compounds have a lack of inversion symmetry hence one can directly use $Z_2$ topological invariants method to analyze robust topological behavior.\textsuperscript{[27]} HH compounds are known for their magnificent thermoelectric\textsuperscript{[28]} superconducting,\textsuperscript{[29]} and half metallicity\textsuperscript{[30]} properties. A large number of the compounds have a very wide range of energy band gaps (insulating to semi-metallic behavior) which are prerequisites to analyze the quantum indication. Using first-principles calculations, a large numbers of TIs have been proclaimed in HH family keeping conventional hybridization between -s and -p orbitals and some of them have potent band inversion strength (higher than HgTe).\textsuperscript{[21–31]} However, very few HH compounds possess an intrinsically topological insulating nature which arises due to the significant SOC effect between
core and valence electrons.\textsuperscript{32}

We have been at work on this transition metal-based TIs due to their \(-d\) orbital valence electrons.\textsuperscript{32,34} As a consequence, novel orbital inversion including \(-d\) orbital plays an important role in the topological phase transition and magnetostructural phase transition\textsuperscript{35} which leads to a caloric effect in HH compounds.\textsuperscript{36} In particular, using \textit{first-principles} calculations we aim to find a non-trivial topological phase in nine XX’O (X= Li, K, Rb, X’= Cu, Ag, Au) HH compounds in equilibrium state of matter. Recently, Gruhn has investigated nine XX’O HH compounds for their optoelectronic properties\textsuperscript{37} In addition, Shi-Yuan Lin et al. predicted the topological insulating phase in more than 2000 HH compounds based on their band inversion strength.\textsuperscript{32} But, a systematic study is absent regarding their topological signature. This inspired us to thoroughly interrogate XX’O compounds in terms of the SOC induced robust topological phase.

Thus, here we try to investigate the structural, electronic and topological properties of all nine HH compounds using \textit{first-principles} density functional theory calculations. Without SOC effect, XX’O compounds manifest semi-metallic nature. When we inflict the SOC effect, novel \(-s\) and \(-d\) orbital inversion including gapless conducting surface states are observed. We find that the XX’O can turn into an ideal non-trivial TI without applying any external disturbance. Furthermore, this non-trivial nature is confirmed by computing their \(Z_2\) invariant as \((\nu_0, \nu_1, \nu_2, \nu_3) \equiv (1, 0 0 0)\), surface states, Wannier charge centers and slab band structure. Thus, indicating that, XX’O HH compounds are a potential candidate for novel applications in the field of nanoelectronics and spintronics.

2 Methodology

Electronic properties of XX’O HH compounds are investigated by the \textit{first-principles} density functional theory calculations implemented within the Quantum Espresso simulation package.\textsuperscript{38} In order to elucidate exchange correlation functional we use generalized-gradient approximation based on Martins-Troullier method with Perdew-Burke-Ernzerhof (GGA-PBE) type.\textsuperscript{39} This pseudopotential appraise 4s\(^1\) orbitals of alkali metal (X), 4s\(^2\)3d\(^9\) orbitals of transition metal (X’), and 2s\(^2\)2p\(^4\) orbitals of non-metal (O). To get a clear vision, we perform both without and with SOC calculations. In SOC, the effect of core electrons on the valence electrons is considered by using \textit{fully relativistic} pseudopotential based on the projector augmented wave (PAW) method.
Our calculated the energy gap due to SOC in the well-known HH compound NaAuS is 0.22 eV, which affirms the accuracy of our calculations. We adopted a plane wave basis with a kinetic energy cut-off of 90 Ry and the convergence threshold criteria is $<10^{-8}$ Ry. A Monkhorst-Pack grid with $10 \times 10 \times 10$ k-points was used for ground state electronic calculations. We also performed ab-initio molecular dynamics (AIMD) simulations for 3 picoseconds (3000 femtoseconds) time step with the temperature of thermostat set to 300 K. Based on maximally localized Wannier functions, we generate a tight binding model for XX’O HH compounds using wannier90 code. Our tight-binding band structures are well matched with DFT results. To investigate topological properties, we calculate $\mathbb{Z}_2$ classifications, slab band structure, and WCC employing WannierTools code.

### 3 Results and Discussion

Figure 1 (a) and (b) shows the conventional crystal structure and irreducible Brillouin zone of the face-centered cubic HH compounds. The crystal structure of the compound emphasizes the topological and electrical properties of a compound. Crystalline HH compounds XX’O in which X, X’, and O atoms occupy the Wyckoff positions 4b, 4a, and 4c correspondingly.

![Crystal structure of XX'O](image)

Figure 1: Crystal structure of XX’O: (a) conventional and (b) irreducible Brillouin zone.

It should be noted that the electronic properties of HH compounds are purely lean on the total valence electron counting (VEC), the atomic number (Z) and the pauli electronegativity of the elements. Pauling electronegativity of the elements occupy an important place in the crystal structure of HH compounds. The element X (more electropositive) gives n electrons to the X’ and O (more electronegative) elements. Therefore, a HgTe-like zincblende lattice is
Table 1: First-principles results for the nine HH compounds. Calculated lattice parameters, average nuclear charge per unit cell $<Z>$, $Z_2$ topological invariant, Energy gap (meV), Band inversion strength (eV).

| Compounds | a (Å) | $<Z>$ | $Z_2$ | Energy gap (meV) | $E_{\Gamma_7} - E_{\Gamma_8}$ (eV) |
|-----------|-------|-------|-------|------------------|-------------------------------|
| LiCuO     | 4.95  | 13.33 | 1     | 65.3             | -1.25                         |
| LiAgO     | 5.45  | 19.33 | 1     | 110              | -0.97                         |
| LiAuO     | 5.50  | 30    | 1     | 84.5             | -2.37                         |
| KCuO      | 5.74  | 18.66 | 1     | 76.6             | -0.72                         |
| KAgO      | 5.99  | 24.66 | 1     | 76.8             | -0.19                         |
| KAuO      | 6.05  | 35.33 | 1     | 186              | -1.47                         |
| RbCuO     | 5.98  | 24.66 | 1     | 65.9             | -0.59                         |
| RbAgO     | 6.19  | 30.66 | 1     | 53.6             | -0.08                         |
| RbAuO     | 6.24  | 41.33 | 1     | 190              | -1.29                         |

formed by $X'$ and O atoms $(X'O)^{n-}$ and an empty void within the zincblende structure is filled by X atoms $(X)^{n+}$. Roughly, 18-VEC (non-18-VEC) manifest a semiconducting (metallic) electronic properties. The crystal structure of XX'O HH compounds has been taken from the literature (already reported in the F43m phase) and re-optimized by performing a proper convergence test \cite{32,37}. The optimized value of lattice constant is listed in Table 1. To emphasize the non-trivial band topology of XX'O HH compounds, we started our investigation with known compound NaAuS\cite{32} (similar band topology) and compute their electrical and topological properties. Since the structural stability of the compounds is emergent for practical application, for each compound, we perform ab initio molecular dynamics simulations (as evident from Fig. 2) at room temperature (300 K) for time step of 3 picoseconds (3000 femtoseconds) and found that the system to be structurally stable (except LiAuO and RbCuO) without any structural deformation.

As observed, XX'O compounds own semi-metallic behavior when SOC is excluded. However, when SOC is employed, it transits into the TI and band inversion (exchange of valence and conduction band characteristic) appears at high symmetric point $\Gamma$ of the Brillouin zone. The $\Gamma_7$ ($j = 3/2$ state) and $\Gamma_8$ ($j = 1/2$) states (Lowest conduction and highest valence bands respectively) are mainly composed with the -d and -p orbitals and $\Gamma_6$ state (inner valence band) is influenced by -s orbitals. Moreover, band inversion takes place between $\Gamma_7$ and $\Gamma_6$ states. As we discussed, the XX'O compounds maintain analogues band topology to those of NaAuS. Accordingly, the non-trivial band topology of the compounds can be defined in terms of their band
inversion strength ($\Delta = E_{\Gamma_6} - E_{\Gamma_8}$). A $\Delta < 0$ stipulate that the compounds hold a non-trivial topological phase, while a trivial topological phase elucidates by $\Delta > 0$.

All compounds have inverted band characteristics at their equilibrium lattice constant ($\Gamma_6$ states stay lower than the $\Gamma_8$). The calculated value of $\Delta$ for all the compounds are tabulated in Table 1, which clearly demonstrates topologically non-trivial insulating nature (further confirmed by computing $Z_2$ invariant). We calculated band inversion strength and SOC-induced energy gap (listed in table 1) of XX’O compounds. We can perceive that the band inversion in XX’O compounds takes place as a consequence of the lighter anionic element (O) with strong electronegativity. This is contrary to the literature, which correlated band inversion and relativistic effect due to core electrons with a heavy constituent element. What, we may still wonder, a comprehensive study of band inversion with electronegativity has not yet come across.
Figure 3: The calculated electronic band structures with SOC effect indicating band inversion at high symmetric point $\Gamma$.

However, the electronegativity accompanying SOC has a predominant place in non-trivial insulating phase in XX’O HH compounds. In all nine compounds, we notice an indistinguishable electronic band structures (as shown in Fig 3) and many sorts of similar non-trivial topological phases (as shown in Fig 4). In contrast to other HH compounds, the RbAuO, LiAgO and KAuO possess a large energy gap ($> 0.1$ eV). Among all the XX’O compounds, seven (LiCuO, LiAgO, LiAuO, KCuO, KAuO, RbCuO, RbAuO) of them have Mexican hat-like band dispersion in their CBM and VBM by the topological phase transition which results in stronger band inversion than an energy gap that arises between the two energy bands.

In the following section, we will discuss throughly regarding RbAuO compounds. See the supplementary material for additional information regarding electronic band structure, density of states (DOS), partial density of states (PDOS), surface states, Slab band structure, and WCC of other eight compounds.
Figure 4: Computational surface states of the XX’O compounds demonstrate conducting surfaces.

3.1 Electronic Properties: RbAuO

The HH compound RbAuO has a cubic $C1_b$ type crystal structure with $F\bar{4}3m(216)$ space group. The optimized lattice constant found by the energy minimization algorithm is 6.24 Å. Our equilibrium lattice constant matches well with the previous theoretical studies. The electronic band structure (Without and With SOC) of RbAuO compounds is shown in Fig 5(a) and (d). Without admittance of SOC effect, RbAuO acquire semi-metallic behavior (conduction and valence bands are just touched at the Fermi level) and possesses doubly degenerate bands along the high symmetric point $\Gamma$ (Fig 5(a)). When the SOC influence is involved, conduction and valence bands are separated by the pseudo energy gap and Fermi energy lies in region.
The angular momentum analogous $l$ degeneracy of the electronic band is lifted off due to the substantial SOC effect (Fig 5 (d)). Since the DOS of RbAuO, without the inclusion of SOC is zero at the Dirac points (as shown in Fig 5 (c)). In the presence of SOC, the gap appears and the DOS reduces near the Fermi level (Fig 5(f)). Importantly, band ordering and orbital inversion near the Fermi level are essential characteristics to analyze the topological phase transition in any compounds and be of critical concern in the surface study as well as spin relaxation properties. Furthermore, low energy excitation results are analyzed near the Fermi level, we restrict our investigation to this region only.

![Figure 5: Electronic band structure of the RbAuO compounds (a) without SOC indicating semimetallic behaviour (d) with SOC effect demonstrating band inversion at high symmetric point Γ (b) PDOS without SOC (e) PDOS with SOC (c) DOS without SOC (f) DOS with SOC (inset zoomed version DOS).](image)

Owing to lack of inversion symmetry in HH compounds, one of the ways is to recognize the band inversion at high symmetric point of Brillouin zone is based on their orbital character of the elements. For TIs without(with) inversion symmetry, the band inversion takes place at unpredictable points of the BZ (at specific time reversal invariant momenta (TRIM) of the Brillouin zone). Without SOC effect, in PDOS plot, the conduction band is composed of -p and -s orbitals, and in the valence band -d and -p orbital contribution is escalating (Fig 5 (b)). However interesting anomaly is observed in the presence of SOC effect, a large amount of Au-d and Au-s orbital contribution arises in the conduction bands and at $\sim -1.4$ eV in
the valence band -s orbital contribution escalates (Au-d orbital contribution is decreasing) as shown in Fig 5(e). Our analysis stipulates that band inversion observed in RbAuO is -s and -d band inversion (Unconventional compared to ordinary -s-p band inversion). As shown in the electronic band structure (Fig 5(d)) the conduction band Γ₇ and Γ₆ are formulated with -d and -s orbitals respectively. However, Γ₈ is composed from the -p and -d hybridized orbitals. Here band inversion is observed between Γ₇ (minima of the conduction band) and Γ₆ (inner valence band). Due to Mass-Darwin relativistic effect, materials like RbAuO having large -d orbital character force Γ₆ state to stay below the Γ₈ and Γ₇ states. To accomplish Mass-Darwin relativistic effect, we observed a similar kind of behavior in all other C₁₆ type HH compounds. This type of band ordering was observed in previously explored HH compounds NaYO (Y = Ag, Au, and Cu). XX'O compounds are more superior than other HH compounds such as LaPtBi, LaAuPb, and LuPdBi by virtue of their large non-trivial energy gap. However, the effect of SOC can be further enhanced by applying strain in a specific crystal plane which increase the energy gap. Although the identification of crystal planes (apply strain on that distinct plane) and the study of their topological properties had been valuable development in material science.

3.2 Strain engineering: RbAuO

In the final step, without breaking cubic symmetry of HH compound, we now explore the effect of hydrostatic strain (compressive and expansive) on the robust topological phase of RbAuO. In the hydrostatic compression(expansion), equally decreasing(increasing) the lattice constant along all the three axes of the cubic unit cell (a=b=c). We have analyzed the electronic and topological properties of RbAuO compounds over a wide range of a = ao - 6%ao to a = ao + 6%ao and observed that the RbAuO retains it’s non-trivial characteristic and band ordering. The electronic band structures with the inclusion of SOC at a = ao ± 6%ao are shown in Fig. 6(a) and (b). Bandgap can be further tuned appreciably by compressive and expansive pressure as evident from Fig 6(c).

Interestingly, hydrostatic compression(expansion) gives increment(decrement) in energy gap. Thus, RbAuO preserves its robust topological phase and conducting surface states leading to a no trivial phase transition that has taken place during this process. The strain tuned large
energy gap (with SOC) at $a = ao - 6\% ao$ is more predominant to well-known another 3D TIs, i.e., we notice that the energy gap increases from 0.19 eV (at equilibrium lattice constant) to 0.23 eV. We find that conducting surfaces with $Z_2=1$ exist at two extrema of hydrostatic strain (as evident from Fig 6 (c) inset) directing us to a potential candidate for spintronics devices.

### 3.3 $Z_2$ analysis and Surface states

Apart from the basic premises of band inversion near the Fermi level due to SOC, the concept of a band topology created agreeable certainties in the introspection of topological phase transition. Topological materials can be distinguished based on their non-trivial band topology. To get accurate topological properties of all nine HH compounds, we compared our electronic band structure (from first principle calculations) with previously reproduced band structure through the maximally localized Wannier wavefunctions (MLWFs) by minimizing spread and generating the accurate tight-binding model (see Fig 7 (a)). Due to the lack of inversion symmetry in cubic HH compounds, we calculated the $Z_2$ indices along six time reversal invariant planes (TRIP) i.e., $k_x = 0, \pi$, $k_y = 0, \pi$ and $k_z = 0, \pi$ in the BZ using equation (1) and (2).

\[
\nu_0 = \left( Z_2(k_i = 0) + Z_2(k_i = 0.5) \right) \mod 2 \quad \ldots (1)
\]
\[
\nu_i = Z_2(k_i = 0.5) \quad \ldots (2)
\]

The 3D $Z_2$ indices ($\nu_0$, $\nu_1 \nu_2 \nu_3$) are normally composed using one strong ($\nu_0$) and three weak ($\nu_1 \nu_2 \nu_3$) topological indices. The $Z_2$ indices ($\nu_0$, $\nu_1 \nu_2 \nu_3$) for all nine systems were found to be (1, 000) which suggests that, all compounds are non-trivial topological insulators.
at their equilibrium lattice constant. However, during a time reversal pumping process, we
}can directly measure the $\mathbb{Z}_2$ invariants by tracing the evolution of WCCs.\textsuperscript{[49]} We calculated the
evolution of WCCs (Fig 7 (d)) using Wilson loop method and one of the advantage is that, it
can be applied to any material irrespective of the inversion symmetry. We can get direction
regarding the trivial or non-trivial band topology of the 2D plane by observing WCC between
two TRIM points in a plane. Electronic states in a periodic system can be described by the
Bloch function $|\psi_{nk}\rangle = e^{i\mathbf{k} \cdot \mathbf{r}} |u_{nk}\rangle$ ; Where n is the band index and $u_{nk}$ is the lattice-periodic
part. However, the set of localized orbitals can be obtained by taking Fourier transformation
of Bloch functions which is defined as-

$$|W_n(R)\rangle = \frac{1}{(2\pi)^3} \int_{BZ} d\mathbf{k} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{R})} |u_{nk}\rangle \quad ...(3)$$

We can choose specific direction of Wannierization in 3D (here, let’s say z). The Wannier
function is localized in z direction and it’s position is known as WCC which can be represented
by

$$\bar{z}_n(k_x, k_y) = \langle W_n(0, k_x, k_y) | \hat{z} | W_n(0, k_x, k_y) \rangle \quad ...(4)$$

The non-trivial uniqueness of the topological insulator is based on the Kramers doublets
exchange partners during the evolution of WCC. In the evolution of WCC, three left(right)
planes with odd(even) number of crossing elucidate topologically nontrivial phase with $\mathbb{Z}_2 = 1$. The qualitative information of the surface states can be obtained by resolving evolution of WCC. Computationally, there are two methods to get surface states and slab band structure. In contrast to first-principle calculation by taking thick enough slab (computationally expensive), the surface Green’s function ($G_s (k_{||}, \omega)$), bulk Green’s function ($G_b (k_{||}, \omega)$) and dual surface Green’s function ($\tilde{G}_s (k_{||}, \omega)$) methods for a semi-infinite system (depicted in eq (5), (6) and (7)) can save an ample amount of computational time by using iterative procedure.

$$G_s (k_{||}, \omega) \simeq (\omega - \varepsilon_{s}^n)^{-1} ...(5)$$
$$G_b (k_{||}, \omega) \simeq (\omega - \varepsilon_{n})^{-1} ...(6)$$
$$\tilde{G}_s (k_{||}, \omega) \simeq (\omega - \tilde{\varepsilon}_{s}^n)^{-1} ...(7)$$

As executed in WT code, by using imaginary part of the surface green function we can obtain the surface spectrum function ($A (k_{||}, \omega)$).

$$A (k_{||}, \omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \text{Im} \text{Tr} G_S (k_{||}, \omega + i\eta) ...(8)$$

Topological surface states consist a single Dirac cone at the $\Gamma$ point as depicted in Fig 7(b) and (c). Additional confirmation for the existence of the dissipation less quantum transportation came expectedly from the conducting surface states. Thus we conclude that, RbAuO undergoes a topological phase transition at their equilibrium lattice constant under the effect of SOC.

4 Conclusion

In conclusion, we have demonstrated the non-trivial insulating phase in XX’O HH compounds using first-principle-based DFT calculations. The LiAgO, KAuO, and RbAuO compounds are initiated to be a large gap 3D TI originated due to the strong electronegativity and SOC strength. The most engrossing aspects is their non-trivial insulating gap in their equilibrium lattice constant. The predicted topological phase in the RbAuO compound retains its robustness over a wide range of hydrostatic strain $a = a_0 - 6 \% a_0$ to $a = a_0 + 6 \% a_0$ with the maximum energy gap of 0.23 eV. In addition, the non-trivial characteristic is further confirmed by computing gapless surface states and the evolution of WCC which indicates that all nine compounds
are categorized to be strong TI in nature with $\mathbb{Z}_2$ invariants (1, 000). The robust topological properties of these compounds can be used for spintronics and nanoelectronics application. We expect our work will guide experimental validation.

**Conflicts of interest**

There are no conflicts to declare.

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