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Electronic structure of the antiferromagnetic topological insulator candidate GdBiPt

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We studied the electronic structures of antiferromagnetic (AFM) GdBiPt with propagating vectors $\vec{Q}_1 = (0,0,\pi)$ (A-type) and $\vec{Q}_2 = (\pi,\pi,\pi)$ (G-type) by performing first-principles calculation based on density-functional theory with modified Becke and Johnson local-density approximation potentials plus Hubbard U (MBJLDA+U). With the total energy calculation, the G-type AFM spin-ordered state is relatively more stable than the A-type AFM spin-ordered state, although the difference in total energy is minute. Our band-structure calculation predicts that the A-type AFM state is topologically nontrivial due to a single *s*-character band inversion at the Γ point, which is similar to the band inversions in half-Heusler topological insulator candidates and bulk HgTe semiconductors, while the G-type AFM state is topologically trivial due to the absence of *s/p* band inversion. With a realistic tight-binding model calculation with 20 bands coupled to an AFM Zeeman field, GdBiPt with A-type AFM spin order presents a metallic surface state on the terminations with AFM aligned Gd ions, and this surface state is independent of the strength of the AFM Zeeman field, i.e., this surface state will be preserved in a nonmagnetic case. Upon terminating the ferromagnetic spin-aligned Gd ions, the surface state is dependent on the strength of the Zeeman field, and the metallic surface can recover when the Zeeman field approaches zero.

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I. INTRODUCTION

With the discovery of the integer quantum Hall effect (IQHE), the topological classification of insulators has become a surging research topic in the field of condensed-matter physics. As we know, the quantization of Hall conductivity is related to the Chern number of a two-dimensional (2D) electronic gas system in a magnetic field, which has broken time-reversal symmetry (TRS) [1]. Recently, several topological invariants were proposed, including the $\mathbb{Z}_2$ topological invariant protected by TRS [2–4] and the mirror Chern number protected by mirror symmetry [5–8]. So far, almost all the predicted topological insulator materials have been nonmagnetic, including the noninteracting Sb_2Te_3 , Bi_2Te_3 , and Bi_2Se_3 semiconductors [9], which can be described by a single-particle picture, and the heavy fermion material SmB_6 [10,11], which can be described by the periodic Anderson-Kondo lattice model. In contrast to these topological band insulators protected by single TRS or point-group symmetry [12–14], an antiferromagnetic (AFM) topological insulator (AFMTI) protected by the combined operation of TRS and a lattice translation by vector $\vec{D}$ was proposed by Roger *et al.* [15]. The AFMTI is a novel material because of the coexistence of a topologically protected metallic surface state and magnetic order. In addition, the AFMTI represents a trivial boundary state upon the termination of ferromagnetic (FM) spin alignment and a topologically metallic surface state upon the termination of AFM spin alignment [15,16].

The first proposed AFMTI candidate was the half-Heusler compound GdBiPt [15]. Ternary Heusler compounds have attracted a great deal of research interest due to their rich

physical properties [17]. About 50 ternary Heusler compounds with nonmagnetism, including LnAuPt , LnPdBi , LnPtSb , and LnPtBi , all with the rare-earth element Ln, are predicted to be topological insulators by first-principles calculation [18–22], and all the predicted topological insulators exhibit a single *s*-character band inversion at the time-reversal-invariant-momentum (TRIM) point Γ , which is similar to that of HgTe [23,24]. Nonmagnetic GdBiPt is also predicted to be a topological metal by density-functional theory (DFT) calculation with the modified Becke and Johnson local density approximation (MBJLDA) [25]. However, many of the Half-Heusler compounds have additional properties at low temperature, e.g., the superconductivity of LaPtBi and LuPtBi below 1.0 K [26,27], and the heavy fermion behavior of YbBiPt [28–31]. GdBiPt is face-centered-cubic (fcc) material with MgAgAs structure (cubic space group $F\bar{4}3m$) [29]. It is paramagnetic with free local spin at room temperature, and it is AFM spin ordered with propagating vector $\vec{Q} = (\pi,\pi,\pi)$ below 8 K [32,33].

Since GdBiPt is AFM material at low temperature, it is problematic whether the single *s*-character band inversion in nonmagnetic GdBiPt can be preserved in the AFM GdBiPt. On the other hand, the electronic correlation of *4f* orbitals is very strong, but the effect of this electronic correlation has not been considered in previous work. In this work, we study the electronic structure of AFM GdBiPt bulk with two different propagating vectors $\vec{Q}_1 = (\pi,0,0)$ (A-type) and $\vec{Q}_2 = (\pi,\pi,\pi)$ (G-type) via first-principles calculation with MBJLDA and MBJLDA plus the Hubbard U (MBJLDA+U). Our results show that the energy difference between the A-type and G-type AFM spin orders is minute, and GdBiPt with A-type AFM spin order is topologically nontrivial, as indicated by the single *s*-character band inversion at the Γ point, while GdBiPt with a G-type AFM state is topologically trivial. We also study the surface states of A-type AFM GdBiPt using

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a realistic tight-binding (TB) model with 20 bands, which is coupled to a magnetic field from the localized $4f$ orbitals of Gd. Our results show that A-type AFM GdBiPt presents a metallic surface state upon termination of AFM aligned Gd ions, and this surface state is independent of the strength of the Zeeman field. In contrast, the surface state upon termination of FM Gd ions is dependent on the strength of the Zeeman field.

II. COMPUTATIONAL METHOD

The DFT calculations employed the all-electron, full-potential linearized augment plane wave (FPLAPW) method with MBJLDA implemented in the WIEN2K code [34,35]. The MBJLDA calculations are crucial for the correct determination of the topological insulator. While the MBJLDA describes accurately the correlation effects of the weak interacting electrons [21,25,36], it cannot capture well those of the more localized $4f$ electrons, whose treatment still requires a small Hubbard U value [37–39]. This is similar to the $GW + U$ approach [40], which was also put forward to fix the GW problems for $4f$ systems. To account for the on-site $4f$ -electron correlations, we apply the MBJLDA + U scheme that incorporates an effective on-site Coulomb repulsion $U_{\text{eff}} = 6.0$ eV with a double-counting correction based on the self-interaction correction (SIC) for the Gd $4f$ orbitals [41]. The spin-orbit coupling (SOC) was included in the self-consistent calculations. We used $R_{\text{MT}} \times K_{\text{max}} = 9.0$, muffin-tin radii of 2.50 a.u. for all elements in GdBiPt, and a 4096 k -point Monkhorst-Pack mesh for both types of AFM GdBiPt. We used the experimental lattice parameter $a = 6.68$ Å for the lattice parameter [29]. The basis set consisted of the Gd $4f$, $5d$, $6s$, and $6p$ valence states, the Gd $5s$ and $5p$ semicore state, the Bi $6s$ and $6p$ valence states, the Bi $5s$ and $5p$ states semicore states, and the Pt $4f$ semicore and $5s$, $5p$, $5d$, and $6s$ valence states. For the total energy calculation, the generalized gradient approximation (GGA) is adopted, since the total energy calculated by MBJLDA has no physical meaning.

III. BULK STATE

At room temperature, GdBiPt is paramagnetic and the localized $4f$ does not form spin order. For nonmagnetic GdBiPt with the $F\bar{4}3m$ space group [shown in Fig. 1(a)], it is predicted to be a topological metal with a single s/p -band inversion at the Γ point via first-principles calculation with MBJLDA [25]. To include the effect of spin order, we consider A-type AFM spin order (the magnetic structure of CeBiPt) [42] and G-type AFM spin order (proposed in GdBiPt) [32,33]. The A-type AFM spin order consists of AFM aligned ferromagnetic (FM) layers perpendicular to the $(1,0,0)$ direction, and the G-type AFM order consists of AFM aligned FM layers perpendicular to the $(1,1,1)$ direction. The magnetic unit cells of A-type and G-type AFM are shown in Figs. 1(b) and 1(c), respectively, and the magnetic unit cells have lowered crystal symmetry because of different spin directions on the two Gd atoms. The magnetic space groups of the two magnetic unit cells are $P\bar{4}2m$ and $R\bar{3}m$, and the latter is very close to the space group of Bi_2Te_3 $R\bar{3}m$, which has an additional spatial inversion symmetry [9]. In AFM GdBiPt, Kramers' degeneracy should be satisfied for the definition of topologically invariant $\mathbb{Z}_2$, and this Kramers'

FIG. 1. (Color online) The crystal structure of the cubic GdBiPt unit cell with the $F\bar{4}3m$ space group. (a) The magnetic unit cell of AFM GdBiPt with propagating vector $\vec{Q}_1 = (0,0,\pi)$ (A-type) and lowered space group $P\bar{4}2m$ resulting from the inequivalent Gd atoms with different spin direction, and (b) the magnetic unit cell of AFM GdBiPt with propagating vector $\vec{Q}_2 = (\pi,\pi,\pi)$ (G-type) and lowered space group $R\bar{3}m$ resulting from splitting the magnetic Gd atoms in a hexagonal representation (c) and a rhombohedral representation (d).

degeneracy requires a combined symmetric operation of time reversal and a lattice translation $\vec{D}$, which inverts the direction of spin [15,44]. In the A-type AFM order, vector $\vec{D} = (1/2, 1/2, 1/2)$ (defined in a magnetic unit cell) inverts the spin direction. In the rhombohedral representation of the G-type AFM order, vector $\vec{D} = (1/2, 1/2, 1/2)$ also inverts all the directions of spin in the magnetic rhombohedral unit cell [shown in Fig. 1(d)]. Therefore, in both types of proposed commensurate AFM spin orders, Kramers' degeneracy is indeed satisfied, and this degeneracy makes it possible to define $\mathbb{Z}_2$ as topologically invariant. Our total energy calculation shows that the FM spin-ordered state has higher total energy than the A-type AFM state by 70 meV. The energy difference between the A-type and G-type AFM states is minute, and it is less than 7 meV even though we include Hubbard U up to 9.0 eV. This minute energy difference indicates that the spin fluctuation should be very strong at finite temperature, and it is also consistent with the very low AFM transition temperature $T_N \sim 8$ K [32,33]. We note here that the energy difference among different AFM states is also very minute by LSDA+ U in GdBi materials, where $U = 6.8$ eV [45]. The band structures with A-type AFM spin order calculated by MBJLDA+ U is shown in Fig. 2(a), and it is similar to the band structure of G-type AFM spin order [shown in Fig. 2(b)]. However,

FIG. 2. (Color online) Band-structure magnetic GdBiPt with A-type AFM spin order (a) and G-type AFM spin order (b) calculated by MBJLDA+U. The weight of s orbitals and p orbitals from Bi and Pt atoms and $5d$ orbitals from Gd is represented by red, blue, and green, respectively.

there exists an essential difference between them, viz. the position of the band with s -orbital character at the Γ point. Both types of AFM GdBiPt are predicted to be a semimetal by MBJLDA+U calculation. In contrast to band structure calculated by MBJLDA [25], the f -electron dominating bands are pushed away by the AFM Zeeman field and correlation from MBJLDA+U, which is dominating compared to the SOC of f orbitals. The Hubbard U is set to be 6.0 eV here, a value that is also adopted in the work of Gd X ($X = \text{N, P, As, Sb, or Bi}$) by Duan *et al.* [43]. However, the sequence of occupied bands is irrelevant with an even larger effective Hubbard U , which just shifts the centers of gravity of the upper Hubbard band (UHB) and the lower Hubbard band (LHB). The calculated local spin moment per Gd is about $6.9\mu\text{B}$ in both types of AFM order, indicating the f orbitals are well localized while the Bi and Pt atoms are nonmagnetic. We find that the single s/p -band inversion at the Γ point is preserved in the A-type AFM state, and this s -orbital dominating Γ_6 and p -orbital dominating Γ_7 (represented by red and blue in band structures) band inversion is essentially similar to the case of half-Heusler topological insulators with zinc-blende structure [18–22], a HgTe/CdTe quantum well [23,24], and strained bulk HgTe [46,47]. However, this s -orbital character band inversion is not predicted in the band structure of the G-type AFM state, in which all the occupied bands have the same $\Gamma_3 + \Gamma_4$ representation resulting from s - d hybridization at the Γ point. The $5d$ orbitals of Pt dominating bands are fully occupied in the energy window $-5.0 \sim -3.0$ eV, while the $5d$ orbitals of Gd are almost slightly hybridized with s orbitals and p orbitals from Bi and Pt around the Fermi level [48].

IV. SURFACE STATE

Since the s and p orbitals make the main contribution to the electronic structure near the Fermi level, and the localized f electrons play the role of local spin, AFM GdBiPt is equivalent to nonmagnetic LaBiPt coupled to an AFM Zeeman field. The nonmagnetic LaBiPt topological insulator candidate shares a similar characteristic of electronic structure with the HgTe semiconductor, i.e., the band inversion between s -orbital dominating Γ_6 and p -orbital dominating Γ_8 at the Γ point [19,20,23]. The band inversion in a 2D HgTe/CdTe

FIG. 3. Surface state on the [101] surface with AFM aligned Gd ions and Zeeman field strength $B = 2.0$ eV.

quantum well can be described by the Bernevig-Hughes-Zhang (BHZ) model [23,46,49]. Here, LaBiPt is 3D material, and the low-energy electronic structure near the Fermi level can be described using the extended BHZ model in three dimensions. With a four-component spinor wave function $\Psi(i) = (\psi_{i,s}, \psi_{i,p})^T$ on a fcc lattice, the s/p -band inversion can be reproduced by this extended BHZ model with approximate hopping parameters. In the work of Roger *et al.* [15], a metallic surface state upon the termination of an AFM aligned Gd ion and an insulating surface state upon the termination of FM aligned Gd ions are predicted, respectively. However, this extended BHZ model is too simple to describe the surface state of paramagnetic GdBiPt determined by angle-resolved

photoemission spectroscopy (ARPES) [50]. The ARPES experiment detected a pair of metallic surface states near the $\bar{\Gamma}$ on the [111] surface, instead of a single Dirac cone predicted by the extended BHZ model. To explain the experimental result and determine the surface state of AFM GdBiPt, we adopt a realistic TB model with 20 bands, including the s and p orbitals and excited s^* orbitals on the Bi and Pt lattice points and spin freedom [47,51]. The single-particle energy and hopping parameters are extracted via first-principles calculation using maximally localized Wannier functions (MLWFs) [52,53], and the SOC term is added manually. In the $|\mathbf{L}\mathbf{S}\rangle$ representation, the SOC is expressed as

$$H_{so} = \frac{\lambda}{2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i\sigma_z & i\sigma_y & 0 & 0 & 0 & 0 & 0 \\ 0 & i\sigma_z & 0 & -i\sigma_x & 0 & 0 & 0 & 0 & 0 \\ 0 & -i\sigma_y & i\sigma_x & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -i\sigma_z & i\sigma_y & 0 \\ 0 & 0 & 0 & 0 & 0 & i\sigma_z & 0 & -i\sigma_x & 0 \\ 0 & 0 & 0 & 0 & 0 & -i\sigma_y & i\sigma_x & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (1)$$

Here, σ_x , σ_y , and σ_z are the Pauli matrices. The AFM Zeeman field with prorogating vector $(0,0,\pi)$ from the local spin moment of Gd is expressed as

$$J(z) = B \cos(2\pi z) \vec{e}_z. \quad (2)$$

The strength of the Zeeman field $B = 2.0$ eV is estimated from the energy splitting of f orbitals induced by AFM order in the first-principles calculation. Since there is no AFMTI in two dimensions, we need sufficient layers that can safely be regarded as 3D material to calculate the surface state. With 60 layers of a unit cell, we find that there is a pair of surface states from the top and bottom of the layers, respectively,

coexisting with the bulk state at the $\bar{\Gamma}(0,0)$ point on the [101] surface with AFM aligned Gd atoms, as shown in Fig. 3. The pair of surface states is degenerated at $\bar{X}(0,\pi)$ and $\bar{M}(\pi,\pi)$, except the $\bar{\Gamma}$. Around the $\bar{\Gamma}$ point, one surface state submerges into bulk states and the other one crosses the Fermi level. Interestingly, this pair of surface states can be preserved under a weak AFM Zeeman field, even though the strength $B = 0.0$ eV. The surface state on the [001] surface with FM aligned Gd atoms is shown in Fig. 4, and this surface is metallic because of the metallic bulk state. In contrast to the [101], this surface state is very sensitive to the external Zeeman field, and it will be similar to the [101] surface state when the Zeeman

FIG. 4. Surface state on the [001] surface with FM aligned Gd ions and Zeeman field strength $B = 2.0$ eV.

FIG. 5. Surface state on the [001] surface with FM aligned Gd ions and Zeeman field strength $B = 0.0$ eV.

field vanishes, as shown in Fig. 5. This predicted surface state with a vanishing Zeeman field is consistent with the pair of metallic surface states in nonmagnetic GdBiPt and strained bulk HgTe observed by ARPES experiment [50,54]. We note that the pair of topologically protected metallic surface states is independent of the choice of surface ending, although the trial surface state resulting from a dangling bond is dependent on the Pt or Bi surface ending.

V. SUMMARY

In summary, we used a first-principles calculation and a model calculation to study the electronic structure of the AFM topological insulator candidate GdBiPt with two different types of commensurate AFM order. The *s/p* band inversion in nonmagnetic GdBiPt can be preserved in A-type AFM states instead of a G-type AFM state, and this band inversion is irrelevant with the electronic correlation. Using a realistic

tight-binding model with 20 bands, a pair of surface states is predicted on the surface with an AFM aligned Gd ion, and this surface state is independent of the strength of the Zeeman field. This pair of surface states agrees with the experimental result very well. However, on the [001] surface with FM aligned Gd atoms, the surface state is sensitive to the strength of the Zeeman field, and it will be similar to the [101] surface state when the Zeeman field vanishes.

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