Lifshitz transitions and hybrid Weyl points in RbAg$_5$Se$_3$

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Abstract

We explore the topological phase transitions of RbAg$_5$Se$_3$ using first-principles calculations in combination with the maximally localized Wannier function method. Our computations reveal that the type-II Dirac cone in RbAg$_5$Se$_3$ protected by the inversion and time-inversion (PT) symmetry in addition to the C$_{4z}$ rotation symmetry can be regulated to type-III and type-I Dirac points by applying strain along the [001] direction. More interestingly, when the inversion symmetry is lifted by intercalating a Pt atom into the unit cell, sixteen hybrid Weyl points emerge accompanied by the Fermi arcs connecting the adjacent Brillouin zones and surface states on the (010) surface. The type-II Weyl point has the chirality of 1, while the type-I Weyl point has the chirality of $-1$. Our work suggests that RbAg$_5$Se$_3$ serves as a promising platform for study of topological phases transitions with curious transport phenomena.

1. Introduction

Topological semimetals featured by Dirac or Weyl points in electronic band structures have aroused great interest in condensed matter physics, because of the intriguing physical properties such as negative magnetoresistance [1–4], quantum anomalous Hall effect [5–7], Fermi arcs [8–11] and chiral anomaly [12–17]. In Dirac semimetals, the valence bands and conduction bands touch at fourfold degenerate points (Dirac points) accompanied by linear energy–momentum relations near the Dirac points. Typical examples include graphene [18], Na$_3$Bi [19, 20], Cd$_3$As$_2$ [21, 22] and so on. While for Weyl semimetals, the degenerate points (Weyl points) become twofold, as evidenced in TaAs family [10, 23], Y$_2$Ir$_2$O$_7$ [24], WTe$_2$ [25, 26]. Weyl points have the chiralities of +1/−1 corresponding to the source/sink of Berry curvature in momentum space [27], which can be treated as the monopoles of Berry magnetic field. The Weyl points with opposite chirality always appear or annihilate in pairs. The unusual surface states featured by Fermi arcs connecting Weyl nodes of opposite chirality are closely related to the nontrivial topology of Weyl semimetals.

According to the tilt of the linear energy–momentum relations, Dirac and Weyl points can be classified into three types (I, II and III) [27–31]. Most of the Dirac (or Weyl) points proposed in previous works belong to type-I with a point-like Fermi surface. Type-II Dirac and Weyl semimetals have electron and hole pockets at the Fermi level where the Lorentz invariance is broken [27], which lead to some unusual scenarios, such as topological superconductivity [32, 33], chiral anomaly related to the current direction [27] and Lifshitz transitions [34]. Type-III Dirac (or Weyl) point can be regarded as the critical state between type-I and type-II where the Fermi velocity vanishes along a certain direction. The coexistence of the three types of Dirac cones in a single material has been predicted to be promising for mimicking the event-horizon evaporation in solid state system with a high Hawking temperature [30, 35].

The stability of Dirac and Weyl cones is closely related to the specific symmetries of materials. For example, the fourfold degenerate Dirac cone is protected by spatial inversion (P) and time inversion symmetry (T) and sometime additional rotation symmetry [36–38], while either inversion symmetry or time-inversion symmetry is lifted for the twofold degenerate Weyl points. Therefore, when time-reversal or
inversion symmetry is lifted, e.g., by means of magnetic doping [39], magnetic field [40] or light irradiation [38], the transition from Dirac points to Weyl points could occur, offering a promising platform for study of topological transition and relevant fascinating scenarios. Moreover, Dirac points can also be gapped by applying external strain [41, 42]. Despite of these efforts, achieving topological phase transition remains a challenging task in experiments, partially due to the rarity of suitable candidate materials.

In this work, we explore the potential of silver selenide-based RbAg5Se3 which has been demonstrated to be a type-II Dirac semimetal [43], in achieving topological transition. Our computations demonstrate that the tensile strain along the [001] direction can lead to the Lifshitz between different types of Dirac cones in RbAg5Se3, where type-III Dirac cones are obtained at a moderate strain of about 2.86%. More interestingly, as the inversion symmetry is lifted by intercalating a Pt atom into the unit cell, Dirac points vanish and hybrid Weyl points emerge. The Weyl points with a chirality of 1 are type-II, while the Weyl points with a chirality of −1 are type-I. The coexistence of different types of fermions in RbAg5Se3 suggest a feasible system for study of topological transition and interaction between different quasiparticles.

2. Method and computational details

The first-principles calculations are performed on the basis of density functional theory in combination with the projector augmented wave method [44] as implemented in Vienna ab initio simulation package (VASP) [45, 46]. The generalized gradient approximation in the form of Perbew–Burke–Ernzerhof (PBE) is adopted for the exchange–correlation functional [47]. Considering the metallic nature of RbAg5Se3, we use the PBE + U approach of Dudarev [48] with $U – J = 3$ eV to describe the effects of Pt dopants which has been verified in previous works [49, 50]. The cutoff energy of plane-wave basis set is 500 eV. The Brillouin zone is sampled by using the Monkhorst–Pack k-point mesh [51] of $7 \times 7 \times 3$ for structure relaxation. The maximally localized Wannier functions (MLWF) [52, 53] is constructed using the WANNIER90 tool [54] interfaced with the VASP code to obtain the tight-binding model Hamiltonian, with which we investigate the topological properties.

3. Results and discussion

The RbAg5Se3 synthesized in experiments has a tetragonal lattice structure with the space group of P4/nbm (No. 125), as shown in figure 1(a). In addition to the inversion and time-inversion symmetry, it also has a $C_{4v}$ rotation symmetry along the [001] direction, which have been demonstrated to be responsible for the emergence of Dirac cones near the Fermi level [43]. The optimized lattice constants are respectively $a = b = 6.081$ Å and $c = 11.112$ Å from the present calculations, in good agreement with the experimental results [55]. Notably, the inversion center of RbAg5Se3 is not at the center of the unit cell but at $(0.75, 0.75, 0.5)$. The void in the center of the unit cell is available for hosting foreign atoms, which may regulate the electronic band structures [56, 57].

The electronic band structure of RbAg5Se3 with SOC is plotted in figure 1(c). A Dirac cone resides at $k_z = 0.21 \pi/a$ in the z-axis, which is about 40 meV below the Fermi level. The tilts of the Dirac cone exhibit the characteristics of type-II Dirac point, with the Fermi velocities of $2.7 \times 10^5$ m s$^{-1}$ and $1.9 \times 10^5$ m s$^{-1}$ of the two Dirac bands ($\circ$ and $\square$) along the $\Gamma$–Z direction. The dispersive Dirac band arises mainly from the $p_z$ orbitals of Se atoms along with minor contribution from the $d_{x^2,y^2}$ orbitals of Ag atoms, while the rather flat Dirac band comes mainly from the $p_{x,y}$ orbital of Se atoms, as shown in figure 1(d). The Dirac cones of RbAg5Se3 are protected by the inversion and time-inversion (PT) symmetry in addition to the $C_{4v}$ rotation symmetry along the [001] direction [43].

The two Dirac bands exhibit different response to the uniaxial strain along the [001] direction which preserves the $C_{4v}$ rotation symmetry, due to the different atomic orbital features of these bands, as shown in figure 2(a). For the dispersive Dirac band ($\circ$), the increasing strain along the [001] direction enhances the interaction of between the $p_z$ orbitals of adjacent Se atoms and thereby increases the Fermi velocity along the $\Gamma$–Z direction. For the flat Dirac band arising mainly from the $p_{x,y}$ orbital of Se atoms, however, the Fermi velocity along the $\Gamma$–Z direction decreases and vanishes at the tensile strain of 2.86%, displaying the characteristics of type-III Dirac cones. When the tensile strain exceeds the critical value, the slope of the flat Dirac band becomes negative and the Dirac cone converts to type-I. The position of the Dirac point is also tunable under the strain. As the applied strain increases, the variation of the position of the Dirac point relative to the $\Gamma$ point is plotted in figure 2(b). When the strain increases from $-2\%$ (compression) to 6$\%$ (tensile), the position of the Dirac point varies from 0.14 $2\pi/c$ to 0.34 $2\pi/c$, exhibiting a linear relation to the strain, as indicated by the red fitting line. The strain-induced Lifshitz transition of the band structure of RbAg5Se3 is more evident from the electronic band structures, as shown in figure 2(c). The band dispersion
profiles near the Dirac point and Fermi surfaces depicted in the insets of this figure verify the types of the Dirac cones. The quasiparticle in a type-II Dirac cone travels unidirectional, but bidirectionally in a type-I Dirac cone in momentum space. Type-III Dirac cone is the critical state between them. These interesting features are akin to the block-hole-horizon in high-energy physics, making the system a fermionic block-hole-horizon analog [58–60]. The electron/hole tunneling between a type-II and a type-I Dirac cones separated by a type-III Dirac cone is analogous to the Hawking radiation of a block hole. The benefits of the fermionic block-hole-horizon analog lie in the relatively high and adjustable Hawking temperatures which depend on the electronic band structures of the solid-state systems [35]. Therefore, the strain-induced topological Lifshitz transition in RbAg₅Se₃ offers a promising platform for mimicking black-hole-horizon scenarios in solid state systems. Notably, the Dirac points are in the valence band region. Hole doping is therefore required to regulate the Fermi level to the Dirac points, in order to detect the fascinating scenarios.

The topological Lifshitz transition of RbAg₅Se₃ under uniaxial strain can be described by the minimal four band Hamiltonian near the Dirac point [43], which gives a Dirac point at \( k = 0 \),

\[
H_D(k) = \begin{pmatrix}
\epsilon_1(k) & 0 & A(k) & B(k) \\
\epsilon_1(k) & -B*(k) & A*(k) & 0 \\
\epsilon_2(k) & 0 & 0 & \epsilon_2(k) \\
\epsilon_2(k) & 0 & 0 & \epsilon_2(k)
\end{pmatrix}, \tag{1}
\]

where \( \epsilon_1(k) = a_1 k_x k_y + b_1 k_y^2 + c_1 k_z, \epsilon_2(k) = a_2 k_x k_y + b_2 k_y^2 + c_2 k_z, A(k) = ik_z (d_1 + d_2 k_z), \\ B(k) = i(d_3 k_y^2 + d_4 k_z^2) \) with \( k_x = k_x + ik_y \). The above parameters can be obtained by fitting the first-principles bands around Dirac points. Along the \( \Gamma-Z \) direction \( (k_z = k_y = 0) \), the above the Hamiltonian has twofold degenerate bands, \( E_1(k_z) = b_1 k_z^2 + c_1 k_z \) and \( E_2(k_z) = b_2 k_z^2 + c_2 k_z \) that construct the Dirac cone near the Dirac point. Omitting the \( k_z^2 \) term near the Dirac point \( (k = 0) \), one can get the Fermi velocities \( v_F = \hbar^{-1} dE/dk_z \) of the two bands, \( v_{F1} \equiv c_1/h \) and \( v_{F2} \equiv c_2/h \), respectively. Clearly, the type of the Dirac cone is determined by the signs of \( c_1 \) and \( c_2 \). If \( c_1 \) and \( c_2 \) have the same sign, one gets a type-II Dirac cone. If \( c_1 \) or \( c_2 \) is zero, a type-III Dirac cone emerges. If \( c_1 \) and \( c_2 \) have different signs, a type-I Dirac cone is formed. For the unstrained RbAg₅Se₃, the fitting parameters are \( a_1 = 51.1 \text{ eV Å}^2, b_1 = 0.5 \text{ eV Å}^2, b_2 = 32.2 \text{ eV Å}^2, c_1 = 0.08 \text{ eV Å}^2, c_2 = 3.2 \text{ eV Å}^2, d_1 = 0.41 \text{ eV Å}^2, \)

\( d_2 = 0.1 \text{ eV Å}^2, d_3 = 4.0 \text{ eV Å}^2, d_4 = 4.0 \text{ eV Å}^2 \), which give a type-II Dirac cone. When tensile strain is applied along \( z \) direction, \( c_1 \) decreases with the increase of tensile strain and becomes negative as the tensile strain exceeds 2.86%, leading to the topological Lifshitz transition between the three-type of Dirac cones.
Figure 2. (a) Variation of the Fermi velocity of the two Dirac bands along the $k_z$ direction under external strain. (b) Variation of the position of the Dirac point relative to the $\Gamma$ point in response to the external strain. (c) The electronic band structures of RbAg$_5$Se$_3$ under tensile strain along the [001] direction. The band dispersion profiles near the Dirac points and the Fermi surfaces are plotted as the insets of this figure. The energy of the Fermi level is set to zero.

The electronic structures of topological materials can also be regulated by intercalating foreign atoms [56, 57]. We therefore placed a Pt atom in the center of the unit cell of RbAg$_5$Se$_3$ (corresponding to a doping concentration of $2.4 \times 10^{21}$ cm$^{-3}$) to demonstrate such effect, as shown in figure 3(a). The space group of the resulted PtRbAg$_5$Se$_3$ converts to P422 (No. 89) compared to P4/nbm (No. 125) of the undoped RbAg$_5$Se$_3$. Nonmagnetic Pt atom has remarkable SOC effect and suitable atomic radius matching with the voids in RbAg$_5$Se$_3$. The incorporation of Pt atoms lifts the inversion symmetry of the host material. The binding energy of the Pt atom to the host RbAg$_5$Se$_3$ is about $-3.80$ eV/Pt, indicating the stability and plausibility of PtRbAg$_5$Se$_3$.

The electronic band structure of PtRbAg$_5$Se$_3$ with SOC is shown in figure 3(b). Obviously, the Dirac cone of the host RbAg$_5$Se$_3$ vanishes, due to the contribution of Pt and symmetry reduction. The bands around the Fermi level are mainly contributed by Pt-d, Ag-d and Se-p orbitals, as shown in figure 3(c). We also construct the MLWF of Pt-d, Ag-d and Se-p orbitals using a Monkhorst–Pack $k$-point mesh of $7 \times 7 \times 3$. The relevant Wannier-based tight-binding bands are plotted as the red dotted lines in figure 3(c), which conform the origins of the bands near the Fermi level.

To uncover the possible intersection of the two bands, we scan the whole Brillouin zone based on Wannier-based tight-binding bands using the WANNIERTOOLS package. The Wannier charge center (WCC) on longitudinal loops around a sphere enclosing the crossing point is calculated to characterize topological properties and the chirality of Weyl points, as shown in figures 3(d) and (e). WCC describes the variation of Wilson loop with longitudinal $\theta$ angle. When the angle $\theta$ varies from zero to $\pi$, the value of the WCC is shifted by $2\pi$ or $-2\pi$, indicating that the crossing point is indeed a Weyl point with a chirality 1 or $-1$. Notably, sixteen Weyl points are formed at the energies of 0.11 and 0.22 eV below the Fermi level. The positions of these Weyl points in the Brillouin zone are plotted as the red dotted lines in figure 3(c), which conform the origins of the bands near the Fermi level.

The linear
Figure 3. (a) Crystal structure of PtRbAg$_5$Se$_3$. (b) Electronic band structure of PtRbAg$_5$Se$_3$ with SOC. (c) Orbital-resolved bands with SOC for PtRbAg$_5$Se$_3$. (d) Evolution of the WCCs around the sphere enclosing of Weyl points with a chirality of 1. (e) Evolution of the WCCs around the sphere enclosing of Weyl points with a chirality of $-1$.

Figure 4. (a) The position of these Weyl points in the Brillouin zone. The red/blue dots represent Weyl points with 1/$-1$ chirality. The 2D band dispersions around Weyl points with (b) 1 and (c) $-1$ chirality.

dispersion around a Weyl point is shown in figures 4(b) and (c). Weyl points with a chirality of 1 are type-II, and points with a chirality of $-1$ are type-I, which display the features of hybrid Weyl semimetals as reported in YCoC$_2$ [61] and HfCuPb [62].

We calculate the surface states and Fermi arcs of PtRbAg$_5$Se$_3$ which are treated as the landmarks in the topological properties of Weyl semimetal. The surface states of the (100) surface are shown in figure 5(a). Although partially obscured, the surface states connecting Weyl point can be clearly seen. Figure 5(c) depicts the Fermi arcs of the (001) surface. The Fermi arc connecting the Weyl points is clearly visible in the figure. To visualize the Fermi arcs more clearly, we plot the Fermi arcs in the $2 \times 2$ Brillouin zone where the
boundaries of the Brillouin zone are indicated by the dotted lines. Obviously, the Fermi arcs are connected to the Weyl points in two adjacent Brillouin zones, similar to the case of Co-terminated Co3Sn2S2 [63]. This also reflects the diversity of Fermi arc shapes, such as the spoon-head and bowtie-like Fermi arcs found in TaAs family [10]. Besides, the surface states are close to Fermi level and thus detectable in ARPES experiments.

Weyl points can be regarded as monopoles of Berry magnetic field, corresponding to the source and sink of Berry curvature, which can be visualized by the Berry curvature near the Weyl points. Therefore, to further determine the topological properties of Weyl points, we calculate the Berry curvature using the Kubo formula based on the Wannier-based tight-banding Hamiltonian $H(k)$ [64, 65]:

$$\Omega_n(k) = -2\text{Im} \sum_{m \neq n} \frac{\langle \phi_{nk} | v_x | \phi_{nk} \rangle \langle \phi_{nk} | v_y | \phi_{nk} \rangle}{\left[ \omega_m(k) - \omega_n(k) \right]^2},$$

(2)$$\Omega(k) = \sum_n f(\omega_n(k)) \Omega_n(k),$$

(3)$$v_x(y) = \frac{1}{h} \frac{\partial H(k)}{\partial k_{x(y)}},$$

(4)

where $v_x(y)$ is the velocity operator along the $x(y)$ direction, $\omega_n(k)$ is the eigenvalue of the Bloch function $\phi_n(k)$, $f$ is the Fermi–Dirac distribution function. Berry curvature $\Omega$ is obtained by summing over all the occupied valence bands. We calculate the Berry curvature of on the $x$–$y$ plane at $k_z = 0.078 \frac{2\pi}{c}$, as shown in figure 5(d). It is clear from the figure that the Berry curvature in momentum space diverges and converges near the Weyl points with chirality of $+1$ and $-1$, which demonstrates that the Weyl points with a chirality of $+1/-1$ are the source/sink of the Berry curvature in momentum space.

4. Conclusion

In summary, we reveal the topological phase transitions of the experimentally-synthesized RbAg$_5$Se$_3$ induced by tensile strain and dopants using first-principles calculations in combination with the maximally localized Wannier function method. The Dirac points of RbAg$_5$Se$_3$ are protected by the inversion and time-inversion (PT) symmetry in addition to the C$_{4z}$ rotation symmetry. As a tensile strain along the [001] direction is applied to RbAg$_5$Se$_3$, the type-II Dirac points will convert into type-III and type-I Dirac points, which are promising for black-hole-horizon analog in high-energy physics. Moreover, the Dirac points of RbAg$_5$Se$_3$ can be regulated to hybrid Weyl points by intercalating a Pt atom to the center of the unit cell,
which lifts the inversion symmetry. Eight pairs of Weyl points corresponding to the space group P422 (No. 89) emerge in the resulted PtRbAg$_5$Se$_3$. The topological properties of the Weyl points are confirmed by the chirality, Berry curvature, surface states and Fermi arcs. Our work provides a platform for experimental realization of topological phase transition and the coexistence of different types of Weyl points may lead to fascinating transport phenomena as the Fermi level is regulated to the Weyl points.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the author.

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