Topological semimetal in honeycomb lattice LnSI

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Recognized as elementary particles in the standard model, Weyl fermions in condensed matter have received growing attention. However, most of the previously reported Weyl semimetals exhibit rather complicated electronic structures that, in turn, may have raised questions regarding the underlying physics. Here, we report promising topological phases that can be realized in specific honeycomb lattices, including ideal Weyl semimetal structures, 3D strong topological insulators, and nodal-line semimetal configurations. In particular, we highlight a semimetal featuring both Weyl nodes and nodal lines. Guided by this model, we showed that GdSI, the long-perceived ideal Weyl semimetal, has two pairs of Weyl nodes residing at the Fermi level and that LuSI (YSI) is a 3D strong topological insulator with the right-handed helical surface states. Our work provides a mechanism to study topological semimetals and proposes a platform for exploring the physics of Weyl semimetals as well as related device designs.

Results

Our tight binding (TB) model is built on an $A$–$A$ stacked honeycomb lattice containing two inequivalent sublattices with $[p_z]$ orbitals ($j_z = \pm 1/2$) occupied on A sublattice located at $(0, 0, 0)$ and $[d_{z^2}]$ orbitals ($j_z = \pm 1/2$) occupied on B sublattice located at $(1/3, 2/3, 0)$, as shown in Fig. 1A, in which only threefold rotation around the $z$ axis ($C_z$) and mirror symmetry with respect to the $xy$ plane ($M_z$) as well as time-reversal symmetry ($T$) are preserved. Under the symmetry restrictions, the TB Hamiltonian up to the next nearest (NN) intralayer and interlayer hoppings takes the form

$$H = H_A + H_B + H_{AB}$$

$$H_A = \sum_i \sum_{\alpha} t^{\alpha+}_i C_{\alpha i}^\dagger C_{\alpha i} + \sum_i t^\alpha_{intra} C_{\alpha i}^\dagger C_{\beta j}$$

$$H_{AB} = \sum_{\langle ij \rangle_{inter}} \sum_{\alpha, \beta} \left[ t_{C_{\alpha i}} C_{\alpha i} (C_{\beta j}) + h.c. \right] + \sum_{\langle ij \rangle_{intra}} \sum_{\alpha \neq \beta} \left[ t_{C_{\alpha i}} C_{\alpha i} (C_{\beta j}) + h.c. \right] .$$

where $\mu = A$, and $B$ labels the sublattice; $\alpha, \beta = \uparrow, \downarrow$ labels the spin. $C_{\alpha i} (C_{\beta j})$ creates a spin $\alpha$ electron in the $p_z (d_{z^2})$ orbital of A (B) sublattice at site $i$. The first, second, and third terms in $H_A$ are onsite energy, NN intralayer hopping, and nearest interlayer hopping, respectively. The first term in $H_{AB}$ means NN interlayer hopping, while the second term is the nearest surface of GdSI, which are easily confirmed by angle-resolved photoemission spectroscopy (ARPES) experiment. Such ideal WSM phase in GdSI provides great facility for research of the chiral anomaly physics as well as the device design based on WSMs.

Significance

We show that fruitful topological states can be realized in a special honeycomb lattice model. Guided by this model, we find that GdSI, the long-perceived ideal Weyl semimetal, has only two pairs of Weyl nodes and that LuSI (YSI) is a topological insulator with the right-handed helical surface states. Our work provides a mechanism to study topological semimetals and proposes a platform for exploring the physics of Weyl semimetals as well as related device designs.

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PNAS Early Edition | 1 of 5
intralayer hopping induced by the spin-orbit coupling (SOC) interaction. More detailed definitions of parameters in Eq. 1 can be found in Fig. 1A and SI Methods.

Compared with the Kane–Mele model (46, 47), there are three obvious differences in our model. First, our model is based on a 3D system, which is a necessary condition to realize the WSM. Second, the nearest intralayer hopping between the same spin is forbidden because of the restriction of $M_i$ symmetry. Thus, the nearest intralayer SOC ($\lambda_1$) rather than the NN SOC in the Kane–Mele model plays a crucial role for the band gap opening in the $k_z = 0$ plane. Third, inversion symmetry is broken in our model. Because of the Rashba effect, all bands are split into two branches, which can be distinguished by the eigenvalue of $M_i$ [i.e., $m_s = \pm 1$ as shown in Eq. 1 by dashed ($m_s = 1$) and dotted lines ($m_s = -1$)]. Accordingly, we can define two different splitting configurations: configuration I, $p_i$, and $d_{\pm 2}$ orbitals have the same Rashba splitting as shown in Fig. 1B and G; and configuration II, $p_i$, and $d_{\pm 2}$ orbitals have opposite Rashba splitting as shown in Fig. 1C, E, and H. As we will show below, different Rashba splitting configurations would lead to different topological states.

For configuration I, we first study the case that bands only invert with each other around the $\Gamma$ point (named as case 1). For this case, $p_i$ and $d_{\pm 2}$ orbitals with the same $m_s$ cross each other at the Fermi level in the $k_z = 0$ plane; then, they reopen a topological nontrivial insulating gap caused by the nearest intralayer SOC ($\lambda_1$) as shown in Fig. 1B, which means that a 3D strong TI phase is achieved. If the band inversion keeps increasing and if all bands are inverted at the $K$ ($K'$) point (named as case 2), two pairs of unstable double-Weyl points ($|C| = 2$) should be realized on the $H - K - (-H)$ and $H' - K' - (-H')$ lines as shown in Fig. 1G. The realization of such double-Weyl points can be understood as following: without loss of generality, we choose $A$ (0,0,0) as the rotation center and define $R_{\tilde{K}}^Z = e^{-i 2\pi / 3} \tilde{Z}$ with $J_z = L_z + S_z$, where $L_z$ and $S_z$ are the $z$ components of the angular momentum operator and spin operator, respectively. Then, we get $R_{\tilde{K}}^Z |d_{\pm 2}^{(1/3,2/3,0)}(j_z)_{K} = e^{-i 2\pi / 3} |d_{\pm 2}^{(1/3,1/3,1/3)}(j_z)_{K} = e^{-i 2\pi / 3} |d_{\pm 2}^{(1/3,2/3,2)}(j_z)_{K} = e^{-i 2\pi / 3} |d_{\pm 2}^{(1/3,2/3,0)}(j_z)_{K} = e^{-i 2\pi / 3} |d_{\pm 2}^{(1/3,2/3,2)}(j_z)_{K}$, where $K = (-1/3,2/3,0)$ is defined with respect to the reciprocal lattice vectors. This means that the effective $j_z$ for the $d_{\pm 2}$ bands at $K$ point have to decrease by 1, namely becoming $-1/2 (|d_{\pm 2}^{(1/3,1)}\rangle \langle j_z | - 3/2\langle d_{\pm 2}^{(1/3,1)} | j_z \rangle)$. Respectively. Meanwhile, the effective $j_z^B$ of the $p_i$ bands located at $A$ site do not change at all. As a result, the band crossing between $|j_z = 3/2\rangle$ and $|j_z = 1/2\rangle$ on the $H - K$ line should give rise to one double-Weyl point yielding to the requirement that chiral charge $|C| = 2$. We emphasize that such type of effective $j_z$ jumping on the high-symmetry line provides a mechanism for the exploration of the topological semimetals.

As discussed in ref. 5, each double-Weyl point has quadratic in-plane (along $k_x$, $k_y$) dispersion and linear out-plane ($k_z$) dispersion. However, different from HgCr$_2$Se$_4$ with $C_4v$ symmetry (5), the double-Weyl point (e.g., $C = 2$) in the $C_3$ symmetric system is usually unstable and will split into one negative Weyl point ($C = -1$) and three positive Weyl points ($C = 1$) (48) (details are in SI Methods and Fig. S1).

For configuration II, if the bands only invert around the $\Gamma$ point (i.e., case 1), it is that the opposite $m_s$ bands cross each other at the Fermi level in the $k_z = 0$ plane as shown in Fig. 1C. No interactions can open band gaps for this case because of the $M_i$ symmetry protection. Therefore, the system becomes a nodal-line semimetal with two nodal lines circled around the $\Gamma$ point as shown in Fig. 1D. Given that most proposed nodal-line semimetals exist only by neglecting the effect of SOC (33–36), our finding paves a way for exploration of the SOC-included nodal-line semimetal.

Next, we would like to study the topological states realized for case 2 band inversion with configuration II Rashba splitting. For this case, owing to the decrease of $j_z^B (d_{\pm 2})$ by one and the requirement of effective $j_z$ jumping, the system becomes an ideal WSM phase, in which four pairs of linearly dispersive WNs emerge on the $H - K - (-H)$ and $H' - K' - (-H')$ lines as shown in Fig. 1E, while all of the nodal lines are eliminated. More interestingly, a semimetal coexisting of both WNs and nodal lines can be realized in a specific parameter region between case 1 and case 2. In this case, one band inversion crossing occurs on the $H - K - (-H)$ line, while the other one is still limited in the $k_z = 0$ plane (named as case 3), as shown in Fig. 1E; in this, the left crossing on the $H - K$ line gives rise to a linearly dispersive WN as illustrated for case 2, while the right crossing in the $k_z = 0$ plane is still protected by the $M_i$ symmetry and forms a nodal line around the $K$ point as explained for case 1. As a result, two nodal lines circled around $K$ and $K'$, and two pairs of WNs located on the $H - K - (-H)$ and $H' - K' - (-H')$ lines can be found in this topological semimetal as illustrated in Fig. 1F.

Guided by this model and clear picture, we find a class of topological materials LaSI ($Ln = Lu, Y,$ and Gd), among which LuSI and YSI are 3D strong TIs, and GdSI is the long-pursuing ideal WSM with only two pairs of WNs crossing the Fermi level. As shown in Fig. S2 A and B, LaSI crystallizes in the space group.
Fig. 2. Band structures and WNs. (A and B) The band structures of LuSI calculated by GGA and GGA + SOC, respectively. A, Inset shows the schematic of the nodal line when SOC is neglected. (C and D) Band structures of the ground state in GdSI calculated by GGA + U and GGA + U + SOC, respectively. The red dots in D are the fitted TB results. (E) Chiral charge evolution of the WNs located on $K - H$ (red dots) and $K' - H'$ (blue dots) of GdSI. (F) Summary of the WNs distribution for $k_z > 0$ BZ of GdSI, where green and magenta balls mean the negative ($C = -1$) and positive ($C = +1$) WNs, respectively. The projections of the WNs on the (010) face are shown as well.

$P6$ (49, 50) (same point group as our model), in which Ln atoms (Fig. S2 A and B, silver white) and S atoms (Fig. S2 A and B, yellow) locate in the $z = 0$ plane and form a honeycomb lattice and I atoms (Fig. S2 A and B, purple) intercalate between two LnS layers. Our DFT calculations indicate that the low-energy bands near the Fermi level are mainly contributed from the $p_z$ orbitals of S atoms and the $d_{z^2}$ orbitals of the Ln atoms [the projected density of states and fitted band analyses are shown in Fig. S3]. In particular, although there are four S atoms and four Ln atoms in one unit cell, only one pair of $p_z$-type molecular orbital $|p_z\rangle$ with $j_z = \pm 1/2$ and one pair of $d_{z^2}$-type molecular orbital $|D_{z^2}\rangle$ with $j_z = \pm 1/2$ dominate and invert with each other at the Fermi level, owing to the chemical bonding and crystal field effects. Therefore, our TB model discussed above can be properly applied to LnSI crystal and capture its essential topological properties effectively. Detailed evolution from the atomic orbitals to the molecular orbitals is shown in Fig. S4.

Since LuSI and YSI have almost the same results, we choose LuSI as an example in the following demonstration. The calculated band structures of LuSI by the generalized gradient approximation (GGA) and GGA + SOC are shown in Fig. 2 A and B and Fig. S3B, respectively, which show that a very deep band inversion between $p_z$-type $|p_z\rangle$ bands and $d_{z^2}$-type bands $|D_{z^2}\rangle$ happens at the $\Gamma$ point. If we exclude the SOC interaction, this band inversion will result in a nodal line centered around the $\Gamma$ point in the $k_z = 0$ plane, as shown in Fig. 2A, Inset by the GGA calculations. When the SOC is considered, we have calculated the eigenvalues of the mirror symmetry $M_z$ for the $|p_z\rangle$ and $|D_{z^2}\rangle$ bands. The calculated results show that $|p_z\rangle$ and $|D_{z^2}\rangle$ bands have the same Rashba splitting in LuSI (i.e., LuSI conforms to case 1 band inversion of configuration I splitting). Therefore, GGA + SOC calculations for LuSI show a 32-meV topological nontrivial band gap as shown in Fig. 2B. To check its topological properties, we have carried out the calculations of surface states for LuSI by constructing the Green’s functions (51, 52) based on the maximally localized Wannier function (MLWF) method (53). The calculated results in Fig. 3A indicate that there is a surface Dirac cone in the band gap connecting the occupied and unoccupied bulk states at the $\Gamma$ point on the (001) face of LuSI, which confirms that LuSI is a 3D strong TI clearly. It is worth noting that, different from most 3D TIs with the left-handed helical Dirac cones, the surface states of LuSI exhibit a right-handed helicity of the spin momentum locking, as shown in Fig. 3B, which indicates a negative SOC in LuSI (54).

In the next step, we study the topological properties of GdSI. Considering that the $f$ orbitals of Gd are partially occupied, GdSI is very likely to stabilize in a magnetic phase. To deal with the correlation effect of the $f$ electrons, the GGA + Hubbard U (GGA + U) method has been used. We have calculated five different magnetic configurations for GdSI by the GGA + U + SOC, including the ferromagnetic, three collinear antiferromagnetic (AFM) configurations (AFM1–AFM3), and one noncollinear collinear AFM configuration (AFM4), as shown in Fig. S5. The calculated total energies and moments are summarized in Table S1, which shows that all magnetic states
are lower than the nonmagnetic state about 28 eV/unit cell (7 eV/Gd) and that the AFM4 configuration is the most stable one, further lowering the total energy about 1.8–9.1 meV compared with in the other collinear magnetic states. This is because that AFM4 configuration has eliminated the frustrations as much as possible, and it agrees with the 2 × 2 reconstruction of the crystal mostly (49, 50).

The GGA + U and GGA + U + SOC band structures of AFM4 are plotted in Fig. 2C and D, respectively, which shows a similar dispersion to LuSI at a quick glance. However, after a meticulous analysis, we find three substantial differences from LuSI. First, our calculations indicate that \( |P_4| \) and \( |D_2| \) bands in GdSI take the opposite Rashba splitting configuration II. Second, band inversion in GdSI not only exists at the \( \Gamma \) point but also happens at the \( K \) (\( K' \)) point (i.e., GdSI belongs to band inversion case 3). Third and most importantly, both time-reversal symmetry \( T \) and mirror symmetry \( M_3 \) are broken in the ground-state AFM4 of GdSI as a result of the noncollinear magnetic configuration. Therefore, the band crossing in the \( k_z = 0 \) plane has lost the \( M_3 \) protection and opens a gap, because \( m_0 \) is not a good quantum number again. Based on this symmetry analysis and as will be shown below, GdSI becomes an ideal WSM, with two pairs of WNs originating from the band crossing occurring on the \( K--K'--\Gamma--\Gamma'--K \) line, although GdSI is categorized in case 3 of configuration 6. For describing GdSI’s band structures and topological properties accurately, a Zeeman splitting term \( H_z = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix} \times \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \) that breaks the time-reversal symmetry \( T \) and a nearest intralayer hopping \( t_2 = \langle \Psi_{(001)} | \hat{H}_{NN}(1/3, 0, 1/2) | \Psi_{(1/3, 0, 1/2)} \rangle \) that breaks the \( M_3 \) symmetry are added to the TB model Eq. 1. The explicit form of this new Hamiltonian and the fitted parameters for GdSI are described in SI Methods. The fitted band structures (red dots in Fig. 2D) are plotted together with the GGA + U + SOC bands (blue lines in Fig. 2D), which show that the effective model reproduces the DFT calculations quantitatively well. Based on this effective TB model and the fitted parameters, we have calculated the chiral charges for the WNs located above the \( k_z = 0 \) plane and plotted their evolution (55) in Fig. 2E, which manifests that the charge center for the WN located on the top of \( K \) point shifts downward (red dots in Fig. 2E), indicating the Chern number \( C = -1 \), while the charge center for the WN located on the top of \( K' \) point shifts upward (blue dots in Fig. 2E), corresponding to \( C = 1 \). The WNs distribution in the \( k_z > 0 \) Brillouin zone (BZ) is summarized in Fig. 2F, and we find their counterparts at the same \( k_z \) and \( k_0 \), but opposite \( k_x \), because the inverted bands are approximately symmetrical around the \( K \) (\( K' \)) point as shown in Fig. S6, despite the \( M_3 \) symmetry breaking in GdSI. Such conclusion is completely consistent with our DFT calculations, which indicate that GdSI holds only two pairs of WNs located at \((-1/3, 2/3, \pm 0.023) \) and \((1/3, -2/3, \pm 0.021) \) crossing the Fermi level. Note that the small difference between the dispersions around \( K \) point and \( K' \) point is induced by the time-reversal symmetry breaking.

Based on the effective TB model, we have calculated the (001) surface states and Fermi arcs on the (010) surface of GdSI and plotted them in Fig. 3C and D, respectively. The (001) surface-state calculation exhibits a clear band touching at the \( K \) point and Fermi level, indicating that GdSI is an ideal WSM. However, because two bulk WNs carrying opposite chiralities and same in-plane coordinates are projected to the same point, no Fermi arc can be found on the (001) face, as shown in Fig. S7A. In contrast, as shown in Fig. 3D, two long Fermi arcs connecting the opposite WNs exist on the (010) face unambiguously, which provide great facility for the ARPES experiment to confirm its topological properties.

In summary, we have studied a specific 3D honeycomb model, in which fruitful topological phases can be realized, including ideal WSM, 3D strong TI, nodal-line semimetal, and the semimetal consisting of both WNs and nodal lines, suggesting a mechanism for exploring the topological semimetals. Guided by this model, our DFT calculations predict that LuSI and YSI are 3D strong TIs with unusual right-handed helical Dirac cones and that GdSI, which stabilized in a noncollinear AFM state, is the long-pursuing ideal WSM with two pairs of WNs residing at the Fermi level. Furthermore, there are two very long Fermi arcs on the (010) surface of GdSI, which are well-suited for the ARPES measurement. Such ideal WSM phase in GdSI provides a good platform to study the physics of the chiral anomaly and great facility for the applications of the WSMs.

Methods

The DFT calculations are performed by the projector augmented wave method implemented in Vienna ab initio simulation package (56, 57). The cutoff energy is 500 eV. GGA of Perdew–Burke–Ernzerhof type (58) is used to treat with the exchange and correlation potential. SOC is taken into account self-consistently. The \( k \)-points sampling grid of the BZ is 5 × 5 × 11. The GGA + U scheme (59) is used to induce an effective onsite Coulomb potential of 6.0 eV for the \( f \) orbitals of Gd. MLWFs have been generated to construct the TB Hamiltonians of the semimfinite sample (53). The projected surface states are obtained from the TB Hamiltonians by using an iterative method (51, 52).

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