Topological semimetals predicted from first-principles calculations

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Abstract

We have given a summary on our theoretical predictions of three kinds of topological semimetals (TSMs), namely, Dirac semimetal (DSM), Weyl semimetal (WSM) and node-line semimetal (NLSM). TSMs are new states of quantum matter, which are different from topological insulators. They are characterized by the topological stability of the Fermi surface, whether it encloses hand crossing points, i.e. Dirac cone-like energy nodes, or not. They are distinguished from each other by the degeneracy and momentum space distribution of the nodal points. To realize these intriguing topological quantum states is quite challenging and crucial to both fundamental science and future application. Na\textsubscript{3}Bi and Cd\textsubscript{3}As\textsubscript{2} were theoretically predicted to be DSM in 2012 and 2013 respectively. Their experimental verification in 2014 have ignited intensive studies on TSMs. The subsequent theoretical prediction of a nonmagnetic WSM in the TaAs family stimulated a second wave and many experimental works were released out in 2015. In 2014, a kind of three dimensional crystal of carbon was proposed to be an NLSM due to negligible spin–orbit coupling and coexistence of time-reversal and inversion symmetry. Though the final experimental confirmation of NLSM is still missing, there have been several theoretical proposals, including Cu\textsubscript{3}PdN from us. In the final part, we have summarized the whole family of TSMs and their relationships.

Keywords: topological semimetals, chiral anomaly, Dirac semimetal, Weyl semimetal, node-line semimetal, topological insulator, first-principles calculation

1. Introduction

Classification of electronic states is one of the key concepts in condensed matter physics. The usual way to classify the electronic states in solids is based on the symmetry principle, by which most of the states as well as the transitions among them can be understood. For example, the ferro-electric and ferromagnetic states can be understood as states that break the spatial inversion and time reversal symmetries respectively. The Landau theory for phase transitions is very successful in condensed matter physics, and is built entirely on the symmetry principle. In the last thirty years, another way to classify condensed matter systems has been developed through a completely different point of view, i.e. topology. The first type of system that can be classified by its topological features is the 2D electron gas (2DEG) under high magnetic field. Once there are integer number of Landau levels being fully occupied, the system is in the \textit{n}th integer quantum Hall state (IQHS) with quantized Hall conductance \cite{1}. Further analysis of the IQHS by TKNN revealed that the IQHS has a very deep topological origin \cite{2, 3}. Although different IQHS are the same in terms of symmetry, they can be characterized by different integers
(TKNN number or Chern number), which can be expressed by the integral of the Berry’s curvature over the whole magnetic Brillouin zone (BZ) [2]. This integer number is called topological invariance, which cannot be changed without closing the energy gap of the system.

After the discovery of IQHS, it was anticipated that the concept of topological electronic states should not be limited only to 2DEG under external magnetic field [4]. The idea ought to be generalized to realistic materials as well. Since about ten years ago, the idea of finding electronic states that can be classified by topological invariance in solid state materials has been realized in a class of band insulators—topological insulators (TIs) [5–9]. Similar to the IQHS, the TI can be characterized by topological invariances or indices but the difference is that these indices, called Z2 indices, can only take two possible values, even or odd. The TI characterized by odd Z2 indices has unique Dirac-like surface (or edge) states, which is unavoidable as long as the time reversal symmetry is preserved. The first TI proposed by theorists is graphene [10], but due to its extremely small energy gap (about 10⁻³ meV) opened by spin–orbit coupling [11], it is hard to observe any physical properties of TI in graphene. The prediction of a TI state in a HgTe/CdTe quantum well was made by the Stanford group [12] and had been confirmed experimentally a year later [13]. The discovery of the 3D TI Bi2Se3 family [14–16] makes it much easier to study all kinds of properties of TIs including transport under magnetic field, thermal electric properties [17, 18] as well as the possible topological superconductor phase induced by the proximate effect [19–21]. With doping of the magnetic elements into Bi2Te3 family thin films, another long-awaited topological phenomenon, the quantum anomalous Hall effect (QAHE) [4, 22–24], has been theoretically predicted [25] and experimentally observed [26]. The QAHE can be viewed as a kind of IQHS without Landau levels (no external magnetic field) [24].

With the successful discovery of those TI states, it is natural to ask whether or not metals can be classified by topological invariances as well. Although to date the general topological classification for metals is still unclear, we now have ways to classify a special type of metal, the semimetals, where the zero energy contour in energy dispersion or Fermi surface contains only isolated points (or lines for 3D systems) rather than surfaces. These Fermi nodes (or nodal lines) are caused by the band crossing points (also called as nodes or nodal points) right at the Fermi level. The semimetal can be viewed as a special type of ‘insulator’ as well, where the energy gap only closes at those isolated k-points or lines. In 2D systems, graphene can be viewed as the first well studied topological semimetal (TSM), where the low energy physics can be well described by the 2D massless Dirac equation. The line integral of the Berry connection along any closed loops in the BZ will accumulate a phase \( \pi \) (0) if the loop (does not) enclose(s) the Dirac point and this phase can be used as the topological invariance, which manifests itself in the unique Landau level structure under a magnetic field. As we will introduce below, band crossing points can also occur in 3D materials, similarly to graphene. Although the band crossings in 3D and 2D do share some similarities, they are nevertheless very different. The most essential difference comes from the fact that, without extra degeneracy, i.e. the spin degeneracy for fermions, the band crossings in 3D can only be shifted but not removed by small perturbations in the Hamiltonian. In comparison, the band crossing points in 2D are caused by crystalline symmetry on some special k-points in the BZ and will disappear immediately once a small perturbation is added to break that symmetry. Therefore in 3D, the crossing points between two non-degenerate bands can be viewed as ‘topological defects’, which are the stable objects like vortices in a fluid. Such crossing points are called Weyl points (Weyl nodes) because the low energy physics around them can be well described by the Weyl equation, which is well known in particle physics and contains only half of the freedom of the Dirac equation [27]. Weyl nodes in crystalline solids were first studied as magnetic monopoles in momentum space in the context of the anomalous Hall effect [28]. As will be illustrated in detail below, Weyl points have chirality defined as the sign of the determinant for the velocity tensor, which is another unique point in 3D. It has been proved mathematically that Weyl points generated in any lattice model can only come in pairs with opposite chirality [29–31]. In fact, the only way to remove Weyl points is to move a pair of Weyl points with opposite chirality to the same k-point and annihilate them. The most important effect generated by these ‘chiral electrons’ is the so-called ‘chiral anomaly’ describing the adiabatic electron pumping caused by the joint effect of the external magnetic and electric fields between Weyl points with opposite chirality [32]. The chiral anomaly (or ABJ anomaly) will generate current along the direction of the magnetic field leading to negative magno-resistance when the magnetic and electric fields are parallel to each other [33, 34]. Besides the negative MR, the chiral anomaly can also generate more effects in transport [35] and optical properties, [36–40] as well as the chiral magnetic effect [41, 42], nonlocal transport [43], and chiral gauge anomaly [44].

The nodal point behaves like a magnetic monopole in crystal momentum space, being a ‘source’ or ‘sink’ of Berry curvature, the field of Berry flux [24, 28, 45, 46]. Figure 1 shows the typical band structure and the topological relationship between the Fermi surface (with the Fermi level slightly off the node) and magnetic monopoles. The Dirac semimetal (DSM) has its Fermi surface enclosing two monopoles with opposite topological charge ‘kissing’ at the same k-point, while the Weyl semimetal (WSM) always has opposite monopoles in pairs and they are well separated [31]. The nodal line semimetal (NLSM) is a special case with nodal points forming a periodically continuous line or closed ring in the momentum space. After a loop of adiabatic evolution along a closed path interlocked with the nodal ring, eigenstates on one of the crossing bands will acquire a Berry phase of \( \pi \), which stabilizes its ring-like Fermi surface. Therefore, these three kinds of TSM can be identified by the degeneracy and distribution of nodal points.

These exotic nontrivial TSMs are expected to have intriguing quantum phenomena and physical properties. Their material realization has become very important and crucial to bring them into the realm of experimental study and potential
application in future. As we have pointed out in [47], the rapid development of first-principles calculation methods and software packages, together with the intrinsic robustness of band topology—immune to perturbation and numerical error—ensure the predictive power of the state-of-art first-principles calculation for topological materials. The remarkable successful stories include the 2D TIs [12, 13], 3D TIs [14–16], Chern insulators supporting the QAHE [25, 26], 3D topological crystalline insulators [48, 49] and so on. In this topical review, we will briefly summarize our theoretical material proposals for three types of TSMs, namely DSM, WSM and NLSM. Some of these have been confirmed by experimental observations following our predictions. Experimentally, the most direct and efficient way to observe the TSMs is to use the angle resolved photoemission spectroscopy (ARPES) technique, which can detect the band structure and even its spin polarization. There are basically three important hallmarks of TSMs to be observed by ARPES, including the 3D Dirac/Weyl points, the Fermi arcs on the surface [50] and the spin texture of Fermi arcs.

2. Dirac semimetal

The Dirac equation describing electrons with relativistic effect [51] is written as

\[
\begin{pmatrix}
\hat{E}(\mathbf{k}) - \sigma \cdot \mathbf{k} & 0 \\
0 & \hat{E}(\mathbf{k}) + \sigma \cdot \mathbf{k}
\end{pmatrix} \psi = mc^2 \begin{pmatrix} 0 & I_x \\
I_x & 0 \end{pmatrix} \psi.
\]

Here \( m \) represents the mass term and couples the two massless Weyl fermions described by \( \pm \sigma \cdot k \) with opposite chirality [27, 52, 53]. If \( m \) is finite, this equation describes a massive Dirac fermion as shown in figure 1, assuming the Fermi level to be inside of the gap. If \( m \) is zero, it describes the massless Dirac fermion composed by two massless Weyl nodes overlapping each other. If the Fermi level is slightly shifted off the Dirac node, the Fermi surface encloses a pair of Weyl nodes. The number of pairs can be viewed as a topological invariance to identify DSM.

In a general band inversion mechanism as shown in figure 2, the band inversion between two spin degenerate bands can cause four-fold degenerate energy nodal points. However, in the general situation as discussed by Murakami [54, 55], including spin–orbit coupling (SOC) will open a band gap at the four-fold degenerate band crossing points. This leads to an insulating state and most probably the system becomes a TI, or a topological crystalline insulator, or any other insulator. However, we think such a band gap opening is not inevitable and it can be well protected by some crystal symmetry as long as the two spin degenerate bands belong to two different 2D irreducible representations of the small group at the \( k \)-point where the band crossing occurs. Therefore, the candidate DSM must have at least two different 2D irreducible representations in its double space group. This is a necessary, but not sufficient, condition. This finding is crucial and directly guides the theoretical prediction of DSM in Na\(_3\)Bi [56] and Cd\(_3\)As\(_2\) [57].

2.1 Na\(_3\)Bi

In 2012, the present authors and their collaborators predicted that DSM might be realized in some hexagonal phase of alkali pnictides \( A_3B \) (\( A = \) alkali metal, \( B = \) As, Sb or Bi) represented by Na\(_3\)Bi [56]. Its crystal structure is shown in figure 3. There are two nonequivalent Na sites, Na(1) and Na(2), in one unit cell. Na(1) and Bi form simple honeycomb lattice layers stacking along the \( c \)-axis. Na(2) atoms are inserted at the interlayer position, connecting these layers on top of Bi atoms. From the ionic picture, due to the closed-shell configuration where the number of valence electrons (3 \( \times \) Na-\( s^1 \) + Bi-\( p^3 \)) is equal to 6, one may expect Na\(_3\)Bi to be a semiconductor, similar to Na\(_3\)Sb [58]. However, the electronegativity of Bi is weaker than Sb, which makes Na\(_3\)Bi a DSM rather than a semiconductor like Na\(_3\)Sb.

The calculated band structures of Na\(_3\)Bi are shown in figure 4. They suggest that the valence and conduction bands are dominated by Bi-\( 6p \) and Na-\( 3s \) states. Around the Fermi level, the top valence band is mostly from Bi-\( 6p_{x,y} \) states and...
the lowest conduction band is mostly from Na(1)-3s orbitals. These features are similar to those of Na$_3$Sb [58] except that in Na$_3$Bi, the Na-3s band is lower than Bi-6px, by about 0.3 eV at Γ, and this value is enhanced to be 0.7 eV in the presence of SOC. This is a typical picture of band inversion [47] but absent in Na$_3$Sb. The band inversion is due to the heavier Bi, which has higher 6p-states and larger SOC compared to Sb. Since GGA usually underestimates the band gap and results in the overestimation of band inversion, the band inversion is further confirmed by the calculation using hybrid functional HSE [59, 60]. The band inversion persists and the Na-3s band is around 0.5 eV lower than Bi-6p ones. K$_3$Bi and Rb$_3$Bi have similar band structure and band topology, with band inversion around 0.33 eV and 0.42 eV respectively.

Unlike topological insulators such as Bi$_2$Te$_3$ and Bi$_2$Se$_3$ [14, 61], Na$_3$Bi is a semimetal with two nodes (band-crossings) exactly at the Fermi level as shown in figure 4. Its Fermi surface consists of two isolated Fermi points, which are located at $(0, 0, k'_z \approx \pm 0.26 \times \frac{\pi}{a})$ along the Γ-A line. Around each node the band dispersion is linear, resulting in a 3D Dirac cone. It is different from the Dirac cone in graphene not only in dimensionality, but also in its robustness, because the Fermi points here survive in the presence of SOC, but a tiny band gap opens in graphene [11].

The crossing bands along the Γ-A line belong to two different irreducible representations distinguished by the three-fold rotational symmetry around the Γ-A axis. Breaking this symmetry will introduce interaction between them and make the structure insulating. It has been tested that 1% compression along the y axis will open up a gap $\approx 5.6$ meV. This insulating state, however, is topologically non-trivial with $Z_2 = 1$ [7, 8] due to the inverted band structure around the Γ point. This fact leads to coexistence of both a bulk 3D Dirac cone and topological surface states (a single pair) as long as the crystal symmetry protecting band crossings stands. As shown in figure 5(a), the solid Dirac cone results from the projection of the bulk 3D Dirac cone onto the [0 0 1]-surface overlapped with the topological surface states. This distinguishing property of DSM is more obvious if inspecting its side surface, on which two Dirac cones are projected at two

Figure 2. Schematic plot of band inversion mechanism. (Left) The case without SOC, band inversion between two spin degenerate (dashed line for up spin, solid one for down spin) bands. + and − indicates the parity of the states at time-reversal invariant moment. (Right) After including SOC, the band crossings are lifted and band gap is open.

Figure 3. (a) Crystal structure of Na$_3$Bi with P6$_3$/mmc symmetry. Na(1) is at 2b position $\pm(0,0,\frac{1}{4})$, and Bi is at 2c position $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{4})$. They form honeycomb lattice layers. Na(2) are at 4f position $\pm(\frac{1}{3},\frac{2}{3},u)$ and $\pm(\frac{2}{3},\frac{1}{3},u)$ with $u = 0.583$, threading Bi along c axis. (b) Brillouin zone (BZ) of bulk and the projected surface BZs of (0 0 1) and (0 1 0) plane.
Figure 4. Calculated electronic structures of Na$_3$Bi. (a) The total and partial density of states; (b) and (c) are the band structures without and with spin–orbit coupling respectively. The red circles indicate the projection to the Na-3$s$ states. The orbital characters of wave-functions at Γ point are labeled in the inset (see effective Hamiltonian for details).

Figure 5. Projected surface states and their fermi surfaces of Na$_3$Bi; (a) and (b) are the projected surface density of states for [0 0 1] and [0 1 0] surfaces, respectively. (c) Fermi surfaces (Fermi arcs) and their spin texture (in-plane component) for the [0 1 0] surface states. (d) Fermi arcs of [0 1 0] surface obtained from fitted effective Hamiltonian with additional exchange field $h_1 = 6$ meV (see phase diagram for details). The discontinuity around the singular Fermi points now becomes obvious (enlarged in the insets).
different points. As shown in figure 5(b), the solid Dirac cone from bulk states is well separated from the topological surface Dirac cone, while the surface states merge into the bulk states at the Dirac points where the bulk band gap closes. Thus, if the Fermi level passes through the bulk Dirac nodes, the Fermi surface has Fermi arc structures as shown in figure 5(c).

It seems that the entire Fermi surface is closed, while its derivative and Fermi velocity are all defined at the two singular points (corresponding to the projection of bulk Dirac points to the surface). The spin texture of surface states has helical structure, quite similar to that of topological insulators, but the magnitude of the spin vector vanishes at the singular points. This kind of Fermi surface has never been found before, and it can be understood following the discussions for the Weyl semimetal [50, 62]. If the $4 \times 4$ Dirac point is split into two separate $2 \times 2$ Weyl points in momentum space by breaking time reversal or inversion symmetry [63, 64], the Fermi surface of surface states will also split into open segments which are Fermi arcs (discussed in [50, 62]). In figure 5(d), an exchange field breaking time-reversal symmetry separates the touch of two Fermi arcs.

All these characteristics in contrast to conventional metals and topological insulators have been experimentally confirmed by successive ARPES measurements [65–67]. The extraordinary magneto transport property in DSM Na$_3$Bi due to chiral anomaly has also been confirmed experimentally [68–70].

2.2. Cd$_3$As$_2$

After the theoretical prediction of DMS in Na$_3$Bi, experimental works to confirm it have been intensively performed. It was soon found to be unstable in air. Therefore, the present authors and their collaborators were motivated to find other, better materials to be more suitable for experimental studies. The well known compound Cd$_3$As$_2$ was re-investigated in 2013 and was found to be another DSM candidate [57]. Similarly, it has a single pair of Dirac points in bulk and Fermi arcs on the surface. In particular, in one of its phases the spin degeneracy of crossing bands is lifted away from the Dirac points, in stark contrast to other examples [56, 71]. It is further suggested that its quantum well structure can naturally support the quantum spin Hall (QSH) effect. The other nice aspect of Cd$_3$As$_2$ is its high carrier mobility up to 15 000 cm$^2$ V$^{-1}$ s$^{-1}$ at room temperature and 80 000 cm$^2$ V$^{-1}$ s$^{-1}$ at 4 K, reported about 50 years ago [72]. These advantages make it a promising candidate for future experimental studies and potential applications.

The crystal structure of Cd$_3$As$_2$ is complicated. As shown in figure 6, there are hypothetical anti-fluorite Cd$_6$As$_4$ and zinc blende Cd$_4$As$_4$. The Cd$_6$As$_4$ is obtained with two diagonal sites of Cd vacancy in Cd$_8$As$_4$. This is the basic building block of real Cd$_3$As$_2$ crystal structure. If the arrangement of building blocks is random, i.e. the distribution of these vacancies is random, one may treat it by virtual crystal approximation (VCA) for simplicity [73, 74]. However, the vacancies are in fact ordered even at room temperature, leading to a tetragonal structure with $D_{4h}^{15}$ ($P4_2/nmc$) symmetry with 40 atoms per unit cell being a $\sqrt{2} \times 2 \times 2$ supercell of building block (called Structure I hereafter), or a body centered tetragonal structure with $C_{4h}^{12}$ ($I4_1/cd$) symmetry with 80 atoms per unit cell being a $2 \times 2 \times 4$ supercell of building block (called Structure II hereafter). The latter is more favored [75] and we noticed there is a correction [76] to the crystal structure after our original published work. This vacancy ordering and very large unit cell of Cd$_3$As$_2$ has brought serious problems for theoretical studies historically, and there has been no first-principles calculation before [57].

Cd$_3$As$_2$ belongs to the II-V$_2$-types narrow gap semiconductor family [72]. It has drawn much attention since it is believed to have inverted band structure [77–80], whereas Cd$_5$P$_2$, Zn$_3$As$_2$ and Zn$_3$P$_2$ have normal band ordering. In contrast to other inverted band compounds (like HgTe, HgSe, and α-Sn), Cd$_3$As$_2$ has tetragonal symmetry, and is representative of this group, which has a split valence band top at $k = 0$.

Similar to most semiconductors with anti-fluorite or zinc-blende structures, the low energy electronic properties of Cd$_3$As$_2$ are mostly determined by the Cd-5s states (conduction bands) and the As-4p states (valence bands), as shown in Figure 7. However, there are two distinct features: (1)
The band-inversion around $\Gamma$ with the $s$-band (red solid cycle) lower than the $p$, which is an important sign of non-trivial topology; (2) it is semimetallic with band crossings along the $\Gamma$–Z path. This band-crossing is unavoidable since the two bands belong to different ($\Lambda_6$ and $\Lambda_7$) representations, as distinguished by $C_4$ rotational symmetry around the $k_z$ axis. The different representation prohibits hybridization between them, resulting in the protected band-crossing. The crossing points are located exactly at the Fermi level due to the charge neutrality requirement and the Fermi surface has only a single pair of Dirac points (two symmetric points along $\Gamma$–Z related by TR). Structures I and II share these common features with small but remarkable differences as will be addressed in the following.

As has been demonstrated by the perturbation method [81], vacancy ordering and BZ folding play important roles in band-inversion, in contrast to the cases of HgTe or Ag$_2$Te [82], where it was driven by the shallow $d$ states. To prove this, Cd$_3$As$_2$ with hypothetical anti-fluorite structure without vacancy as in figure 6(a) has been calculated by using VCA, compared with the usual first-principles calculation for Cd$_3$As$_2$ in the same anti-fluorite structure but with Cd vacancy as in figure 6(b). It was found that the VCA calculation gives normal band ordering at $\Gamma$ but the one with Cd vacancy results in inverted band ordering. At the BZ boundary X point of the hypothetic anti-fluorite structure with Cd vacancy, there exist shallow $s$ and $p$ states, which will be folded to $\Gamma$ in the real structure with Cd vacancy ordering. Therefore, hybridization among the states with the same representation will push them away from each other, i.e. make the lowest $s$-state even lower and highest $p$-state higher, resulting in robust band inversion at $\Gamma$. The band-inversion calculated from the generalized gradient approximation (GGA) is about 0.7 eV for both Structures I and II. The possible underestimation of the $s$–$p$ gap within GGA is improved by the calculations with HSE method [59, 60]. Band-inversion is obtained around 0.3 eV, being consistent with most of the existing experimental evidence, such as the optical and transport measurements [77, 78].

The inverted band structure discussed above suggests that Cd$_3$As$_2$ is topologically non-trivial. However, due to the four-fold rotational symmetry, it is in fact a 3D DSM with a pair of 3D Dirac points at the Fermi level. This is slightly different from Na$_3$Bi. Similarly, if the four-fold rotational symmetry is broken, two Weyl fermions with opposite chirality will annihilate each other, resulting in a massive Dirac fermion with finite band gap. The resulting insulator is a strong TI.

Similar as Na$_3$Bi, Cd$_3$As$_2$ has coexistent bulk and surface Dirac cones in its surface state. The semi-infinite ($0\ 0\ 1$) and ($1\ 1\ 0$) surfaces of the Structure II Cd$_3$As$_2$ are presented in figure 8. For the ($0\ 0\ 1$) surface, the surface projection of continuous bulk states superposes with the non-trivial surface.
states. The Fermi surface of this surface is just a point as shown in figure 8(b). For the (1 1 0) surface, the non-trivial surface states are clear. The Fermi surface of this topological surface states has two half-circle Fermi arcs touching at the singularity points where the surface projection of bulk Dirac points exists.

It is noted that Structure II has no inversion symmetry and no Kramer degeneracy at general momenta. As shown in figure 9, the bulk Dirac cone in Structure II has spin splitting as momentum deviates from the rotation axis due to the broken inversion symmetry. Such a spin polarized bulk Dirac cone is quite similar to the Weyl cone in WSM of TaAs family.

Soon after this theoretical prediction, the present authors and their collaborators observed the 3D bulk Dirac cone [83, 84] and surface states [85] in Cd$_3$As$_3$ through ARPES measurement. Other experimental works include [86–90].

Yang and Nagaosa have classified Na$_3$Bi and Cd$_3$As$_2$ as DSM carrying quantized topological invariants [91], and BiO$_2$ [71] and distorted spinel [92] as the class having only a single Dirac point at a time-reversal invariant momentum. The classification of DSM has been further investigated by Gibson et al [93] and several similar DSM candidates have also been proposed by Du et al [94]. As originally pointed out by Murakami [54, 55], DSM can also be obtained at the topological phase transition point for an inversion symmetry (IS) conserved system. Bi$_{1-x}$Sb$_x$ [95, 96] is believed to be a DSM at the phase transition point from TI to normal insulator. We have proposed that ZrTe$_5$ and HfTe$_5$ are DSM only at the phase transition point from weak to strong TI [42, [97–99].

3. Weyl semimetal

As discussed before, DSM has Dirac nodes composed of two opposite chiral Weyl nodes, which ‘kiss’ at the same $k$-point due to the degeneracy in spin degree of freedom. In condensed matter, such spin degeneracy at a general $k$-point is usually protected by the coexistence of time-reversal symmetry (TRS) and inversion symmetry (IS). This is known as Kramer degeneracy. Breaking either TRS or IS might result in two-fold degenerate Weyl nodes. This leads to two types of WSM, i.e. magnetic WSM and nonmagnetic noncentrosymmetric WSM. The first WSM was proposed to exist in pyrochlore iridates with all-in/all-out magnetic ordering by Wan et al [50] in the same year, we and our collaborators [62] proposed that ferromagnetic half-metal HgCr$_2$Se$_4$ might be a WSM with pair of Weyl nodes having topological charge of 2, so-called double WSM [100]. However, ARPES measurement of the magnetic WSM suffers difficulty due to the complex domain structure. There is still no material definitely confirmed to be a magnetic WSM. Finding a nonmagnetic WSM is thus very important. In this section, we will introduce our theoretical predictions for the FM HgCr$_2$Se$_4$ and noncentrosymmetric nonmagnetic TaAs family. Recent progress in nonmagnetic WSM includes...
the proposal of type-II WSM [101] in WTe$_2$ [102] and MoTe$_2$ [103]. The discovery of Weyl points in photonic crystal [104] is not discussed here.

3.1 Magnetic Weyl semimetal: HgCr$_2$Se$_4$

In 2011, it was proposed that a spinel structural compound HgCr$_2$Se$_4$ might be a WSM under its ground state. Compared with the former proposal of WSM [50], HgCr$_2$Se$_4$ has only one pair of Weyl cones around the Fermi level and each Weyl cone has topological charge 2. HgCr$_2$Se$_4$ has quite simple ferromagnetic (FM) ordering and is robust against the choice of on-site Coulomb interaction parameter U. Before the WSM state was proposed in HgCr$_2$Se$_4$, it was known as a FM spinel exhibiting large coupling effects between electronic and magnetic properties [105]. It shows quite interesting properties like giant magnetoresistance [106], anomalous Hall effect [107], and red shift of optical absorption edge [108]. Its experimental Curie temperature $T_c$ is high (around $106 \sim 120$ K), and the saturated moment is around 5.64 $\mu_B$ f.u. $^{-1}$ [109, 110], approaching the atomic value expected for high-spin Cr$^{3+}$. Its transport behavior is different from other FM chalcogenide materials like giant magnetoresistance [106], anomalous Hall effect [107], and red shift of optical absorption edge [108]. Its experimental Curie temperature $T_c$ is high (around $106 \sim 120$ K), and the saturated moment is around 5.64 $\mu_B$ f.u. $^{-1}$ [109, 110], approaching the atomic value expected for high-spin Cr$^{3+}$. Its transport behavior is different from other FM chalcogenide materials like giant magnetoresistance [106], anomalous Hall effect [107], and red shift of optical absorption edge [108].

The spinel structure, with space group Fd$ar{3}$m, can be related to the zinc blende and/or diamond structures. As shown in figure 10, taking the Cr$_2$Se$_4$ cluster as a single pseudo-atom (called X) located at the center of mass, HgX becomes a typical zinc blende structure. The pseudo-atom X is actually a small cube formed by four Cr atoms and four Se atoms located at alternate cube corners. The cubes are connected by sharing the Cr atoms at the corners. As a result, each Cr atom is octahedrally coordinated by the six nearest Se atoms. There are two HgX formula units (f.u.) in each unit cell, and they are connected by inversion symmetry similarly to two atoms in the diamond structure.

The first-principles calculation confirms that the FM solution is considerably more stable than the non-magnetic solution, being about 2.8 eV f.u. $^{-1}$ lower in total energy. The magnetic moment obtained (6.0 $\mu_B$ f.u. $^{-1}$) agrees with experimental values [109, 110] very well. The electronic structures shown in figures 11(a) and (b) suggest that it can be approximately characterized as a ‘zero-gap half-metal’ in the case without SOC. It is zero-gap because there is band touching around $\Gamma$ at the Fermi level in spin down channel; it is half-metal since there is a band gap in the up-spin channel. The 3d-states of Cr$^{3+}$ are in the configuration of $t^3_2g^1e^{01}_g$. The band gap is due to crystal field splitting of the $t^3_2g$ and $e^{01}_g$ manifolds. The Se-4$p$ states are from $-6$ to 0 eV, being fully occupied and contribute dominantly to the valence band maxima. By hybridizing with Cr-3$d$ states, Se-4$p$ are slightly spin-polarized but with opposite moment (about $-0.08 \mu_B$/Se) to that on Cr. The zero-gap behavior in the spin-down channel is the most important characteristic. It suggests an inverted band structure around $\Gamma$, which is similar to the case in HgSe or HgTe [113, 114].

The four low energy states (eight after considering spin degree of freedom) at $\Gamma$ can be labelled as $|P_x|$, $|P_y|$, $|P_z|$, and $|S|$, which are linear combinations of atomic orbitals: $|P_{\alpha}| \approx \frac{1}{3} \sum_{i=\alpha}^{3} |s^{\alpha}_{f}\rangle$, and $|S| \approx 0.4 \sum_{j=x,y,z}^{3} |s^{j}\rangle + 0.24 \sum_{k=1}^{4} |d^{k}_{t}\rangle$, where $\alpha = x, y, z$ and $i, j, k$ runs over Se, Hg, Cr atoms in the unit cell; $|s_{f}\rangle$, $|P_{\alpha=x,y,z=2,3}\rangle$, $|d_{t}^{k=x,y,z,3}\rangle$ are the orbital orbitals of each atom. Taking these four states as a basis, the same situation is found in HgSe and HgTe. The only difference is the presence of exchange splitting in HgCr$_2$Se$_4$. The band inversion, $|S, \downarrow\rangle$ being lower than $|P, \downarrow\rangle$ at $\Gamma$ as shown in figure 11(c), is due to the following two factors. Firstly, the Hg-5$d$ states are very shallow (located at about $-7.0$ eV in figure 11(a)) and its hybridization with Se-4$p$ states pushes the antibonding Se-4$p$ states higher, similar to that in HgSe. Secondly, the hybridization between unoccupied Cr-3$d^4$ and Hg-6$s^1$ states in the spin-down channel pushes the Hg-6$s^1$ state lower in energy.
(figures 11(b) and (c)). Therefore, the $|S, \uparrow\rangle$ is about 0.4 eV lower than $|P, \downarrow\rangle$ states at $\Gamma$, and it is further enhanced to 0.55 eV in the presence of SOC. It is important to check the correlation effect beyond GGA. It has been shown that semiconducting CdCr$_2$S$_4$ and CdCr$_2$Se$_4$ can be well described by the LDA+$U$ calculations with effective $U$ around 3.0 eV [115, 116]. The same LDA+$U$ calculations for HgCr$_2$Se$_4$ show that the band-inversion remains unless the $U$ is unreasonably large (>8.0 eV).

Considering SOC, the new low energy eigen states at $\Gamma$ are given as $|\frac{3}{2}, \pm \frac{1}{2}\rangle$, $|\frac{1}{2}, \pm \frac{1}{2}\rangle$, and $|\pm \frac{1}{2}\rangle$, which can be constructed from the $|P\rangle$ and $|S\rangle$ states. Using this effective Hamiltonian, the low energy band structures of HgCr$_2$Se$_4$ can be well reproduced. Due to the exchange splitting, the eight states at $\Gamma$ are all energetically separated, with $|\frac{3}{2}, \frac{1}{2}\rangle$ having the highest energy, and $|\frac{1}{2}, c\rangle$ the lowest. Several band-crossings are observed as shown in the band structure of figure 11(d). Among them, two kinds of band-crossings (called A and B) are important for the states very close to the Fermi level. The crossing A gives two points located at $k_z = \pm k_z^c$ along the $\Gamma$-$Z$ line, and the trajectory of crossing B is a closed loop surrounding the $\Gamma$ point in the $k_z = 0$ plane, as schematically shown in figure 12(a). For the 2D planes with fixed-$k_x$ ($k_x = 0$ and $k_x = \pm k_x^c$), the band structures are all gapped in the sense that a curved Fermi level is defined. Thus, the Chern number $C$ for each $k_x$-fixed plane can be evaluated. It is found that $C = 0$ for the planes with $k_x < -k_x^c$ or $k_x > k_x^c$, while $C = 2$ for the planes with $-k_x^c < k_x < k_x^c$ and $k_z = 0$. The crossing A points locate at the phase boundary between $C = 2$ and $C = 0$ planes, i.e. $k_z = \pm k_z^c$ plane, and they are topologically unavoidable Weyl nodes. On the other hand, however, the crossing B points forming the closed loop in the $k_z = 0$ plane are just accidental, due to the presence of crystal mirror symmetry with respect to the $k_z = 0$ plane. Crossing B is not as stable as crossing A in the sense that it can be altered by changing the crystal symmetry. This node-line has become a hot topic recently, as we will discuss in the next section.

Considering the minimum two bases $|\frac{3}{2}, \frac{3}{2}\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle$ which catch the band-inversion nature, the $8 \times 8$ Hamiltonian can be downfolded into an effective $2 \times 2$ model by only keeping these two states and integrating out all the other bands, which reads

$$H_{\mathbb{G}} = \begin{pmatrix} M & Dk_xk_z^c \\ Dk_xk_z^c & -M \end{pmatrix}. \quad (1)$$

Here $k_{\pm} = k_x \pm ik_y$, and $M = M_0 - \beta k_z^2$ is the mass term up to the second order. $M_0 > 0$ and $\beta > 0$ are the condition to ensure the band inversion. Since the two bases have opposite parity, the off-diagonal element has to be odd in $k$. The $k_z^c$ term is necessary to conserve the angular momentum along the $z$-direction. Therefore, to the leading order, the $k_z^c$ is the only possible form for the off-diagonal element. This two-level Hamiltonian has eigenvalues $E(k_z) = \pm \sqrt{M^2 + D^2(k_x^2 + k_z^2)^2}$. Two gap-less solutions exist: one is the degenerate points along the $\Gamma$-$Z$ line with $k_z = k_x^c = k_z^c = \sqrt{M_0/\beta}$; the other is a circle around the $\Gamma$ point in the $k_z = 0$ plane determined by the equation $k_x^2 + k_z^2 = M_0/\beta$. These are consistent with the first-principles calculations. The presence of $k_x^2$ in the off-diagonal term [117] makes the Chern number $C = 2$ for the planes of $-k_x^c < k_x < k_x^c$ except the $k_x = 0$ plane where node-line exists. The in-plane band dispersions near the Weyl nodes at
$k_z = \pm k_z'$ are quadratic rather than linear, with a phase of $4\pi$ for the chiral spin texture as shown in figure 12(c). The two Weyl nodes located at $\pm k_z'$ have opposite chirality, and they form a single pair of magnetic monopoles carrying gauge flux in $k$-space as shown in figure 12(d). The band-crossing loop in the $k_z = 0$ plane is not topologically unavoidable—however, its existence requires that all gauge flux in the $k_z = 0$ plane (except the loop itself) must be zero.

This Chern semimetal state realized in HgCr$_2$Se$_4$ will lead to novel physical consequences, which can be measured experimentally. The eight-band Kane model fitted from first-principles calculations is used for the numerical demonstration. First, each $k_z$-fixed plane with non-zero Chern number can be regarded as a 2D Chern insulator, and there must be chiral edge states for such a plane if an edge is created. By replacing $k_z$ with $-i\hbar \partial_z$ and using open boundary conditions.

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**Figure 12.** Weyl nodes and Berry flux in momentum space of HgCr$_2$Se$_4$. (a) Band-crossing points $\pm k_z'$; (b) Chern number of occupied states in 2D planes perpendicular to $k_z$ axis; (c) schematic plot of the band dispersion around the Weyl nodes in the $k_z = \pm k_z'$ plane, and the inset shows the chiral spin texture. (d) Berry flux evaluated as Berry’s curvature in the $(k_x, k_z)$ plane with $k_y = 0$.

**Figure 13.** Edge states and Fermi arcs of HgCr$_2$Se$_4$. (a) Calculated edge states for the plane with $k_z = 0.06\pi$. A ribbon with two edges is used, and there are two edge states for each edge (because $C = 2$). States located at different edges are indicated by different colors. (b) Calculated Fermi arcs for the $(k_y, k_z)$ side surface.
along the x (or y) direction, one can obtain the edge states for each fixed-\(k_z\). The number of edge states is two for the case of \(C = 2\) as shown in figure 13(a), or zero for the case of \(C = 0\). If the chemical potential is located within the gap, only the chiral edge states can contribute to the Fermi surface, which are isolated points for each Chern insulating plane but do not exist for the plane with \(C = 0\). Therefore the trajectory of such points in the \((k_x, k_z)\) surface or \((k_y, k_z)\) surface form non-closed fermi arcs, which can be measured by ARPES as shown in figure 13(b). This is very different from the conventional metals,

**Figure 14.** Quantized anomalous Hall effect in HgCr\(_2\)Se\(_4\) thin film. (a) Subband energy levels at \(\Gamma\) point as a function of film thickness. (b) Hall conductance as a function of film thickness.

**Figure 15.** Crystal structure and BZ. (a) The crystal symmetry of TaAs; (b) bulk BZ and projected surface BZ for both (0 0 1) and (1 0 0) surfaces; (c) band structure of TaAs calculated by GGA without including SOC; (d) Band structure of TaAs calculated by GGA with SOC.
where the Fermi surfaces must be either closed or interrupted by the BZ boundary. The possible Fermi arcs have recently been discussed from a viewpoint of accidental degeneracy for pyrochlore iridates [50]. In general, any magnetic system with band-crossing nodes at the Fermi level may show Fermi arcs on its surface. As demonstrated in figure 13, the calculated Fermi arcs for HgCr$_2$Se$_4$ not only end at $k_z = \pm k_z^c$, but also are interrupted by the $k_z = 0$ plane, where the node-line exists. Nevertheless, for WSM the Fermi arcs should be stable because the Weyl nodes are topologically unavoidable.

The QAHE, however, is a unique physical consequence characterizing the WSM nature in ferromagnetic HgCr$_2$Se$_4$ quantum-well structure [24]. For 2D band insulators, the transverse Hall conductance should be quantized as $\sigma_{xy} = C e^2/h$, where $C$ is the Chern number. Such a quantum Hall effect without magnetic field has been long-pursued [4, 22, 24, 25], but only achieved experimentally in 2013 in magnetic ion doped topological insulator films (as theoretically predicted in 2010 [24–26]). In HgCr$_2$Se$_4$, considering the $k_z$-fixed planes, the Chern number $C$ is non-zero for limited regions of $k_z$ due to the band inversion around $\Gamma$ as discussed above. In the quantum well structure, the low energy states around $\Gamma$ are quantized into subbands, with $|H_n\rangle$ and $|E_n\rangle$ for hole and electron subbands respectively. All the subbands’ energy levels change with film thickness. As shown in figure 14, when the thickness of the film is very thin the band inversion in the bulk band structure will be removed entirely by the finite size effect. With increase of the thickness, the band inversion among these subbands is restored, which results in jumps in the Chern number or the Hall coefficient $\sigma_{xy}$ [23, 24]. As shown in figure 14(b), the critical thickness of the film is around 21 Å. The subsequent jump of $\sigma_{xy}$ in unit of $2e^2/h$ is due to the change of 2 in Chern number. This brings an interesting way to realize high plateau quant um Hall conductivity of 2 in QAHE, being distinguishing from present experimentally achievable magnetic doped TI systems [24]. In fact, a strong anomalous Hall effect (AHE) has been observed for the bulk samples of HgCr$_2$Se$_4$ [107]. This is in sharp contrast to pyrochlore iridates, where the AHE should be vanishing due to the AF ordering.

![Figure 16. Nodal rings and Weyl points distribution, as well as $Z_2$ and MCN for mirror planes. (a) 3D view of the nodal rings (in the absence of SOC) and Weyl points (with SOC) in the BZ; (b) side view from [1 0 0] and (c) top view from [0 0 1] directions for the nodal rings and Weyl points. Once the SOC is turned on, the nodal rings are gapped and give rise to Weyl points off the mirror planes; (d) top panel: flow chart of the average position of the Wannier centers obtained by Wilson loop calculation for bands with mirror eigenvalue $i$ in the mirror plane ZNi; bottom panel: flow chart of the Wannier centers obtained by Wilson loop calculation for bands in the glide mirror plane ZNi. There is no crossing along the reference line (the dashed line) indicating the $Z_2$ index is even.](image-url)
Inspired by this theoretical proposal, recent detailed transport studies have revealed that the ground state of HgCr$_2$Se$_4$ has nearly full spin-polarized current in its $s$-orbital conduction band, which is strong evidence for its half-metallicity [118].

3.2. Nonmagnetic Weyl semimetal: TaAs family

In addition to the two magnetic WSMs, namely pyrochlore iridate Rn$_2$Ir$_2$O$_7$ [50] and spinel HgCr$_2$Se$_4$ [62] introduced above, other proposals involve a fine-tuned multilayer structure composed of normal insulator and magnetically doped TIs [63] or just magnetic ion doped TIs [119]. All of them involve magnetic compounds and the spin degeneracy of the bands is removed by breaking time reversal symmetry. However, these proposals are still waiting for experimental confirmation.

As mentioned above, WSM can also be generated by breaking the spatial inversion symmetry but keeping time-reversal symmetry. This is nonmagnetic and noncentrosymmetric WSM. Compared with magnetic WSM, nonmagnetic WSM has the following advantages: (1) it can be more easily studied by ARPES measurement since the alignment of magnetic domains is not required; (2) without the spin exchange field, the unique structure of Berry curvature related with magnetic monopoles leads to very unusual transport properties under an external magnetic field. Such properties are not mixed by the self-magnetization of the magnetic sample.

There have been several proposals for WSM in systems without inversion symmetry, such as a superlattice composed of alternately stacked normal and topological insulators [63, 120], elemental tellurium or selenium crystal under proper pressure [121], or a fine-tuned solid solution of $A$Bi$_{1-x}$Sb$_x$Te$_3$ ($A$ = La and Lu) [122] TlBi(S$_{1-x}$R$_x$)$_2$ (R = Se or Te) [123] around the topological transition points [54, 55]. None of the above has been realized experimentally due to the following possible problems: (1) very fine control, such as quantum well thickness and doping concentration, is required in sample preparation; (2) applying pressure makes other measurements very difficult.

At the end of 2014, we and our collaborators posted the theoretical prediction that TaAs, TaP, NbAs and NbP single crystals are natural WSMs and possess 12 pairs of Weyl points [124]. Compared with other proposals, this family of materials are completely stoichiometric without any additional doping, external strain or pressure. High quality samples can be obtained easily and experimental verification becomes much easier. A similar proposal is in [125].

Unlike in the case of pyrochlore iridates and HgCr$_2$Se$_4$, inversion symmetry is kept and the appearance of Weyl points can be immediately inferred from the product of the parities at all the time reversal invariant momenta (TRIM) [126–128]. For the TaAs family, parity is no longer a good quantum number. It is found that the appearance of Weyl points can be inferred by analyzing the mirror Chern numbers (MCN) [49, 129] and $Z_2$ indices [5, 125, 130, 131] for the four mirror and time reversal invariant planes in the BZ. Similarly to many other topological materials, the WSM phase in this family is also induced by

### Table 1. The two nonequivalent Weyl points in the $xyz$ coordinates shown in figure 15(b).

|   | W1              | W2              |
|---|-----------------|-----------------|
| TaAs | (0.520, 0.037, 0.592) | (0.949, 0.014, 0.0) |
| TaP  | (0.499, 0.045, 0.578)  | (0.955, 0.025, 0.0)  |
| NbAs | (0.510, 0.011, 0.593)  | (0.894, 0.007, 0.0)  |
| NbP  | (0.494, 0.010, 0.579)  | (0.914, 0.006, 0.0)  |

Note: The position is given in units of the length of $\Gamma$-$\Sigma$ for $x$ and $y$ and of the length of $\Gamma$-$Z$ for $z$. 

**Figure 17.** Berry curvature from pairs of Weyl points. (a) Distribution of the Berry curvature for the $k_z = 0$ plane, where the blue and red dots denote the Weyl points with chirality of $+1$ and $-1$, respectively; (b) same as (a) but for $k_z = 0.592\pi$ plane. The insets show the 3D view of hedgehog-like Berry curvature near the two selected Weyl points.
band inversion, which, in the absence of SOC, leads to nodal rings in the mirror plane. Once SOC is activated, each nodal ring will be gapped with the exception of three pairs of Weyl points, which lead to fascinating physical properties including complicated Fermi arc structures on the surface.

The experimental crystal structure of TaAs [132] is shown in figure 15. It has body-centered-tetragonal structure with nonsymmorphic space group $I\overline{4}1md$ (No. 109), lacking inversion symmetry. The measured lattice constants are $a = b = 3.4348\, \text{Å}$ and $c = 11.641\, \text{Å}$. Both Ta and As are at $4a$ Wyckoff position $(0, 0, u)$ with $u = 0$ and 0.417 for Ta and As, respectively. To calculate topological invariants such as MCN and surface states of TaAs, we have generated atomic-like Wannier functions for Ta $5d$ and As $4p$ orbitals using the scheme described in [133].

The band structure of TaAs within GGA without including SOC is shown in figure 15(c). There is clear band inversion and multiple band crossing features near the Fermi level along ZN, ZS and ΣS paths. In figure 15(b), the shadowed planes are two mirror planes, namely $M_x$, $M_y$, while the dashed lines indicate two glide mirror planes, namely $M_{x'y'}$, $M_{-x'y'}$. The plane spanned by $Z$, $N$ and $\Gamma$ points is invariant under mirror $M_y$ and the energy bands within the plane can be labeled by mirror eigenvalues $\pm 1$. Further analysis shows that the two bands that cross the $Z$ to $N$ line belong to opposite mirror eigenvalues and hence the crossing between them is protected by mirror symmetry. Similar band crossings can also be found along other highly symmetrical lines in the ZNΓ plane, such as ZS and NS. Therefore, these band crossing points form a ‘nodal ring’ in the ZNΓ plane as shown in figure 16(b). Unlike for the situation in the ZNΓ plane, in the two glide mirror planes ($M_{x'y'}$ and $M_{-x'y'}$), the band structure is fully gapped with the minimum gap around $0.5\, \text{eV}$. The bands near the Fermi energy are mainly formed by Ta $5d$ orbitals, which have quite strong SOC. SOC brings dramatic changes in the band structure near the Fermi level, as plotted in figure 15(d). It seems that the previous band crossings on the nodal rings in ZNΓ plane are all gapped. Detailed symmetry analysis reveals that the bands ‘2’ and ‘3’ in figure 15(d) belong to opposite mirror eigenvalues, indicating the almost touching point along the ZN line is completely accidental. In fact there is a small gap of roughly $3\, \text{meV}$ between bands ‘2’ and ‘3’ as illustrated by the inset of figure 15(d). Therefore, the ZNΓ plane becomes fully gapped with SOC included.

There are three critical questions to be addressed to convincingly identify TaAs as a WSM. (1) Do Weyl nodes really exist? (2) How many of them? (3) Where are they? Since Weyl nodes are at general $k$-points with accidental double degenerate eigenenergy, the numerical method always has error due to discrete sampling of 3D momentum space.

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**Figure 18.** Fermi arcs in the surface states. (a) Surface states for the (0 0 1) surface; (b) corresponding Fermi surfaces on (0 0 1) surfaces; (c) surface states for the (1 0 0) surface. The dots illustrate the projective points of the bulk Weyl points on the surfaces, where the color represents the chirality of the Weyl points (blue for positive and green for negative), small dot represents the single projected Weyl point, and large dot represents two Weyl points with same chirality projecting on top of each other. (d) Corresponding Fermi surfaces on (1 0 0) surfaces. All the dots here are the projective points for a pair of Weyl points with opposite chirality.
dense the sampling grid used, finite numerical error exists and brings difficulty in identifying the existence of a massless Dirac cone like band structure. Some efficient mathematically rigorous method is necessary to make the final conclusion.

Since TaAs has no inversion center, the widely used and most simplified parity configuration method [125–128, 131] cannot be applied to identify the existence of WSM. Another strategy is thus developed in [124]. As previously mentioned, the space group of the material provides two mirror planes (Mx and My), where MCN can be defined. If a full gap exists for the entire BZ, the MCN can directly reveal whether this system is a topological crystalline insulator [48] or not. Interestingly, if the system is not fully gapped MCN is still useful to find out whether the material hosts Weyl points in the BZ or not.

Figure 19. (a) Schwarz minimal P-surface in a $2 \times 2 \times 2$ supercell. (b) Top view of 6-1-1-p MTC in a $2 \times 2$ supercell. (c) Bulk and (0 0 1)-surface BZ, as well as the high symmetrical $k$-points. (d) Band structure from the first-principles calculation. The two triply degenerated eigenstates at $\Gamma$ and $R$ with $T_{1g}$ and $T_{2u}$ symmetrical representation are marked. The band inversion between them can be easily seen.

Figure 20. (a) Band structure from effective tight-binding model calculation, which reproduces all the features of figure 19(d). (b) Fermi surface consists of three lotus root like rings. These rings are centering the $R$ point and parallel to the $k_x = \pm \frac{\pi}{a}$, $k_y = \pm \frac{\pi}{a}$ and $k_z = \frac{\pi}{c}$ plane, respectively. They are formed by the electron pockets (blue) and hole pockets (red) connected by nodal points at the Fermi energy.
Besides the two mirror planes, there are two additional glide mirror planes (M_{xy} and M_{-xy}). MCN is not well defined for the glide mirror planes, but the Z_2 index is still well defined here since these two planes are time reversal invariant and electronic states inside of them are insulators. The Wilson loop method [47, 134] is applied to calculate the MCNs for the two mirror planes and Z_2 indices for the two glide mirror planes.

To determine the MCNs for the mirror plane M_x, Wilson loops along the k_x direction with fixed k_z are defined. All the occupied bands at k-points in this plane can be classified into two groups according to their eigenvalues under mirror operation, i or −i. For the bands having eigenvalue i, the evolution of Berry phases along the periodic k_x direction can be obtained and the MCN is simply the winding number. In figure 16(d), it is clear that MCN is 1 for the ZNΓ plane (M_y) and Z_2 index is even for ZXΓ plane(M_y). Thus, for the (0 0 1) surface, which is invariant under the M_y or M_x mirror, there will appear non-trivial helical edge modes due to non-zero MCN in the ZNΓ plane, which generates a single pair of FS cuts along the projective line of the ZNΓ plane, i.e. the x- or y-axis in figure 16(c). Whether these Fermi cuts will eventually form a single closed Fermi circle or not depends on the Z_2 indices for the two glide mirror planes, which are projected to the dashed blue lines in figure 16(c). Since the Z_2 indices for the glide mirror planes are trivial, there are no protected helical edge modes along the projective lines of the glide mirror planes and the Fermi level cuts along the x- or y-axis must end somewhere between the x- or y-axis and the diagonal lines. That means they must be Fermi arcs, ending at the surface projection of Weyl points in the bulk band structure of TaAs.

The existence of Weyl points is confirmed. The remaining questions are the total number and their exact positions. As mentioned above, this is a hard task since the Weyl points are located at generic k-points without any symmetry. For this purpose, we calculate the integral of the Berry curvature on a closed surface in k-space, which equals the net chirality of the

Figure 21. (0 0 1)-surface state. (a) The nearly flat surface band is nestled between two solid Dirac cones, which are the projection of one of the node-line circles as indicated in the inset (red circle). The other two node-line rings are projected as two orthogonal diameters (green line). (b) Surface density of state. (c) Wave function of surface state indicated by the arrow decays rapidly into bulk. (d) Eigenenergy distribution of surface flat band nestled inside of projected node-line circle, which looks like a vibration model of a ‘drumhead’. The mixing of surface and bulk state leads to discontinuity in this plot.
Weyl nodes enclosed by the given compact surface. Due to the four-fold rotational symmetry and mirror planes that characterize TaAs, one only needs to search for the Weyl points within the reduced BZ, i.e. one eighth of the whole BZ. The total chirality or monopole charge enclosed in the whole reduced BZ is found to be one. This guarantees the existence of an odd number of Weyl points in one eighth of the BZ. To determine the exact location of each Weyl point, the reduced BZ is divided into a very dense \( k \)-grid and the Berry curvature or the ‘magnetic field in momentum space’ \([28, 133, 135]\) is calculated as shown in figure 17. From this, one can easily identify the precise positions of the Weyl points by searching for the ‘source’ and ‘drain’ points of the ‘magnetic field’. Around the Weyl points, the hedgehog-like Berry curvature is clearly shown in figure 17.

Therefore, there are a total of twelve pairs of Weyl points in TaAs as illustrated in figure 16(a). All of them are in the vicinity of the nodal rings on two of the mirror invariant planes in the SOC-free case. There are two types of Weyl nodes. W1 are those located off the \( k_z = 0 \) plane, totally eight pairs. W2 are those located exactly in the \( k_z = 0 \) plane four pairs in total. All W1 Weyl nodes are related by mirror symmetry, four-fold rotational symmetry, and time reversal symmetry, likewise for W2. However, W1 and W2 are not related by any symmetry and they can have different velocity matrix and be located at different energy. For example, in TaAs, W2 nodes are about 2 meV.
above the Fermi energy and form eight tiny hole pockets, while the W1 nodes are about 21 meV below the Fermi level forming sixteen electron pockets. These values are obtained by a dense k-grid band structure calculation based on a tight-binding model from MLWFs of Ta\(d\) and Te\(p\) orbitals. SOC is included as onsite terms with 0.3 eV for Ta\(d\) and 0.2 eV for Te\(p\) as fitted from first-principles calculation with SOC included. The band structures for the other three materials TaP, NbAs and NbP are very similar. The precise positions of the Weyl points for all these materials are summarized in table 1.

Among the hallmarks of WSM are the Fermi arcs on the surface [41, 50, 62]. In the TaAs family, there are multiple Weyl points. When they are projected to one surface, some of them might be on top of each other. It is easy to see that the total number of surface modes at the Fermi level crossing a closed circle in the surface BZ must equal to the sum of the ‘monopole charge’ of the Weyl points inside the 3D cylinder that projects to the given closed circle. Another important fact determining the behavior of the surface states is the MCN, introduced in the above discussion, which limits the number of FSs cutting certain projection lines of the mirror plane as long as this mirror symmetry is still preserved on the surface.

By using the Green’s function method [47], the surface states for both (0 0 1) and (1 0 0) surfaces have been calculated as shown in figure 18 together with its Fermi surface. On the (0 0 1) surface, the crystal symmetry is reduced to \(C_2\) leading to different behavior for the surface bands around \(\bar{X}\) and \(\bar{Y}\) points respectively. Along the \(\bar{M}\text{-}\bar{X}\) or \(\bar{M}\text{-}\bar{Y}\) lines, Fermi surface crosses it twice with opposite Fermi velocity. This satisfies the constraint from the MCN for \(\Gamma\text{ZN}\) plane.
In addition to the MCN, the possible ‘connectivity pattern’ of the Fermi arcs on the surface has to link different projection points of the Weyl nodes with opposite chirality. However, for the (0 0 1) surface of TaAs, the connectivity pattern of the Fermi arcs that satisfy all the conditions discussed is not unique. Only the appearance of ‘Fermi arcs’ on the (0 0 1) surface is guaranteed since all the projective points on the (0 0 1) surface are generated either by a single Weyl point or by two Weyl points with the same chirality. The Fermi arc connectivity pattern for the (0 0 1) surface shown in figure 18(b) is obtained from our ab initio calculation on a non-relaxed surface described by the TB model based on MLWFs of Ta d and Te p orbitals. Changes of surface potentials or the simple relaxation of the surface charge density might lead to modification of the Fermi arc connectivity pattern and result in topological Fermi arc phase transitions on the surface. The extremely long Fermi arcs which cross the zone boundary along the \(\bar{X}\) to \(\bar{M}\) line is quite interesting. Compared with other proposed WSM materials, the Fermi arcs in TaAs families are much longer, which greatly facilitates their detection in experiments.

On the other hand, the surface states on the (1 0 0) surface of TaAs are much more complicated as shown in figure 18(c) and (d). The biggest difference between them is that all the projected Weyl points on the (1 0 0) surface are formed by a pair of Weyl points with opposite chirality, which does not guarantee (but does not disallow) the existence of the Fermi arcs. The only constraint for the (1 0 0) surface states is the nonzero MCN of the \(\Gamma Z N\) plane, which generates a pair of chiral modes along the \(\bar{\Gamma}\bar{Y}\) line, the projection of the mirror plane, as illustrated in figure 18(d).

Following this theoretical prediction, we and our collaborators have reported several experimental works to confirm it. In total, four hallmarks of WSM in the TaAs family have been observed: (1) Fermi arcs on the (0 0 1) surface [136]; (2) Weyl nodes in the bulk state [137]; (3) negative magnetoresistivity due to ‘chiral anomaly’ [138]; (4) spin texture of the Fermi arcs on the (001) surface [139]. Other experimental works include [140–149]. Topological superconductivity [150–153] is also expected for either DSM or WSM, and several experimental efforts [154–156] have been reported.

### 4. Node-line semimetal

In the previous two sections, we have discussed TSMs with isolated Dirac cone like nodes at or close to the Fermi level. However, there is another interesting electronic state having the nodes forming a closed ring or periodically continuous line in momentum space. This kind of semimetal state is now known as topological nodal semimetal [64] or topological node-line semimetal (NLSM) [157]. In 2011, Burkov et al proposed that a fine-tuned superlattice of a normal insulator and TI with broken TRS might realize NLSM [64]. This is basically a model proposal rather than a practically realizable material candidate. In this section, we will introduce some realistic 3D compounds proposed to host NLSM. The underlying mechanism is also based on band inversion, which causes node-lines when both TRS and IS are conserved and SOC is neglected for light element compounds.

### Table 2. An incomplete survey of existing proposals for compounds hosting TSM.

| Type | Candidate compound | Experimental confirmation | Theoretical proposal |
|------|--------------------|--------------------------|----------------------|
| DSM  | Na3Bi              | [65–69]                  | [56]                 |
|      | Cd3As2             | [83–89]                  | [57]                 |
|      | BaAuBi-family      | [93, 94]                 |                      |
|      | LiGaGe-family      | [93]                    |                      |
| Class I | Cu3PtN           | [170]                      |                      |
|      | BiO2               | [71]                    |                      |
| Class II | Distorted spinel   | [92]                    |                      |
|      | HfI2-family        | [93]                    |                      |
|      | TIMo7Te7-family    | [93]                    |                      |
| Magnetic | R13Ir2O7          | [50]                    |                      |
|      | HgCr2Se4           | [62]                    |                      |
| TSM  | TaAs-family        | [136–149]                | [124, 125]           |
| WSM  | Se or Te under pressure | [121]                |                      |
|      | ABl1–xSbxTe2       | [122]                   |                      |
|      | HgTe-class with strain | [183]                 |                      |
|      | Carbon allotropes  | [157, 184]              |                      |
|      | Cu3RN              | [169, 170]              |                      |
| Without-SOC | LaN             | [168]                   |                      |
| NLSM | Black Phosphorus under pressure | [177] |                      |
|      | Ca3P2              | [172]                   |                      |
|      | CaAgX              | [185]                   |                      |
| With-SOC | PtTaSe2, TITaSe2   | [174–176]              |                      |
|      | SrIrO3             | [171]                   |                      |
4.1. All-carbon Mackay–Terrones crystal

In 1992, Mackay and Terrones proposed that [158] graphene can be extended to form 3D networks by placing graphitic tiles consisting of 4- to 8-membered rings onto the Schwarz minimal surface. This kind of 3D all-carbon allotrope is called a Mackay–Terrones crystal (MTC). The Schwarz minimal surface is a 3D periodic minimal surface with its mean curvature \( \frac{H}{k^2} = 0 \) being zero and Gaussian curvature \( K \) being negative everywhere on it. The above \( k_1 \) and \( k_2 \) are the principal curvatures. There are various Schwarz minimal surfaces, such as primitive (P), diamond (D) and gyroid (G) surfaces. One type of MTC based on the P-surface is shown in figure 19. Unlike C\(_{60}\)-like fullerene, which has positive Gaussian curvature, MTC has negative Gaussian curvature and is periodically connected. It has been shown that such all-carbon MTCs can host non-trivial electronic states, including topological node-lines and 3D Dirac points, which are distinct from its 2D counter material graphene. Similar node-lines have also been proposed in optimally tuned photonic crystal composed of gyroid [159], the Schwarz minimal G-surface.

Figure 19 shows a stable structure with simple cubic lattice in the \( \bar{P}m \bar{m} \) space group. It contains 176 atoms per unit cell and was obtained by Tagami et al in [160] and labeled as 6-1-1-p. The electronic band structure of this crystal, calculated based on the local density approximation (LDA), is shown in figure 19(d). It indicates this crystal is a semimetal with band crossings around the Fermi level, similar to the massless Dirac cone in graphene, but they are essentially different. The occupied and unoccupied low energy bands are triply-degenerate at \( \Gamma \), and have \( T_{1d} \) (even parity) and \( T_{2u} \) (odd parity) symmetry respectively. Moving away from point \( \Gamma \) their degeneracy is lifted but at point \( R \) their degeneracy is recovered again. However, the odd and even eigenstates exchange their energy ordering, which is a typical band inversion picture. Thus, band inversion leads to band crossings along both \( X - R \) and \( R - M \) paths as seen from figure 19(d). Including SOC will open a band gap on the nodal points and it becomes a 3D strong TI with \( Z_2 \) index (1;111) [125, 131] if the lower (upper) half of the anti-crossing bands are thought of as occupied (unoccupied). However, the computed SOC splitting is very small, around 0.13 meV or equivalent to 1.5 K temperature, which can be neglected when temperature is higher than 1.5 K.

Without SOC, the most interesting thing found in MTC is that the band crossing points lead to nodal lines rather than nodal points. In fact, the band crossings form closed loops in the 3D momentum space, and generate three circular-like node-lines around the \( R \) point, as shown in figure 20.

Detailed analysis indicates that these node-lines are protected by two factors. One is the coexistence of TRS and IS and the other is that the SOC is negligible. The cubic symmetry of MTC leads to three in-plane nodal rings. The node-lines are not necessarily flat in energy, i.e. the crossing points might be at different energy levels at different \( k \), which leads to compensated electron and hole pockets along the node-lines. This differs from other proposals for the topological node-lines, such as that in [64]—the appearance of node-lines in MTC is very stable and does not require fine tuning of any parameter. This mechanism to generate topological node-lines...
in 3D materials only requires TRS, IS and negligible SOC, which can be easily applied to a large class of materials consisting mainly of light elements.

This topologically stable NLSM state can have nontrivial surface states [64, 161–164]. For the (0 0 1)-surface, the three node-line rings are projected to be a ring and two orthogonal diameter segments inside as shown in figure 21(a). The (0 0 1)-surface state is calculated based on a six-band TB model using both the Green’s function method and slab-model method [47]. There is a nearly flat surface band nestled inside of the projected node-line ring with its band width being about 40 meV due to the particle–hole asymmetry. The peak-like surface density of states contributed by this nearly flat band is clearly shown in figure 21(b). This is proposed to be an important route to high temperature surface superconductivity [165, 166]. The weight function of the surface flat band on each layer is shown in figure 21(c). It penetrates just three layers into bulk with most of the weight on the surface layer. The surface localization of these flat bands is well resolved for those separated from bulk bands. The nested flat surface states have small dispersion and their eigen-energy distribution in surface BZ is shown in figure 21(d), which looks like the vibrational mode of a ‘drumhead’. Such ‘drumhead’-like states are readily detected by angle-resolved photoelectron spectroscopy or scanning tunnel microscopy.

Recently, there have been many other efforts in studying NLSM [167–177], including the theoretical proposal of Cu3PdN to be introduced in the following.

4.2. Anti-perovskite Cu3PdN

In this section, cubic anti-perovskite Cu3PdN is introduced [170]. It is another example of a system hosting a node-line semimetal state protected by the coexistence of TRS and IS in the case with band inversion and negligible SOC. However, Pd is a heavy element and quite strong SOC might open a band gap along the nodal line as discussed in section 3.2. Interestingly, in Cu3PdN, the C4 rotational symmetry will protect the nodal points on the rotation axis and lead to DSM state. This is totally different from the situation in TaAs, where SOC opens a band gap along the whole nodal ring but results in Weyl nodes off the nodal ring plane. Thus, Cu3PdN is a DSM with three pairs of Dirac nodes distinguished from Na3Bi and Cd3As2 with only one pair as shown in sections 2.1 and 2.2 respectively.

Cubic perovskite Cu3PdN is shown in figure 22 together with its BZ and projected BZ. The band structure of Cu3PdN is shown in figure 23. The valence and conduction bands are mainly from Pd-4d (blue) and Pd-5p (red) states, respectively. The fattened bands indicate there is band inversion at R with Pd-5p lower than Pd-4d by about 1.5 eV. This band inversion is checked by hybrid functional [59, 60] calculation. If SOC is neglected the occupied and unoccupied low energy bands are triply degenerate at R. These states belong to the 3D irreducible representations Γ5 and Γ2 of Os group at the R point respectively. The band inversion process in Cu3PdN is shown explicitly in figure 23(b), where the energy levels of Γ5 and Γ2 bands at R point are calculated under different hydrostatic strains. The band inversion happens at $a = 1.11a_0$ ($a_0$ is experimental lattice constant) and the inversion energy increases with further compression of the lattice.

The intriguing point of the Cu3PdN band structure without SOC is that the band crossings due to the band inversion form a nodal ring due to the coexistence of TRS and IS as addressed in section 4.1. Due to the cubic symmetry, there are three mutually perpendicular nodal rings centered at R as schematically shown in figure 22.

When SOC is considered with spin degree of freedom included, the sixfold degenerate states at R are split into one fourfold and one twofold degenerate state. Around the Fermi level, the occupied one has $Γ_4^+$ symmetry and the unoccupied one has $Γ_8^-$ symmetry. Both of them are fourfold degenerate. Along $R − X$ direction, the little group symmetry is lowered to $C_{2v}$. The fourfold degenerate states at R are split into twofold degenerate states. The two bands seem to cross each other, have the same $I_3$ symmetry and a gap $\sim 0.062$ eV is opened at the intersection as shown in the inset of figure 23(b).

However, along the $R − M$ direction, the symmetry is characterized by the $C_{4v}$ double group. As indicated in figure 23(c), the two sets of bands close to Fermi energy belong to the $Γ_7$ and $Γ_5$ representations respectively. They are decoupled, and the crossing point on the $R − M$ path is unaffected by SOC. They form a Dirac node near the Fermi energy as shown in figure 23(c), which is protected by $C_4$ rotational symmetry [56, 57, 178]. If $C_4$ rotational symmetry is broken, the Dirac node will be gapped and the $Z_2$ indices of such gapped system are $(1;111)$, indicating a strong TI. The band structure of Cu3PdN is different from that of antiperovskite Sr3PbO [179] and Ca3PbO [180], where the band inversion happens at $Γ$ point and the bands involved belong to the same irreducible presentation, which leads to anti-crossing along the $Γ-X$ direction.

The band inversion and the 3D Dirac cones in Cu3PdN suggest the presence of topologically nontrivial surface states. The calculated band structures and surface density of states (DOS) on a semi-infinite (0 0 1) surface are presented in figure 24.

Without SOC, the bulk state is the same as MTC [157] and there exists surface flat bands nested inside the projected nodal line ring on the (0 0 1) surface, namely the ‘drumhead’ states as shown in figure 24(a). The peak-like DOS from these nearly flat bands is also clearly shown. The small dispersion of this ‘drumhead’ state comes from the fact that the nodal line ring is not necessarily on the same energy level due to the particle–hole asymmetry [64, 157, 181]. Such 2D flat bands and nearly infinite DOS are proposed as a route to achieving high-temperature superconductivity [165, 166, 181].

In the presence of SOC, each ring is driven into one pair of Dirac nodes. The (0 0 1) surface state band structure in figure 24(b) clearly shows the gapped bulk state along the $Γ-M$ direction and the existence of surface Dirac cones due to topologically nontrivial $Z_2$ indices as seen in Na3Bi [56] and Cd3As2 [57]. The bulk band structures along $R − X$ and $R − M$ overlap each other when projected onto the (0 0 1) surface along the $X-M$ path. The bulk Dirac cones are hidden
by other bulk bands. Therefore, it is difficult to identify the detailed connection of Fermi arcs in the Fermi surface plotting as shown in figure 25, though some eyebrow-like Fermi arcs can be clearly seen around these projected Dirac nodes.

5. Discussion and future prospects

Topological semimetals, as a nontrivial extension of topological classification of electronic quantum state from insulator to metal, have been under the spotlight in the field of condensed matter physics in recent years. The theoretical prediction of these topologically nontrivial quantum states has played a crucial role in greatly stimulating this field. An incomplete survey on the existing theoretical proposals of candidate compounds for each member of TSMs has been listed in table 2. The DSM classification follows those of [182]. Currently widely studied DSM materials Na3Bi and Cd3As2 are both first predicted and then confirmed experimentally. The first WSM of the TaAs family is also predicted by theoretical calculation, and recently they have been under intensive study. The proposed FM half-metal state in HgCr2Se4 has also been confirmed, and it is now much closer to the final confirmation of its double WSM state. To discover an NLSM is the next challenge and the predicted candidates are waiting for experimental verification.

As mentioned in the introduction, the most interesting phenomenon caused by the existence of the Weyl points near the Fermi energy is so-called chiral anomaly, where the electrons under parallel magnetic and electric fields will be pumped from one Weyl node to another with opposite chirality. In the solid state, this pumping process will be eventually balanced by the inter-valley scattering terms generated by the impurities, leading to a steady state carrying extra chiral current along the direction of the magnetic field with the strength being proportional to the inner product of $E$ and $B$ fields. How this chiral pumping effect can manifest itself in experimental measurable quantities is one of the key issues in the study of TSM now. Both theoretical analysis and experimental studies seem to suggest that the chiral anomaly will cause universal negative magnetoresistance proportional to $-B^2$ only in the weak magnetic field limit. In the quantum limit under strong magnetic field, the inter-valley scattering rate will depend on field strength as well, making the behavior of magnetoresistance in the quantum limit related to the detailed properties of the impurity potential and non-universal. Although negative magnetoresistance under parallel magnetic and electric fields has been experimentally observed in several Weyl, Dirac and even massive Dirac materials, how this can be explained uniquely by chiral anomaly is still far from clear. Other effects that may be induced by chiral anomaly, i.e. chiral magnetic effect, nonlocal transport effect and unique optical properties, are still to be observed experimentally.

Throughout this topical review, the relationship among these TSMs is revealed and summarized in figure 26. In the spinless case without including SOC, the coexistence of TRS and IS protects the NLSM state where the band inversion leads to nodal points. Starting from such NLSM, including SOC might lead to DSM (such as Cu3PdN), TI (such as MTC) and WSM (such as the TaAs family). For DSM, introducing different mass terms can drive it to a normal insulator or TI and breaking either TRS or IS will lead to WSM.

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Note added in proof. Since we finished this manuscript, there has been much progress in the field of TSM. For WSM, there are proposals of non-magnetic WSM in chalcoprites [186] and TaS2 [187], and those of magnetic WSM in half-Heuslers under magnetic field [188] and magnetic Heuslers [189], as well as type-II WSM in MoP2 and WP2 [190]. WSM in magnons [191] and phonons [192] are also proposed. For DSM, there is a proposal of LiZnBi [193]. For NLSM, there are proposals for rare-earth elemental metals [194, 195]. There are also proposals for “new fermions” in solids, such as those in [196–198].

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