

Higher-order Dirac fermions in three dimensions

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Relativistic massless Weyl and Dirac fermions exhibit the isotropic and linear dispersion relations to preserve the Pioncaré symmetry, the most fundamental symmetry in high energy physics. In solids, the counterparts of the Pioncaré symmetry are crystallographic symmetries, and hence, it is natural to explore generalizations of Dirac and Weyl fermions compatible with their crystallographic symmetries and then the new physics coming along with them. Here, we study an important kind of generalization, namely massless Dirac fermions with higher-order dispersion relations protected by crystallographic symmetries in three-dimensional nonmagnetic systems. We perform a systematic search over all 230 space groups with time-reversal symmetry and spin-orbit coupling considered. We find that the order of dispersion cannot be higher than three, i.e., only the quadratic and cubic Dirac points (QDPs and CDPs) are possible. We discover previously unknown classes of higher-order Dirac points, including the chiral QDPs with Chern numbers of ± 4 and the QDPs/CDPs without centrosymmetry. Especially the chiral QDPs feature four extensive surface Fermi arcs and four chiral Landau bands and hence leads to observable signatures in spectroscopic and transport experiments. We further show that these higher-order Dirac points represent parent phases for other exotic topological structures. Via controlled symmetry breaking, QDPs and CDPs can be transformed into double Weyl points, triple Weyl points, charge-2 Dirac points or Weyl loops. Using first-principles calculations, we also identify possible material candidates, including α -TeO₂ and YRu₄B₄, which realize the predicted nodal structures.

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I. INTRODUCTION

Weyl and Dirac fermions are elementary particles in high energy physics, where the Pioncaré symmetry is fundamental, and therefore massless Dirac fermions exhibit the isotropic twofold degenerate linear dispersion relation along all directions. Recently, topological metallic phases with protected band degeneracies near the Fermi level have been attracting significant interest [1–12], and particularly, seeking Weyl and Dirac fermions as quasiparticles in such condensed matter systems has been actively performed with various theoretical scenarios and material candidates being proposed [7, 13–22]. Certainly, it is fascinating that the Lorentz-invariant massless Dirac (Weyl) fermions can be realized as quasiparticle excitation in the vicinity of fourfold (twofold) degenerate Fermi points with isotropic twofold degenerate (nondegenerate) linear dispersion, as various celebrated phenomena in high energy physics can lead to remarkable observable effects in Dirac (Weyl) semimetals [23–25]. However, in solids the most fundamental symmetry is the corresponding crystallographic symmetries, which are the counterpart of the Pioncaré symmetry in high energy physics. Therefore, besides straightforwardly looking for faithful Dirac and Weyl

quasiparticles, it is natural to properly extend the definitions of Dirac and Weyl fermions to be compatible with crystallographic symmetries. Since the linearity of dispersion for relativistic particles is required by the Lorentz symmetry, it should not be a surprise that in lots of cases crystallographic symmetries happen to contradict the linear dispersion. In this respect, we focus in this paper on the Dirac points, which have higher order dispersions protected by crystallographic symmetries and are not limited to being twofold degenerate. Here, the term “Dirac” only refers to the fourfold degeneracy of the Dirac point, following the previous convention [26–28].

With the generalization, we can go beyond previous schemes for Dirac semimetals to embrace more diversity for Dirac fermions and related novel physics. For instance, previous works are mostly focused on centrosymmetric nonmagnetic systems [26–30], because it greatly simplifies the analysis: All the bands have an intrinsic Kramers degeneracy due to the combined $\mathcal{PT}$ symmetry [spin-orbital coupling (SOC) considered], such that a Dirac point is formed whenever two bands cross each other. However, this condition is not necessary for our generalized notion of Dirac fermions. As we shall see, for higher-order Dirac fermions, a variety of crystallographic symmetries can lead to fourfold degeneracy at some high-symmetry points in the Brillouin zone, typically with anisotropic behaviors. Especially, in the absence of $\mathcal{P}$, there are birefringent Dirac points with the four crossing

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TABLE I. List of SGs hosting the quadratic and cubic Dirac points. The column with “centrosymmetric” indicates whether the SG contains the centrosymmetry. The C in the penultimate column is the Chern number of the point.

Order	SG	BZ	Location	Generators $\{\mathcal{O} t_1t_2t_3\}$	Centrosymmetric	$ C $	Materials
Quadratic	92	Γ_q	A $\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{C_{4z}^+ 00\frac{1}{4}\}, \{C_{2,1\bar{1}0} \frac{1}{2}\frac{1}{2}\frac{3}{4}\}, \mathcal{T}$	N	4	α -TeO ₂
	96			$\{C_{4z}^+ 00\frac{3}{4}\}, \{C_{2,1\bar{1}0} \frac{1}{2}\frac{1}{2}\frac{1}{4}\}, \mathcal{T}$			
	142	Γ_q^v	P $\{\frac{1}{4}\frac{1}{4}\frac{1}{4}\}$	$\{S_{4z}^+ \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{M_{1\bar{1}0} 10\frac{1}{2}\}, \mathcal{T}\{\mathcal{P} 000\}$	Y	0	YRu ₄ B ₄
	228	Γ_c^f	W $\{\frac{1}{2}\frac{1}{4}\frac{3}{4}\}$	$\{S_{4x}^+ \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{M_z \frac{3}{4}\frac{3}{4}\frac{3}{4}\}, \mathcal{T}\{\mathcal{P} \frac{3}{4}\frac{3}{4}\frac{3}{4}\}$			
Cubic	184	Γ_h	A $\{00\frac{1}{2}\}$	$\{C_{6z}^+ 000\}, \{M_y 00\frac{1}{2}\}, \mathcal{T}$	N	0	
	185			$\{C_{3z}^+ 000\}, \{C_{2z} 00\frac{1}{2}\}, \{M_y 000\}, \mathcal{T}$			
	186			$\{C_{3z}^+ 000\}, \{C_{2z} 00\frac{1}{2}\}, \{M_x 000\}, \mathcal{T}$			
	163	Γ_h	A $\{00\frac{1}{2}\}$	$\{C_{3z}^+ 000\}, \{C_{2y} 00\frac{1}{2}\}, \{\mathcal{P} 000\}, \mathcal{T}$	Y		
	165			$\{C_{3z}^+ 000\}, \{C_{2x} 00\frac{1}{2}\}, \{\mathcal{P} 000\}, \mathcal{T}$			
	167	Γ_{rh}	Z $\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{C_{3z}^+ 000\}, \{C_{2y} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{\mathcal{P} 000\}, \mathcal{T}$			LiOsO ₃ [30]
	226	Γ_c^f	L $\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$\{C_{3,111}^+ 000\}, \{C_{2,1\bar{1}0} 000\}, \{\mathcal{P} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \mathcal{T}$			
	228			$\{C_{3,111}^+ 000\}, \{C_{2,1\bar{1}0} \frac{1}{4}\frac{1}{4}\frac{1}{4}\}, \{\mathcal{P} \frac{3}{4}\frac{3}{4}\frac{3}{4}\}, \mathcal{T}$			
	176 ^a	Γ_h	A $\{00\frac{1}{2}\}$	$\{C_{6z}^+ 00\frac{1}{2}\}, \{\mathcal{P} 00\frac{1}{2}\}, \mathcal{T}$			Tl(MoTe) ₃ [29]
	192			$\{C_{6z}^+ 000\}, \{M_y 00\frac{1}{2}\}, \{\mathcal{P} 000\}, \mathcal{T}$			

^aThe CDP in this SG is not an isolated point but resides on the intersection of three movable but unremovable nodal lines in the $k_z = \pi$ plane [38].

bands fully splitting along certain directions, which were also proposed for linear Dirac fermions [17,31–34].

Actually the importance of higher-order Dirac points has been noticed in a few scattered theoretical works. For example, Yang *et al.* classified Dirac points on a rotational axis or at time reversal invariant momentum (TRIM) points for systems with both time reversal ($\mathcal{T}$) and inversion ($\mathcal{P}$) symmetries [26]. Gao *et al.* performed similar analysis and considered the constraints from seventeen different point groups [28]. Both works reported the possible existence of special Dirac points with linear band splitting in one direction and quadratic/cubic splitting in the orthogonal plane. Such Dirac points hence can be named as quadratic and cubic Dirac points (QDPs and CDPs). Notably, the CDPs were later predicted in realistic materials, such as Tl(MoTe)₃ [29] and LiOsO₃ [30].

Despite the progress mentioned above, higher-order Dirac points have not been thoroughly studied yet, and therefore our current understanding of them is still limited. Particularly, it is worth emphasizing the importance of taking the whole crystallographic group into consideration. A fundamental weakness in the previous works is that only certain subsets of the full crystallographic groups were considered, but the remaining symmetries may cause serious problems for the existence of Dirac fermions possibly from the following aspects. First, certain additional symmetries, although they do not affect the degeneracy at a Dirac point, may generate nodal lines or nodal surfaces that cover the fourfold degenerate point [35,36]. Second, the nonsymmorphic symmetries, such as screw axis and glide mirror, have not been fully considered in previous studies, and their existence may strongly affect the symmetry conditions for Dirac points [30].

Motivated by these questions and challenges, here, we present a systematic investigation of higher-order Dirac points in three-dimensional (3D) systems. The time-reversal symme-

try is assumed, and the SOC is fully considered. We search through all the 230 SGs of nonmagnetic materials, looking for higher-order Dirac points stabilized at the high-symmetry points of the Brillouin zone (BZ). The results are listed in Table I. Our key findings include the following: (i) We find that beyond the linear Dirac point, QDP and CDP are the only stable possibilities, namely, there are no symmetry-protected Dirac points with leading order dispersion (along any direction) higher than the third order. (ii) We discover a *chiral* QDP which carries a topological charge (Chern number) of ± 4 in SG 92 and 96. Such kind of chiral higher-order Dirac point has not been known before. (iii) We show that both QDP and CDP can be realized in crystals *without* $\mathcal{P}$ symmetry, as in SG 92, 96, and 184–186. For these cases, the four bands generally split along generic directions deviating from the point. This behavior is in sharp contrast to the previously studied QDPs/CDPs. (iv) For SG 142 and 228, although $\mathcal{P}$ is preserved, we find that QDP can be realized at points (P and W , respectively) other than the TRIM points.

Furthermore, for each case in Table I, we present the $k \cdot p$ effective model to characterize the low-energy emergent fermions. We discuss the physical signatures for the chiral QDP discovered here, including topological surface Fermi arcs and chiral Landau bands. We further explore the possible topological phase transitions for QDPs and CDPs, and show that they may transform into double Weyl points, triple Weyl points, charge-2 Dirac points [37], or Weyl loops under proper symmetry breaking. With first-principles calculations, we also identify concrete material examples including α -TeO₂ and YRu₄B₄ for realizing some interesting cases in Table I. Our work not only reveals previously unknown types of higher-order Dirac points, it also provides concrete symmetry guidelines for the materials search. Together with previous efforts [26–28], as far as we can see, this completes the classification of all possible higher-order Dirac points for 3D

nonmagnetic systems. Some remaining questions and possible future directions are commented at the end.

Before diving into detailed analysis, let us briefly comment on other promising directions beyond conventional Weyl and Dirac fermions. First, one can think of degenerate Fermi points forming higher dimensional manifolds, such as nodal lines (which can take the form of nodal rings [39–48], nodal links [49], nodal chains [50–52]), and even nodal surfaces [35,53–59], especially with quadratic and cubic dispersion relations [60]. Second, one can study different degrees of degeneracy, such as threefold and sixfold nodal points [61–69]. Third, another promising direction is to explore the interplay between crystallographic-symmetry representations and anisotropic dispersion relations, which would extend previous examples in the context of Weyl points. It has been shown that certain rotational symmetries can enforce the band splitting to be linear along the rotation axis, whereas in the plane orthogonal to the axis, the leading order splitting is of quadratic or cubic order [70–72].

II. APPROACH

Unlike the Weyl points which are topologically protected as long as the discrete translational symmetry is preserved, the Dirac points must require additional crystal symmetry protection. The condition is more stringent for higher-order Dirac points, because they require some symmetries to eliminate the lower-order terms in the band energy splitting. Therefore, such Dirac points have to reside at high symmetry points or on high-symmetry axis of the BZ. The case with high-symmetry axis has been discussed in previous works [26–28], so here we focus on the high-symmetry points. Distinct from the previous approaches, here we fully consider the SG symmetry, including the nonsymmorphic operations that play a crucial role for degeneracies at high-symmetry points on the BZ boundary [15,30,51,73,74]. As we have mentioned in the Introduction, this reveals types of higher-order Dirac points which have not been reported before.

The search approach is similar to the one developed in our previous work [60]. For each SG, we scan through its high-symmetry points and look for symmetry-protected four-fold degeneracy. This is inferred from the dimension of the irreducible representations (IRRs) of the little group at the point. The generators of the little group can be found, e.g., in Ref. [75]. The matrix representations of the symmetry operators can be established by analyzing the algebra formed by these operators. Since we are concerned with nonmagnetic systems with SOC, we deal with the double-valued SG representations, where a 2π rotation produces a minus sign and $\mathcal{T}^2 = -1$. Then, for each four-dimensional IRR, we construct the most general symmetry-allowed $k \cdot p$ Hamiltonian expanded around the degeneracy point, from which the order of the Dirac point can be directly read off. This procedure is applied to all the 230 SGs, which leads to the results presented in Table I. The detailed derivations of the effective models for these higher-order Dirac points are presented in Supplemental Material (SM) [76]. The obtained models are also double checked by using the kdotp-symmetry tool [77]. In the following section, we shall use detailed examples to illustrate the approach.

III. QUADRATIC DIRAC POINT

A. Chiral QDP

As an illustration, let us consider SG 92, which can host a chiral QDP locating at the A point. The little group at A contains three generators: a screw rotation along the z axis $\tilde{C}_{4z} \equiv \{C_{4z}^+ | 00\frac{1}{4}\}$ and a rotation axis along the $(1\bar{1}0)$ direction $C_{2;1\bar{1}0} \equiv \{C_{2;1\bar{1}0} | \frac{1}{2}\frac{1}{2}\frac{3}{4}\}$, as well as $\mathcal{T}$. $\tilde{C}_{4z}$ and $C_{2;1\bar{1}0}$ satisfy the following algebra at A :

$$\tilde{C}_{4z}^4 = 1, \quad C_{2;1\bar{1}0}^2 = -1, \quad \tilde{C}_{4z} C_{2;1\bar{1}0} = -C_{2;1\bar{1}0} \tilde{C}_{4z}^3. \quad (1)$$

The Bloch states at A can be chosen as the eigenstates of $\tilde{C}_{4z}$, which we denote as $|c_{4z}\rangle$ with $c_{4z} \in \{\pm 1, \pm i\}$ the eigenvalue of $\tilde{C}_{4z}$. Based on Eq. (1), one finds that

$$\tilde{C}_{4z} C_{2;1\bar{1}0} |\pm 1\rangle = -C_{2;1\bar{1}0} \tilde{C}_{4z}^3 |\pm 1\rangle = \mp C_{2;1\bar{1}0} |\pm 1\rangle, \quad (2)$$

which indicates that $C_{2;1\bar{1}0} |\pm 1\rangle = |\mp 1\rangle$ and the two states $|1\rangle$ and $|-1\rangle$ would be degenerate. In addition, since $\mathcal{T}^2 = -1$, the state $|\pm 1\rangle$ and its time-reversal partner $\mathcal{T}|\pm 1\rangle$ are linearly independent. Hence, the four states $\{|1\rangle, C_{2;1\bar{1}0}|1\rangle, \mathcal{T}|1\rangle, \mathcal{T}C_{2;1\bar{1}0}|1\rangle\}$ must be degenerate at the same energy, forming a Dirac point.

To fully characterize this Dirac point and the associated emergent fermions, we construct the $k \cdot p$ effective model based on the symmetry. The matrix representations of the generators can be expressed in the above quartet basis as

$$\tilde{C}_{4z} = \sigma_0 \otimes \sigma_z, \quad C_{2;1\bar{1}0} = i\sigma_0 \otimes \sigma_y, \quad \mathcal{T} = i\sigma_y \otimes \sigma_0 \mathcal{K}, \quad (3)$$

where $\mathcal{K}$ is the complex conjugation, σ_i ($i = x, y, z$) are the Pauli matrices, and σ_0 is the 2×2 identity matrix. The Hamiltonian $\mathcal{H}_{\text{eff}}$ is required to be invariant under the symmetry transformations, namely,

$$\tilde{C}_{4z} \mathcal{H}_{\text{eff}}(R_{4z}^{-1} \mathbf{k}) \tilde{C}_{4z}^{-1} = \mathcal{H}_{\text{eff}}(\mathbf{k}), \quad (4)$$

$$C_{2;1\bar{1}0} \mathcal{H}_{\text{eff}}(R_{2;1\bar{1}0}^{-1} \mathbf{k}) C_{2;1\bar{1}0}^{-1} = \mathcal{H}_{\text{eff}}(\mathbf{k}), \quad (5)$$

$$\mathcal{T} \mathcal{H}_{\text{eff}}(-\mathbf{k}) \mathcal{T}^{-1} = \mathcal{H}_{\text{eff}}(\mathbf{k}), \quad (6)$$

where $\mathbf{k}$ is measured from the Dirac point, and R_{4z} and $R_{2;1\bar{1}0}$ are the corresponding rotations acting on $\mathbf{k}$. One notes that from Eq. (4) together with $\tilde{C}_{4z}^2 = \sigma_0 \otimes \sigma_0$, the Hamiltonian must satisfy $\mathcal{H}_{\text{eff}}(-k_x, -k_y, k_z) = \mathcal{H}_{\text{eff}}(\mathbf{k})$. This clearly eliminates terms which are odd in k_x and k_y , indicating that the Dirac point might be a QDP.

It is convenient to write the 4×4 model in the following block form

$$\mathcal{H}_{\text{eff}}^{\text{SG}}(\mathbf{k}) = w(\mathbf{k}) \mathbf{I}_{4 \times 4} + \begin{bmatrix} h_{11}^{\text{SG}}(\mathbf{k}) & h_{12}^{\text{SG}}(\mathbf{k}) \\ h_{12}^{\text{SG}\dagger}(\mathbf{k}) & h_{22}^{\text{SG}}(\mathbf{k}) \end{bmatrix} \quad (7)$$

where each entry in the bracket is a 2×2 matrix. The w term represents an overall energy shift for all the bands, which does not affect the order of the Dirac point. Hence, we will neglect the w term in the following discussion.

With the constraint in Eqs. (4)–(6), the effective model expanded up to the second order is given as

$$h_{11}^{92}(\mathbf{k}) = c_1 k_z \sigma_z + [(c_2 k_+^2 + c_3 k_-^2) \sigma_+ + \text{H.c.}], \quad (8)$$

$$h_{12}^{92}(\mathbf{k}) = \alpha_1 k_z \sigma_z + \alpha_2 k_x k_y \sigma_y, \quad (9)$$

and

$$h_{22}^{92}(\mathbf{k}) = h_{11}^{92*}(-\mathbf{k}) \quad (10)$$

is a time-reversed partner of h_{11}^{92} . Here, $k_{\pm} = k_x \pm ik_y$ and $\sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2$. Note that here and hereafter, we use the Roman letters (such as c_i) and Greek letter (such as α_i) to denote the real and complex parameters, respectively. This effective model confirms that the Dirac point is a QDP, with linear band splitting along k_z and quadratic splitting in the k_x - k_y plane.

More importantly, the diagonal blocks h_{11}^{92} and its time-reversed partner h_{22}^{92} each correspond to a double Weyl point, and they share the *same* topological charge (Chern number) of $2\text{sgn}(|c_2| - |c_3|)$. Therefore, the Dirac point is chiral and has topological charge $\mathcal{C} = \pm 4$. To the best of our knowledge, such a chiral QDP has not been discovered before. Indeed, because the previous studies assume the inversion symmetry, the combined $\mathcal{PT}$ symmetry requires that the Berry curvature and hence the topological charge for any nodal point must be zero. In contrast, the QDP here can be chiral, because the SG considered here explicitly breaks the inversion symmetry. Chiral nodal points and the associated chiral emergent fermions are fascinating subject of research. For example, several types of unconventional chiral fermions have been proposed in chiral crystals [37,78–80]. Later in Sec. V, we shall discuss the interesting physics of this chiral QDP.

Similar analysis applies for SG 96, which results in a $\mathbf{k} \cdot \mathbf{p}$ model $\mathcal{H}_{\text{eff}}^{96}$ of the same form as SG 92 in Eqs. (8)–(10). This proves that the Dirac point in SG 96 is also a chiral QDP with $\mathcal{C} = \pm 4$.

B. QDP at non-TRIM point

Table I shows that QDP may also be realized in SG 142 and 228. However, these two are distinct from SG 92 and 96, as the QDP here appears at a point (P or W) that is not a TRIM point. As a result, the $\mathcal{T}$ symmetry does not belong to the little group at the location of the QDP, and hence it is *not* a symmetry that protects the Dirac point. Nevertheless, as shown in Table I, the combination of $\mathcal{T}$ with inversion does play an important role in stabilizing the Dirac point.

Following a similar method as in the last subsection, we find that the effective model for the QDP in SG 142 reads [76]

$$h_{11}^{142}(\mathbf{k}) = e^{-i\pi/4}(ic_1k_z + c_2k_+^2 + c_3k_-^2)\sigma_+ + \text{H.c.}, \quad (11)$$

$$h_{12}^{142}(\mathbf{k}) = (\alpha_1k_z + \alpha_2k_xk_y)\sigma_y, \quad (12)$$

and

$$h_{22}^{142}(\mathbf{k}) = h_{11}^{142*}(\mathbf{k}). \quad (13)$$

This QDP (and in fact all the bands for SG 142) is not chiral, because the SG contains both $\mathcal{T}$ and $\mathcal{P}$ symmetries. As for the QDP in SG 228, we find that its effective model $\mathcal{H}_{\text{eff}}^{228}$ actually takes the same form as that for SG 142 (connected by a coordinate transformation and a unitary transformation [76]).

Before proceeding, we comment that the symmetry $\mathcal{PT}$ which protects the QDP here is a kind of magnetic symmetry, meaning that it may also be preserved in a magnetic system which explicitly breaks the $\mathcal{T}$ symmetry. Particularly, this $\mathcal{PT}$ may be present in certain antiferromagnetic systems. Previous

works have shown that an antiferromagnet with $\mathcal{PT}$ symmetry may host a linear Dirac point [81–84]. Our discussion here suggests that it is also possible to realize a QDP in the presence of antiferromagnetic ordering with the required symmetry (as in Table I). This would be an interesting topic for future studies.

IV. CUBIC DIRAC POINT

The CDPs in Table I can be put into two classes depending on whether the system contains the $\mathcal{P}$ symmetry or not. Below, we discuss the two classes one by one.

A. CDP without inversion symmetry

We first consider the CDP realized in SG 184–186, for which the inversion symmetry $\mathcal{P}$ is absent. These cases are distinct from the previously reported CDPs which all have the $\mathcal{P}$ symmetry. As a result, the four bands that form the CDP will fully split along a generic direction deviating from the point (twofold degeneracy may still appear along some high-symmetry direction such as the rotational axis).

For SG 184, the CDP resides at the A point at the BZ boundary, and the nonsymmorphic symmetry such as $\{M_y|00\frac{1}{2}\}$ plays an important role in stabilizing the CDP. The corresponding effective Hamiltonian is obtained as

$$h_{11}^{184}(\mathbf{k}) = f(\mathbf{k})k_z\sigma_z + [(\alpha_1k_+^3 + \alpha_2k_-^3)\sigma_+ + \text{H.c.}], \quad (14)$$

$$h_{12}^{184}(\mathbf{k}) = (c_4k_+^3 + c_5k_-^3)\sigma_0 + [g(\mathbf{k})k_z\sigma_+ + \text{H.c.}], \quad (15)$$

$$h_{22}^{184}(\mathbf{k}) = h_{11}^{184}(k_x, -k_y, k_z), \quad (16)$$

where $f(\mathbf{k}) = c_1 + c_2k_{\parallel}^2 + c_3k_z^2$, $g(\mathbf{k}) = \alpha_3 + \alpha_4k_{\parallel}^2 + \alpha_5k_z^2$, and $k_{\parallel} = \sqrt{k_x^2 + k_y^2}$. One observes that the diagonal blocks $h_{11}^{184}(\mathbf{k})$ and $h_{22}^{184}(\mathbf{k})$ describe two triple Weyl points but with *opposite* Chern numbers $\pm 3\text{sgn}(|\alpha_1| - |\alpha_2|)$. Therefore, the net Chern number of the CDP vanishes, which is consistent with the presence of the (glide) mirror that passing through this point.

For SG 185 and 186, the role of the glide mirror is replaced by a twofold screw rotation $\{C_{2z}|00\frac{1}{2}\}$. Together with the $\mathcal{T}$ symmetry, it actually ensures a twofold degeneracy in the $k_z = \pi$ plane. As A is located on this plane, a band crossing at A will naturally have a fourfold degeneracy, making a Dirac point. For SG 185, the effective Hamiltonian reads

$$h_{11}^{185}(\mathbf{k}) = f(\mathbf{k})k_z\sigma_0 + [i(c_4k_+^3 + c_5k_-^3)\sigma_+ + \text{H.c.}], \quad (17)$$

$$h_{12}^{185}(\mathbf{k}) = g(\mathbf{k})k_z\sigma_0 + \alpha_4(k_+^3 - k_-^3)\sigma_x, \quad (18)$$

$$h_{22}^{185}(\mathbf{k}) = h_{11}^{185*}(-\mathbf{k}), \quad (19)$$

where $f(\mathbf{k}) = c_1 + c_2k_{\parallel}^2 + c_3k_z^2$, and $g(\mathbf{k}) = \alpha_1 + \alpha_2k_{\parallel}^2 + \alpha_3k_z^2$. Again, one finds that the diagonal blocks $h_{11}^{185}(\mathbf{k})$ and $h_{22}^{185}(\mathbf{k})$ describe two triple Weyl points with opposite Chern numbers $\pm 3\text{sgn}(|c_4| - |c_5|)$.

Similarly, the effective model of the CDP in SG 186 is related the model of SG 185 by a coordinate transformation,

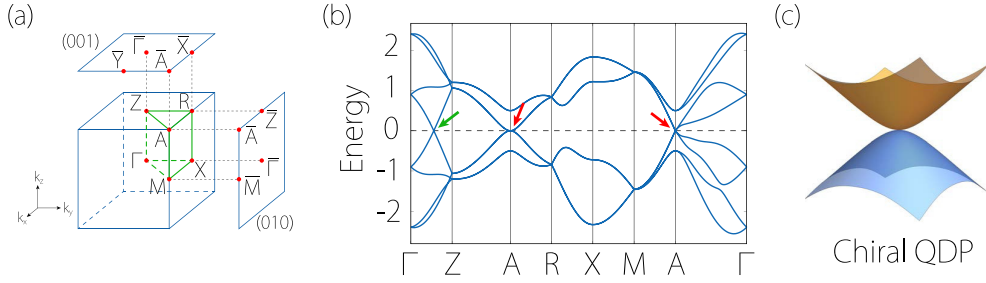


FIG. 1. (a) Bulk and surface BZs for SG 92. (b) Bulk band structure for a lattice model with SG 92. The chiral QDP is located at the A point (as indicated by the red arrows) and it carries a Chern number of -4 . There also exists a pair of double Weyl points on the k_z axis (as indicated by the green arrow), each with a Chern number of $+2$. The quadratic dispersion around the QDP in the plane perpendicular to k_z is plotted in (c).

expressed as

$$\mathcal{H}_{\text{eff}}^{186}(k_x, k_y, k_z) = \mathcal{H}_{\text{eff}}^{185}(-k_y, k_x, k_z). \quad (20)$$

Thus, although the inversion symmetry is broken for these SGs, the CDPs realized here are not chiral (i.e., with vanishing Chern numbers).

B. CDP with inversion symmetry

The remaining cases in Table I are for the CDPs in SGs with inversion symmetry. These include SG 163, 165, 167, 226, 228, and 192. Due to the $\mathcal{PT}$ symmetry, the bands are at least doubly degenerate, and the Berry curvature as well as the net Chern number must vanish. To construct the effective model, we note that for SG 163, 165, 167, 226, and 228, the inversion symmetry anticommutes with the twofold rotation, and it satisfies $\mathcal{P}^2 = 1$. Hence, the fourfold degeneracy at the CDP can be decomposed into the four linearly independent states $\{|p=1\rangle, |p=-1\rangle, \mathcal{T}|p=1\rangle, \mathcal{T}|p=-1\rangle\}$, with p denoting the eigenvalue of $\mathcal{P}$. Specifically, the effective model for SG 163 is obtained as

$$h_{11}^{163}(\mathbf{k}) = [f(\mathbf{k})k_z + c_4k_+^3 + c_5k_-^3]\sigma_+ + \text{H.c.}, \quad (21)$$

$$h_{12}^{163}(\mathbf{k}) = [g(\mathbf{k})k_z + \alpha_4(k_+^3 + k_-^3)]\sigma_x, \quad (22)$$

$$h_{22}^{163}(\mathbf{k}) = h_{11}^{163*}(-\mathbf{k}), \quad (23)$$

where $f(\mathbf{k}) = c_1 + c_2k_{\parallel}^2 + c_3k_z^2$, and $g(\mathbf{k}) = \alpha_1 + \alpha_2k_{\parallel}^2 + \alpha_3k_z^2$. Meanwhile, we find that the effective models for SG 165, 167, 226, and 228 all share the same form as SG 163 (after a coordinate transformation as expressed by Eqs. (S76)–(S78) in SM [76]).

At last, the effective model for the CDP in SG 192 is found to be

$$h_{11}^{192}(\mathbf{k}) = (c_1k_+^3 + c_2k_-^3)\sigma_+ + \text{H.c.}, \quad (24)$$

$$h_{12}^{192}(\mathbf{k}) = g(\mathbf{k})k_z\sigma_x, \quad (25)$$

$$h_{22}^{192}(\mathbf{k}) = h_{11}^{192*}(-\mathbf{k}), \quad (26)$$

where $g(\mathbf{k}) = \alpha_1 + \alpha_2(k_x^2 + k_y^2) + \alpha_3k_z^2$.

Previously, the CDP has been reported in two materials: One is in the centrosymmetric phase of LiOsO_3 [30], the other is in the $\text{Ti}(\text{MoTe})_3$ family materials [29]. The former case belongs to the SG 167, while the latter case belongs to the

SG 176. It should be noted that different from the other cases, the CDP in SG 176 is not an isolated Dirac point. Instead, it resides on the intersection of three movable but unremovable Dirac nodal lines on the $k_z = \pi$ plane [38]. Therefore, strictly speaking, this degeneracy should not be classified as a Dirac point.

V. SIGNATURES OF CHIRAL QDP

We have demonstrated that different kinds of QDPs and CDPs can be stabilized by the space group symmetry. The most interesting discovery here is the chiral QDP which carries a nonzero Chern number ± 4 . Below, we focus on this case and discuss its two interesting physical signatures, including the topological surface Fermi arcs and the chiral Landau bands.

A. Surface Fermi arcs

Because the QDPs in SG 92 and 96 carry nonzero Chern number with absolute value $|C| = 4$, according to the bulk-boundary correspondence [14], on the surface of the material, there should exist four Fermi arcs emerging from the surface projection of the Dirac point. To explicitly demonstrate this, we construct an eight-band tight-binding model for SG 92 (see SM [76]) and calculate its bulk and surface spectra. In Fig. 1(b), one observes the QDP located at the A point. Figure 1(c) shows the quadratic band dispersion around this QDP in the k_x - k_y plane (here, each band is doubly degenerate

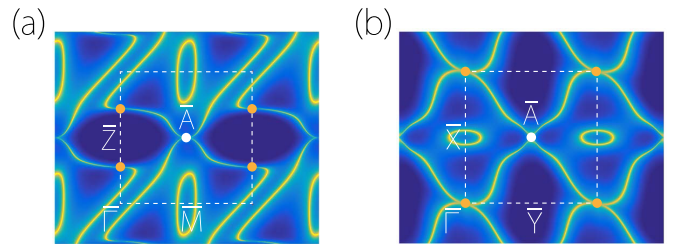


FIG. 2. The Fermi surface contours on (a) the (010) surface and (b) the (001) surface for the lattice model with SG 92. The white and orange dots indicate the surface projections of the chiral QDP and the double Weyl points, respectively. There are four surface Fermi arcs emanating from the projection of the chiral QDP, consistent with its topological charge.

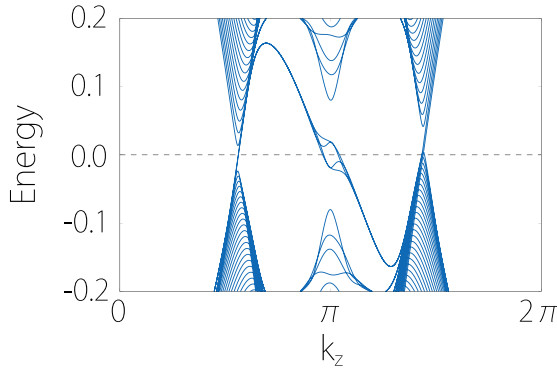


FIG. 3. Landau spectrum calculated from the lattice model for SG 92, with B field along the z direction. The chiral QDP gives four chiral Landau bands crossing the Fermi level with negative slope (near $k_z = \pi$ here). They are accomplished by the four positive chiral Landau bands associated with the two double Weyl points.

because of the $\mathcal{T}\tilde{C}_{2z}$ symmetry). Figure 2(a) shows the surface spectrum for the (010) surface, in which one can clearly observe four surface Fermi arcs emanating from the projected QDP. These arcs are terminated at the projections of two double Weyl points located on the k_z axis [see Fig. 2(a)]. For this tight-binding model, we find that the chiral QDP carries a Chern number of -4 , and each double Weyl point carries a Chern number of $+2$, so the net topological charge in the BZ vanishes, satisfying the no-go theorem. It is also worth pointing out that because these chiral nodal points are sitting at different locations in the BZ (A point and k_z axis) which are far apart, the Fermi arcs connecting them are extensive in the surface BZ. This makes them more accessible in angle-resolved photoemission spectroscopy (ARPES) or scanning tunneling spectroscopy (STS) experiment.

B. Chiral Landau bands

The chiral nature of a nodal point can manifest in the spectrum under a strong magnetic field. For the conventional Weyl point with topological charge of ± 1 , there exists one chiral Landau band with linear dispersion along the magnetic field direction [23]. In Ref. [85], it has been shown that the net number of chiral Landau bands just corresponds to the topological charge. Here, since the QDP has a topological charge of ± 4 , one expects to find four such Landau bands.

In Fig. 3, we show the explicit result of the Landau spectrum based on the tight-binding model. (An analytic solution of the $k \cdot p$ model is presented in SM [76].) Here, we take the same model as in Fig. 1 for SG 92, and the magnetic field is oriented along the z axis. Under the magnetic field, the electron motion in the x - y plane is quantized into Landau levels, so the original 3D band structure transforms into 1D Landau bands with dispersion only along k_z . In the spectrum, one clearly observes four chiral Landau bands with negative slopes around $k_z = \pi$, corresponding to the chiral QDP. Meanwhile, the two double Weyl points residing on the k_z axis give another four chiral Landau bands with positive slopes. Similar to the Weyl case, when further applying an electric field parallel to the magnetic field, electrons will be pumped between the different chiral points, and this can result in a negative contribution to the longitudinal magnetoresistance [86]. Recent works have shown that this chiral anomaly related process would undergo a breakdown when the magnetic field is strong enough such that the inverse magnetic length ℓ_B^{-1} is comparable to the chiral point separation [87–89]. For SG 92 and 96, since the QDP is well separated from the other nodal point in momentum space, one can expect that this chiral anomaly effect will be more robust against the magnetic tunneling.

TABLE II. Topological phase transitions for higher-order Dirac points under symmetry breaking. WPs and DPs stand for the Weyl points and the Dirac points, respectively.

Type	SG	Change of SG	Symmetry breaking	New phase
Chiral QDP	92	$\Rightarrow 76$	$\{C_{2z} 1\bar{1}0 \frac{1}{2}\frac{1}{2}\frac{3}{4}\}$ (retain $\{C_{4z}^+ 00\frac{1}{4}\}$)	A pair of double WPs at $(\pi, \pi, \pi \pm q_z)$
	96	$\Rightarrow 78$	$\{C_{2z} 1\bar{1}0 \frac{1}{2}\frac{1}{2}\frac{1}{4}\}$ (retain $\{C_{4z}^+ 00\frac{3}{4}\}$)	
	92	$\Rightarrow 19$	$\{C_{4z}^+ 00\frac{1}{4}\}$ (retain $\{C_{2z} 00\frac{1}{2}\}$)	A pair of charge-2 DPs
	96	$\Rightarrow 19$	$\{C_{4z}^+ 00\frac{3}{4}\}$ (retain $\{C_{2z} 00\frac{1}{2}\}$)	
non-TRIM QDP	142	$\Rightarrow 110$	$\mathcal{P}$ (retain $\{C_{2z}^+ \frac{1}{2}0\frac{1}{2}\}$ and $\{M_{1\bar{1}0} 10\frac{1}{2}\}$)	Weyl chain
		$\Rightarrow 122$	$\mathcal{P}$ (retain $\{S_{4z}^+ \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ and $\{M_{1\bar{1}0} 10\frac{1}{2}\}$)	
non- $\mathcal{P}$ CDP	185	$\Rightarrow 173$	$\{M_y 000\}$	A pair of triple WPs at $(0, 0, \pi \pm q_z)$
	186	$\Rightarrow 173$	$\{M_x 000\}$	
	184	$\Rightarrow 158/159$	$\{C_{2z} 000\}$	Weyl loops
	185	$\Rightarrow 158$	$\{C_{2z} 00\frac{1}{2}\}$ (retain $\{M_x 00\frac{1}{2}\}$)	
	186	$\Rightarrow 159$	$\{C_{2z} 00\frac{1}{2}\}$ (retain $\{M_y 00\frac{1}{2}\}$)	
$\mathcal{P}$ CDP	163	$\Rightarrow 159$	$\mathcal{P}$ (retain $\{M_y 00\frac{1}{2}\}$)	Weyl loops
	165	$\Rightarrow 158$	$\mathcal{P}$ (retain $\{M_x 00\frac{1}{2}\}$)	
	167	$\Rightarrow 161$	$\mathcal{P}$ (retain $\{M_y \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$)	
	226/228	$\Rightarrow 219$	$\mathcal{P}$ (retain $\{M_{1\bar{1}0} \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$)	
	192	$\Rightarrow 188/190$	$\mathcal{P}$ (retain $\{M_x 00\frac{1}{2}\}/\{M_y 00\frac{1}{2}\}$)	

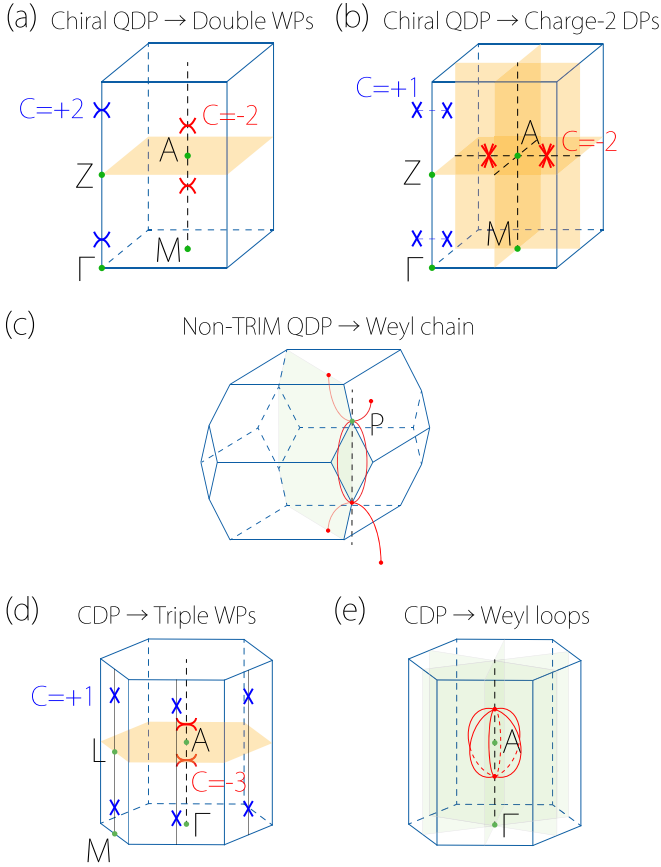


FIG. 4. QDPs and CDPs under symmetry breaking. (a) Breaking $C_{2,1\bar{1}0}$ rotation axis can transform the chiral QDPs of SGs 92 and 96 into a pair of double Weyl points (red crosses), while the double Weyl points on the k_z axis (blue crosses) remain. (b) By breaking the $\bar{C}_{4z}$ screw axis (retaining $\bar{C}_{2z}$), the chiral QDPs can be transformed into a pair of charge-2 Dirac points (red crosses), while the double Weyl points on the k_z axis split into a pair of linear Weyl points (blue crosses). (c) Breaking $\mathcal{P}$ (retaining $\{S_{4z}^+|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ and $\{M_{1\bar{1}0}|10\frac{1}{2}\}$) can transform the QDP of SG 142 to nodal chains with the touching point located at the point P. (d) Breaking M_y mirror can transform the CDP of SG 185 into a pair of triple Weyl points (red crosses). Their topological charges are compensated by three pairs of linear Weyl points on the three M - L path (blue crosses). (e) Breaking $\mathcal{P}$ (retaining $\bar{M}_x$) can transform the CDP of SG 185 into three crossed Weyl loops lying in the three glide invariant planes.

VI. TOPOLOGICAL PHASE TRANSITION

As the higher-order Dirac points are protected by symmetry, they will generally be gapped or transformed to other types of band degeneracies when the symmetry is broken. Several interesting cases are illustrated in Table II and Fig. 4. For example, breaking the $C_{2,1\bar{1}0}$ rotation axis can split the chiral QDP of SGs 92 and 96 into a pair of double Weyl points with the same chirality [Fig. 4(a)]. For SGs 185 and 186, the breaking of mirror symmetry (M_y or M_x) may transform the CDP into a pair of triple Weyl points [Fig. 4(d)]. The triple Weyl points have the same chirality, which would be compensated by three pairs of linear Weyl points with the opposite chirality on the three M - L paths. For SGs 92 and 96, one can also obtain a pair of charge-2 Dirac points [37] with

the same Chern number $|C| = 2$ on a screw invariant axis, via breaking the $\bar{C}_{4z}$ screw axis while retaining the $\bar{C}_{2z}$ screw axis [Fig. 4(b)]. For SG 142, retaining $\{S_{4z}^+|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ and $\{M_{1\bar{1}0}|10\frac{1}{2}\}$ while breaking $\mathcal{P}$, the QDP at non-TRIM can be transformed into nodal chains whose touching point is located at point P [Fig. 4(c)]. This is consistent with the previous study [50]. Moreover, retaining a glide plane while breaking C_{2z} or $\mathcal{P}$ that anticommute with the glide mirror can transform the CDP into Weyl loops traced by the necking point of hourglass dispersions. This explains the appearance of mutually crossed nodal rings in the ferroelectric phase of LiOsO_3 [30]. These results demonstrate that QDP and CDP systems provide a promising playground for studying topological phase transitions and a variety of emergent fermions.

It should be mentioned that the list in Table II is not exhaustive. There may exist other topological gapless or gapped phases realized by symmetry breaking from these higher-order Dirac points [26,90]. The transformation of higher-order Dirac points is an interesting topic which deserves further studies.

VII. MATERIAL REALIZATION

The symmetry conditions summarized in Table I provide useful guides for the material search. As indicated in the table, the previously identified materials LiOsO_3 [30] and $\text{Tl}(\text{MoTe})_3$ [29] belong to two space groups which can host CDPs in the presence of $\mathcal{P}$ symmetry. Here, we identify two material examples that host the kinds of higher-order Dirac points discovered in this work.

The first example is the tetragonal paratellurite, α - TeO_2 , which belongs to SG 92. This material has been synthesized in experiment and exists as the low-pressure phase of TeO_2 [91–95]. Here, we only focus on the tetragonal low-pressure phase. Its structure is built up of asymmetric TeO_4 trigonal bipyramid polyhedron units [see Fig. 5(a)]. We use first-principle calculations to obtain its band structure (SOC included), which has been plotted in Fig. 5(b). Although it is an indirect band-gap semiconductor with a band gap of ~ 2.69 eV, the feature of QDPs can be found at the A point in both conduction and valence bands. From a zoom-in image in Fig. 5(c), one clearly observes the quadratic dispersion within the k_x - k_y plane. The calculated Chern number for this QDP is -4 , which is consistent with our symmetry analysis. On a generic surface, there should be four Fermi arcs emerging from the surface projection of the QDP point. We calculate the projected spectrum for the (001) surface and indeed verify the existence of four topological surface Fermi arcs, as shown in Fig. 5(d).

The second example is YRu_4B_4 , which is a member of the superconducting materials family $M(\text{Rh}, \text{Ru})_4\text{B}_4$ ($M = \text{Y}, \text{Th}$, or Lanthanides) [96,97]. The material has a tetragonal crystal structure with the space group of $I4_1/acd$ (No. 142). In the lattice structure, as shown in Figs. 6(a) and 6(b), the Y atoms form a face-centered-cubic sublattice, while Ru atoms form an array of tetrahedra with B atoms interspersed among them. According to Table I, this SG can host a QDP at a non-TRIM point. In the band structure of YRu_4B_4 plotted in Fig. 6(c), one indeed observes a Dirac point about 0.18 eV above the Fermi level at the non-TRIM point P. The dispersion around

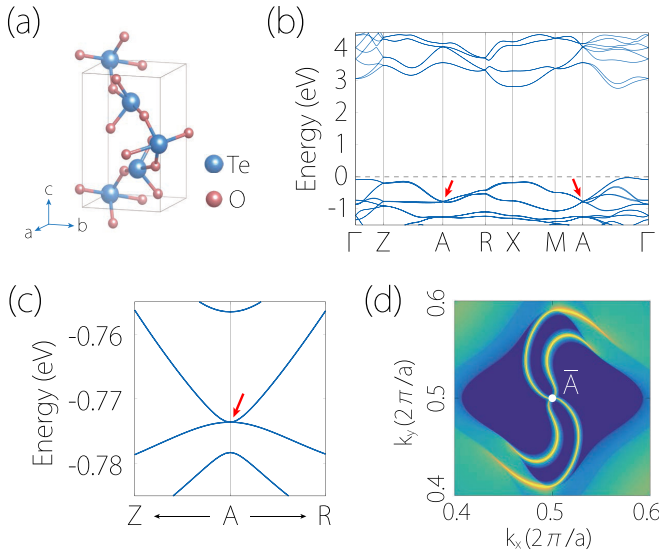


FIG. 5. (a) Crystal structure for α -TeO₂ (SG 92). (b) Calculated band structure for α -TeO₂ (with SOC included). The red arrows indicate the chiral QDP at A. (c) shows the zoom-in image around the QDP. (d) Calculated constant energy slice (at the QDP energy) for the (001) surface shows four surface Fermi arcs emitted from the projected chiral QDP.

the Dirac point [see Fig. 6(e)] confirms that it has a quadratic in-plane dispersion, which is in agreement with our symmetry analysis.

VIII. DISCUSSION AND CONCLUSION

In this work, we have systematically investigated the higher-order Dirac points that can be stabilized at high-symmetry points for nonmagnetic systems. The fourfold degeneracy of a Dirac point must require protection from certain crystalline symmetry, so the Dirac point generally cannot appear at a generic k point in the BZ; instead it might be located at a high-symmetry point (studied in this work), on a high-symmetry path (Refs. [26–28]), or on a high-symmetry (mirror) plane. Regarding the last case, the previous work by Yang *et al.* [39] have indicated that a combination of chiral symmetry, mirror symmetry, $\mathcal{P}$, and $\mathcal{T}$ may stabilize linear Dirac points on a mirror plane. The chiral symmetry is a natural symmetry for the superconducting quasiparticle spectrum, and it may also emerge at low energy for many elemental materials with a bipartite lattice [35,44,53,98,99]. However, to ensure a higher-order dispersion, the condition is more stringent. Additional symmetries must be needed to rule out the linear order terms, and hence a higher-order Dirac point on a mirror plane appears unlikely. Therefore, we speculate that our work, together with previous studies [26–28], has examined all possible higher-order Dirac points in 3D nonmagnetic systems.

We have identified two material examples which contain the higher-order Dirac points. The purpose is to confirm our symmetry analysis. However, these materials are not ideal, in the sense that either the Dirac point is not close to the Fermi

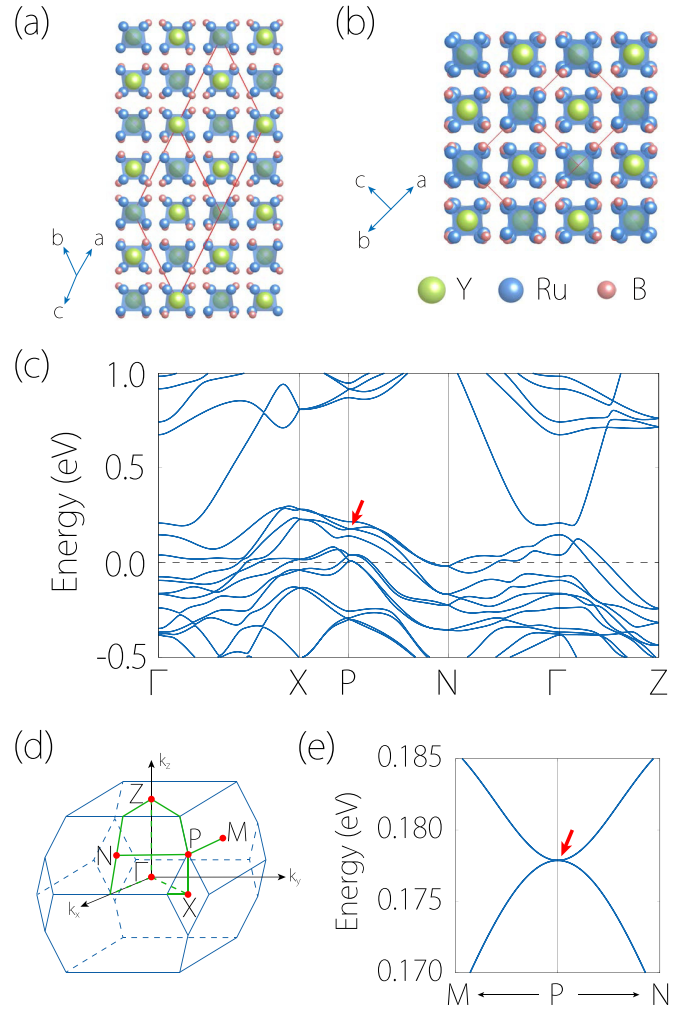


FIG. 6. (a) Side and (b) top view of the crystal structure of YRu₄B₄. The red parallelograms indicate the primitive cell. (c) Calculated band structure for YRu₄B₄ (with SOC included). The red arrows indicate the QDP at P. (d) shows the BZ. (e) Enlarged view of the band dispersion around the QDP in (c).

level (for α -TeO₂), or the low-energy bands are not clean (for YRu₄B₄). To facilitate experimental research on these new nodal points, it is important to search out better material candidates in future studies. Our results here will provide a useful guidance for this task.

In conclusion, via symmetry analysis, we have searched through all 230 SGs and obtained all possible higher-order Dirac points at high-symmetry points for 3D nonmagnetic systems. We show that only QDP and CDP are possible, i.e., there is no stable Dirac point with dispersion higher than the third order. We find several types of previously unknown Dirac points, including the chiral QDP (with Chern number $\mathcal{C} = \pm 4$), QDP at non-TRIM point, and CDP without the $\mathcal{P}$ symmetry. We present the list of SGs that can host these Dirac points as well as their low-energy effective models. For the chiral QDP, we further discuss its interesting physical properties, including the extensive surface Fermi arcs and chiral Landau bands. We also explore the topological phase

transitions for QDPs and CDPs under symmetry breaking, and show that they can give rise to a rich variety of topological band degeneracies, such as double Weyl points, triple Weyl points, charge-2 Dirac points, or Weyl loops. Finally, we identify material examples α -TeO₂ and YRu₄B₄ that exhibit the higher-order Dirac points. Our work discovers topological gapless phases with new kinds of emergent Dirac fermions. The obtained symmetry conditions will be useful to guide material search. The approach adopted here may also be extended to study new kinds of nodal structures in magnetic systems in future works.

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