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New classes of topological crystalline insulators having surface rotation anomaly

Chen Fang1,2,3* and Liang Fu4*

We discover new types of quantum anomalies in two-dimensional systems with time-reversal symmetry (T) and discrete rotation symmetry with order of \( n = 2, 4, \) and 6 (\( C_n \)). The new anomalous states have \( n \) flavors of massless Dirac fermions protected by \( T \) and \( C_n \), whereas any two-dimensional lattices having the two symmetries must have a multiple of 4, 8, and 12 Dirac cones for \( n = 2, 4, \) and 6, respectively. We show that these anomalous states are physically realized on the surface of new classes of topological crystalline insulators, normal to the rotation axis. Moreover, these topological crystalline insulators support \( n \) gapless one-dimensional helical mode on the otherwise fully gapped side surface, connecting the anomalous two-dimensional states on the top and bottom surfaces. The presence of these helical modes enables a new quantum device made from a topological crystalline insulator nanorod, a “helical nanorod,” which has a quantized longitudinal conductance of \( ne^2/h \).

INTRODUCTION

A single flavor of massless relativistic fermion is known to have quantum anomalies such that the conservation of certain global symmetry current is broken at the quantum level (1). Well-known examples include the chiral anomaly of Weyl fermions in three dimensions (2-5) and the parity anomaly in two dimensions (6-8). Because of these anomalies, theories with only one flavor of massless fermions cannot have an ultraviolet (UV) completion that preserves the relevant symmetry. This, in turn, implies that any UV-complete theory with \( U(1) \) charge conservation must have an even number of massless fermions not only in odd spatial dimensions but also in even spatial dimensions if time-reversal symmetry is present.

Massless relativistic fermions also emerge as low-energy excitations in solids, where the lattice spacing provides a natural UV cutoff. The above fermion doubling theorem then enforces that Weyl fermions come in pairs in three-dimensional (3D) semimetals and that Dirac fermions (massless two-component complex fermions in two dimensions and massless four-component complex fermions in three dimensions) must come in pairs in 2D time-reversal invariant systems such as graphene. Unlike the quantum vacuum in particle physics, condensed matter systems are non-Lorentz invariant but satisfy the spatial symmetry of the underlying crystal. Spatial symmetry also constrains the number of massless fermions. For example, recent works (9, 10) have shown that any 2D lattice with either (glide) reflection symmetry, or the composite symmetry of twofold rotation and time reversal, must have an even number of Dirac fermions. The field theory of massless Dirac fermions in these systems is compatible with emergent Lorentz invariance at low energy. Since the above symmetry transformations reverse the orientation of 2 + 1-dimensional spacetime, their actions on emergent relativistic fermions are essentially equivalent to inversion symmetry in parity anomaly.

In this work, we present new quantum anomalies associated with time reversal (\( T \)) and discrete rotational symmetry of crystals (\( C_n = 2, 4, 6 \)). These anomalies can only exist in theories breaking continuous rotation symmetries and lead to a stronger constraint on the number of massless fermions in two dimensions. We show that in time-reversal invariant band structures with \( T^2 = -1 \) and \( n \)-fold rotational symmetry (\( n = 2, 4, \) and 6), the number of stable massless Dirac fermions must be a multiple of \( 2n \). Here, massless Dirac fermion is synonymous with linear band crossing in the Brillouin zone, and “stable” means that these band crossings are robust against arbitrary perturbations preserving \( T \) and \( C_n \). This result, dubbed the fermion multiplication theorem, is a generalization of fermion doubling theorem in particle physics to crystalline solids (throughout the paper, we have assumed the general presence of spin-orbital coupling so that time reversal satisfies \( T^2 = -1 \); the results do not apply to systems without spin-orbital coupling, i.e., the spinless cases).

Despite lacking a lattice regularization, field theories with anomaly can describe boundary states of a topological bulk state in one higher spatial dimension. This provides a powerful approach to identify and classify topologically nontrivial bulk states. A single 3 + 1 Weyl fermion with chiral anomaly appears on the boundary of a 4D quantum Hall state (11), and a single (2 + 1)-d massless Dirac fermion with parity anomaly appears on the surface of a 3D topological insulator (TI) with time-reversal symmetry (12). In both systems, the topological boundary states evade the fermion doubling theorem because their UV completion lies in the bulk. This leads to a bulk-boundary correspondence: Anomalous theory on the boundary implies nontrivial topology in the bulk.

In the similar spirit, the new 2 + 1D anomaly that we found has important implications for 3D topological states protected jointly by rotation and time-reversal symmetry, generally referred to as topological crystalline insulators (TCIs) (13-15). The study of anomaly leads us to theoretically discover new classes of time-reversal invariant TCIs with \( C_n = 2, 4, 6 \) rotation symmetry. These TCIs have anomalous surface states on the top and bottom surfaces perpendicular to the \( n \)-fold axis. Such topological surface states consist of \( n \) Dirac cones that connect to bulk states at high energy, evading the above fermion multiplication theorem. Furthermore, these TCIs in a rod geometry support \( n \) 1D helical modes on the side surface (16). These 1D helical modes are located along \( n \) gapless lines on the otherwise gapped side surface, connecting the top and the bottom surfaces, and are related to each other by \( C_n \)-rotation. For each class of new TCIs, we construct the corresponding \( Z_2 \) topological invariant in terms of Bloch
wave functions in momentum space. We further provide a unified real-space understanding of these TCIs based on dimensional reduction and domain wall states. Last, we predict several materials realizing the anomalous surface states protected by two- and fourfold rotation symmetries, and we propose a new quantum device called “helical nanorod” made from these new TCIs, featuring ballistic longitudinal transport with conductance $ne^2/h$, independent of the radius.

**RESULTS**

**Rotation anomaly**

We consider 2D systems of noninteracting electrons with spin-orbit coupling, time-reversal, and $n$-fold rotational symmetry, where $n = 2, 4, \text{ or } 6$. We aim to establish the number of symmetry-protected Dirac cones—or equivalently the number of stable band crossings—that such systems are allowed to have. For this purpose, it suffices to consider systems with an integer number of electrons per unit cell and with either a bandgap or Dirac points at Fermi energy.

Dirac points can be located at either generic momenta or high-symmetry points in the Brillouin zone. As shown in the Supplementary Materials, one can always choose a $C_n$ symmetric superlattice unit cell such that (i) high-symmetry points fold back to $\Gamma$ in the reduced Brillouin zone and (ii) the number of electrons in the enlarged unit cell is an even integer. The condition of even-integer electron filling makes systems at certain even-integer electron fillings gapless.

Because of time reversal and $C_n$-rotation symmetry ($n$ even), the number of Dirac points at generic momenta must be a multiple of $n$, and each multiplet consists of $n/2$ pairs of Dirac points at opposite momenta that are related by symmetry, as shown in Fig. 1.

We now show that the simplest scenario of $n$ Dirac points is anomalous; i.e., it can only be realized on the surface of a 3D TCI. In any 2D lattice system with time-reversal symmetry, the number of Dirac points away from high-symmetry points must be a multiple of $4, 8, \text{ or } 12$, respectively, when two-, four-, or sixfold rotation symmetry is present.

To prove this fermion multiplication theorem, consider the Berry phase along the closed contours in the Brillouin zone plotted in Fig. 1. Because of time reversal and the twofold rotation symmetry, the Berry curvature vanishes everywhere in momentum space; the Berry phase along the closed contours in the Brillouin zone plotted in $\Gamma, X, Y, M, \text{ and } K$ in the corresponding Brillouin zone. Following the method of (17), we find

\[
e^{i\Theta_2} = \prod_{i=1}^{N_{\text{occ}}} \zeta_i(\Gamma)\zeta_i(X)\zeta_i(Y)\zeta_i(M)
\]

\[
e^{i\Theta_4} = (-1)^{N_{\text{occ}}} \prod_{i=1}^{N_{\text{occ}}} \zeta_i(\Gamma)\zeta_i(M)\zeta_i(X)
\]

\[
e^{i\Theta_6} = (-1)^{N_{\text{occ}}} \prod_{i=1}^{N_{\text{occ}}} \omega_i(\Gamma)\theta_i(K)\zeta_i(M)
\]

where $N_{\text{occ}}$ is the number of occupied bands (counting spin) and $\zeta_i$, $\theta_i$, $\zeta_i$, and $\omega_i$ are the eigenvalues of $C_2$, $C_3$, $C_4$, and $C_6$ operation at the corresponding invariant points, respectively.

Since we deal with even-integer electron fillings, $N_{\text{occ}}$ is even. Because of time reversal, at $\Gamma, X, Y, \text{ and } M$ points, rotation eigenvalues $\zeta, \xi, \text{ and } \omega$ appear in complex conjugate pairs, leading to Kramers degenerate bands. It then follows from Eq. 1 that $e^{i\Theta_2} = e^{i\Theta_4} = 1$. For systems with $C_6$ symmetry, at $K$ point, the allowed $C_3$ eigenvalues are $e^{in/3}, e^{-in/3}$, or $-1$. The first two appear in complex conjugate pairs due to the composite symmetry $C_2T$. The number of the remaining bands with $C_3$ eigenvalue $\Theta = 0$ must also be even, as the total number of occupied bands is even. This implies $e^{i\Theta_6} = 1$. To summarize, we find

\[
\Theta_{2,4,6} = 0 \mod 2\pi
\]

Equation 2 implies that within each contour, there must be an even number of Dirac cones. In other words, all configurations in Fig. 1 are anomalous because they all have one Dirac cone enclosed by the contour. These states can only be realized on the surface of TCIs, to which we turn our attention below.

**New classes of TCIs**

A defining property of TCIs is the presence of topological surface states protected by crystal symmetries. The 230 space groups describing all possible crystal symmetries allow for many different classes of TCIs. One class of TCI protected by reflection symmetry was found in IV-VI semiconductors SnTe and Pb$_{1–x}$Sn$_x$(Se,Te) ($18–22$). Recently, another class of TCI protected jointly by glide reflection and time-reversal symmetry was predicted in KHgSb ($23$), and the experimental signature of its “hourglass” surface states has been reported ($24$). In addition, several other classes of TCIs have been theorized ($9, 10, 23, 25–30$). Here, we predict a new class of TCIs protected jointly by $n$-fold rotation ($n = 2, 4, \text{ and } 6$) and time-reversal symmetry (with $T^2 = -1$). These TCIs exhibit topological surface states consisting of $n$ massless Dirac cones as shown in Fig. 1 on the top and bottom surfaces.

![Fig. 1. The schematics of the gapless states in two dimensions that have rotation and time-reversal symmetries. There are (A) two, (B) four, and (C) six Dirac cones, related to each other by two-, four-, and sixfold rotation symmetries, respectively, in the first Brillouin zone. The contours are the boundaries of the invariant Brillouin zones, along which the Berry phase is quantized to either zero or $\pi$.](http://advances.sciencemag.org/)
Topology in momentum space

Our new TCIs can be constructed by “adding” two time-reversal invariant strong TIs (denoted by a flavor index \( \tau_z = \pm 1 \)), each with \( n \)-fold rotational symmetry. By addition, we take the occupied bands of the desired TCI to consist of valence bands of both TIs. Each TI has a single flavor of Dirac fermion on the surface, and without loss of generality, the two Dirac cones are both centered at the center of the surface Brillouin zone. By considering the symmetry-allowed hybridization between the surface Dirac fermions of the two TIs, we obtain the desired surface states of TCIs as shown in Fig. 1.

We explicitly show how this construction works for \( n = 2 \) and summarize the results for \( n = 4 \) and 6 while leaving details to the Supplementary Materials. With twofold rotation and time-reversal symmetry, the surface state Hamiltonian of a strong TI can be written in the following general form

\[
h_\pm(k) = k_x \sigma_x \pm k_y \sigma_y \tag{3}\]

where \( \sigma_x, \sigma_y, \sigma_z \) are the Pauli matrices and they act on the spin space. Here, we have chosen a basis for the Kramers doublet at \( k = 0 \) such that the twofold rotation and the time-reversal symmetry are represented by \( C_2 = i \sigma_x \) and \( T = i \sigma_y K \). When these symmetries are present, the Hamiltonian \( h_+ \) and \( h_- \) cannot be deformed into each other, describing two types of surface states. The Dirac fermions described by \( h_+ \) and \( h_- \) have vortex-like spin textures in momentum space, with left- and right-handed chirality, respectively (see Fig. 2). \( h_+ \) has an emergent rotation invariance that includes twofold rotation as a subgroup, whereas \( h_- \) does not. To be precise, for \( h_+(k) \), one can define a continuous rotation operator \( U_+(\theta) = \exp(i\sigma_\theta\theta/2) \) such that (i) it commutes with time-reversal operator, (ii) \( R(\pi) = C_2 \), and (iii) \( R(2\pi) = -1 \) for \( \frac{1}{2} \)-spin. This means that the \( C_2 \) rotation symmetry in \( h_+(k) \) can be promoted to an \( O(2) \) rotation symmetry. On the other hand, for \( h_- \), one can define a rotation operator \( U_-(\theta) = \exp(-i\sigma_\theta\theta/2) \), which satisfies (i) and (iii), but \( U_-(\pi) \neq C_2 \). Therefore \( h_- \) does not have continuous rotation symmetry. Here, the reason we require that \( C_2 = i \sigma_x \) is that, otherwise if \( C_2 = -i \sigma_x \), a unitary transform \( U = i \sigma_x \) on the second block sends \( h_- \) to \( h_+ \) and, at the same time, \(-i \sigma_z \) to \(+i \sigma_z \), such that the two blocks are identical, having the same \( h_+ \) and the same choice of \( C_2 \). The presence and the absence of continuous rotation symmetry can be explicitly seen by looking at the pseudospin vector pattern on some equal energy contours of \( h_+ \) and \( h_- \), respectively: The pattern in Fig. 2A is invariant under arbitrary rotation, and the one in Fig. 2B is not, but only invariant under a \( \pi \)-rotation.

The addition of \( h_+(k) \) and \( h_-(k) \) in our construction gives rise to two flavors of Dirac fermions on the surface, described by the Hamiltonian

\[
H(k) = h_+(k) \oplus h_-(k) = k_x \tau_0 \sigma_x + k_y \tau_y \sigma_y \tag{4}
\]

where \( \tau_i \)'s are Pauli matrices acting in the flavor space. One can check that no mass term preserving \( C_2 \) and \( T \) symmetry can be added to gap the spectrum of \( H(k) \) (here and below, we define “mass” terms as momentum-independent terms in the Hamiltonian that gaps out the entire energy spectrum). The only \( T \)-invariant mass term is proportional to \( \tau_3 \sigma_z \), which breaks \( C_2 \). Symmetry-preserving terms, on the other hand, can only split the two Dirac cones sitting on top of each other at \( k = 0 \) to a pair of Dirac cones centered at opposite momenta, which is precisely the desired TCI surface state shown in Fig. 1A. For example, if one adds \( m \tau_3 \sigma_z \) into \( H(k) \), one finds that (i) it commutes with \( k_x \tau_0 \sigma_x \) and hence cannot open a full gap and (ii) it splits the two Dirac points along the \( k_x \) axis by a separation proportional to \( |m| \). This shows that TCIs protected by \( C_2 \) and \( T \) symmetry can be realized by adding two TIs whose surface-state spin textures have opposite chirality.

In contrast, adding two surface states with the same helicity leads to a surface spectrum that can be gapped by a symmetry-preserving mass term \( \tau_3 \sigma_z \). From these considerations, we conclude that band insulators with twofold rotation and time-reversal symmetry are classified by \( \mathbb{Z}_2 \times \mathbb{Z}_2 \) topological invariant [this is consistent with the classification in (31) using K-theory]. The generator of each \( \mathbb{Z}_2 \) group corresponds to a TI whose surface states have left- and right-handed chiral spin textures. For the TCI surface states shown in Fig. 1A, this topological index takes the value (11).

In Table 1, we summarize how to construct the TCI surface states with 2-, 4-, and 6-fold symmetry by adding two TIs. The proof of these results is found in the Supplementary Materials.

Topology in real space

Having established the TCI surface state band structure, in this subsection, we provide an alternative understanding of their topological nature from the perspective of real space, following the approach introduced in (32, 33). The essence of this real-space approach is to add symmetry-allowed perturbations to break translational symmetry and gap the massless Dirac fermions on the surface as much as possible and study what could be left. This reduction gives a “theoretical minimum” realization of the nontrivial TCI surface states and enables us to demonstrate their robustness under electron interactions. Throughout this section, we assume that the bulk state is described by the double-TI model in the previous section, and the surface-state Hamiltonian is the direct sum of \( h_+ \) and \( h_- \) for \( C_2 \) and similarly for the case of \( C_{4,6} \) (see Table 1). We emphasize that the double-TI Hamiltonian represents a rotation-TCI phase, the Hamiltonian of which may be deformed to this model without breaking rotation symmetry, time-reversal symmetry, or closing the gap. Note that specific materials in the rotation-TCI phase may have Hamiltonians different from, and presumably more complicated than, the double-TI model. However, since they have surface states on the top surface that are topologically equivalent to those shown in Fig. 1, by merit of bulk-edge correspondence, we know that they belong to the same topological phase.
We start from considering a double-TI model of a C$_2$-TCI placed in a cylinder, the size of which is much greater than the correlation length and the surface of which is smooth at atomic scale (the argument for C$_{4,6}$-TCI proceeds similarly). Naturally, each surface—top, bottom, or side—has two Dirac cones from the two TIs. On the top surface, as we have argued, because of the presence of rotation symmetry, a mass term is disallowed, but on the side surface, where rotation symmetry is broken, the mass term may be added. The mass term is allowed to be slowly varying with respect to the scale of correlation length so that the massive Dirac Hamiltonian on the side surface becomes

$$H = h_z \oplus h_\tau + \int d\mathbf{r} \, m(\mathbf{r}) \psi^\dagger \tau_z \sigma_z \psi$$

(5)

Since $\tau_z \sigma_z$ anticommutes with $h_z \oplus h_\tau$, the energy spectrum has a local gap as long as $m(\mathbf{r}) \neq 0$. However, since $C_2 = i\sigma_z$ also anticommutes with $\tau_z \sigma_z$, for the whole system to have twofold rotation symmetry, that is, $[C_2, H] = 0$, it is required that

$$m(\mathbf{r}) = -m(C_2 \mathbf{r})$$

(6)

Equation 6 necessitates the presence of domain walls on the side surface where $m(\mathbf{r})$ changes signs. Consider a circumference of the cylinder at any height; then, along this circumference, $m(\mathbf{r})$ must change sign twice, leaving two points far from each other, related by $C_2$, locally gapless, and since the same holds true for any circumference, these gapless points form two gapless domain walls connecting the top and the bottom surfaces, related to each other under $C_2$. A domain wall between gapped double-Dirac cones hosts one pair of helical edge modes (18), and the overall surface states of the cylinder consist of 2D gapless modes on the top and the bottom and two helical edge modes on the side surface, shown in Fig. 3A. For C$_{4,6}$-TCI placed on a cylinder, the surface states are shown in Fig. 3 (B and C) [also see (16) for the discussion of $C_6$ case in detail]. We note that the locations of these modes are not pinned to any physical hinges or intersections of crystalline surfaces like in (34–37). Note that while the cylindrical shape may have continuous rotation symmetry, the system described by the Hamiltonian $h_z \oplus h_\tau$ necessarily breaks it down to discrete rotation symmetry, consistent with the existence of the two 1D gapless lines even on a perfectly atomic-scale smooth cylinder.

In real materials, samples as grown do not take the shape of the cylinder, and the side surface usually contains several flat planes with different Miller indices. For example, a sample grown along the [001] direction naturally has (100) and (010) for the side surfaces. In that case, we comment that each one of the side surface may be fully gapped individually because of the broken rotation symmetry, but as long as the overall twofold rotation symmetry of the crystallite is preserved, the mass terms on two opposite sides related by $C_2$ must have opposite sides. Therefore, there must be domain walls along the hinges

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### Table 1. Superposition of the surface Hamiltonians of two TIs that have two-, four-, and sixfold rotation symmetries and time-reversal symmetry represented by $i\sigma_r K$.

| Rotation symmetry | #1 irreducible representation | #2 irreducible representation | Surface Hamiltonian | Trivial/Nontrivial |
|-------------------|-------------------------------|-------------------------------|---------------------|-------------------|
| C$_2$             | $i\sigma_z$                  | $i\sigma_z$                  | $h_z \oplus h_\tau \oplus h_\tau$ | Trivial          |
|                   | $i\sigma_z$                  | $i\sigma_z$                  | $h_z \oplus h_\tau$    | Nontrivial        |
| C$_4$             | $\pm \exp (i\pi/4)$          | $\pm \exp (i\pi/4)$          | $h_z \oplus h_\tau$    | Trivial          |
|                   | $\exp (i\pi/4)$              | $-\exp (i\pi/4)$             | $h_z \oplus h_\tau$    | Nontrivial        |
| C$_6$             | $\pm \exp (i\pi/6)$          | $\pm \exp (i\pi/6)$          | $h_z \oplus h_\tau$    | Trivial          |
|                   | $\exp (i\pi/6)$              | $-\exp (i\pi/6)$             | $h_z \oplus h_\tau$    | Nontrivial        |
|                   | $\pm \exp (i\pi/6)$          | $\pm \exp (i\pi/6)$          | $h_z \oplus h_\tau$    | Trivial          |
|                   | $\exp (i\pi/6)$              | $-\exp (i\pi/6)$             | $h_z \oplus h_\tau$    | Nontrivial        |

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**Fig. 3. Surface states of rotation TCI.** Schematics of surface states on the top and the bottom surfaces and the edge states on the otherwise gapped side surfaces of the new TCI protected by (A) twofold, (B) fourfold, and (C) sixfold rotation symmetries in rod geometry. The top and the bottom surfaces have Dirac cones shown in Fig. 1 (A to C), and on the side surface, two, four, and six helical edge modes connect the two surfaces; they can have arbitrary shape and position but are related to each other by two-, four-, and sixfold rotations, respectively.
between surfaces that have opposite masses. In that geometry, we expect vertical helical edge modes along at least two hinges on the side surface that connect the top and the bottom surfaces (18).

The existence of the 1D edge modes hints us to write down the bulk $Z_2$ topological invariants following (16), and the details are given in the Supplementary Materials. In the Supplementary Materials, we additionally discuss, as contrast, a related TCI protected by inversion and time reversal (38, 39), where surface states do not exist but a single helical edge mode exists on the surface.

We also note that many topological crystalline states can be understood from a dimensional reduction perspective (32, 40–42), where the 3D state can be considered a set of decoupled layers of 2D topological states. From this perspective, all three types of new TCIs here can also be constructed from 2D TIs. This construction helps extend our theory to include strongly interacting symmetry-protected topological states protected by rotation symmetry and any local symmetry, including, but not limited to, time reversal. The discussion is found in the Supplementary Materials.

**DISCUSSION**

Last, we predict material realizations of TCIs that harbor anomalous surface states in Fig. 1 (A and B), consisting of two and four Dirac cones protected by twofold and fourfold rotation, respectively. These two types of surface states appear in the SnTe class of TCIs, on the (110)-surface and the (001)-surface, respectively. On the (110)-surface, there are two Dirac cones located along $\bar{\Gamma}Z$ in the surface Brillouin zone, which are protected by mirror symmetry (43), but now, we know that even when mirror symmetry is broken (via external strain field, for example), as long as $C_2$ and $T$ are preserved, this surface state is still anomalous and cannot be gapped. Similarly, the four Dirac cones on the (001)-surface are protected by mirror symmetry (18), and we now emphasize that they are stable against all $C_{1v}$- and $T$-preserving perturbations because of the $C_4$-rotation anomaly. When mirror symmetries are broken, the Dirac points are free to move away from the high-symmetry lines to generic momenta on the (110)- and (001)-surfaces, as shown in Fig. 1 (A and B, respectively).

Another line of thinking starts from band inversion in the bulk and from the observation that the new state can be constructed by adding the band structure of two TIs. In the case of $C_4$, it requires that the two surface Dirac points from the two TIs belong to different irreducible representation of $C_4$. In the bulk, this means that two valence bands and two conduction bands have band inversions and that the two valence bands (as well as conduction bands) belong to different irreducible representations of $C_4$. One possible way of realization is through the inversion of two $\Gamma_8$ bands that have opposite parity. $\Gamma_8$ is a 4D irreducible representation, consisting of two Kramers’ doublets with total angular momentum $j_z = \pm 1/2\hbar$ and $j_z = \pm 3/2\hbar$, respectively. Under $C_4$, the two doublets transform differently as $\exp (i\sigma_z\pi/4)$ and $\exp (i\sigma_z\pi/4)$. Band inversion between two $\Gamma_8$ bands having opposite parity has been predicted in antiperovskite material $\text{Sr}_3\text{PbO}_3$ (44). On the (001)-surface of $\text{Sr}_3\text{PbO}_3$, according to our theory, there will be four Dirac cones as shown in Fig. 1B.

On the side surface, the localized 1D helical edge modes require the absence of gapless surface modes, but in all the above examples, the additional mirror symmetries of the lattice make low-index surfaces such as (100) and (210) gapless. To see the helical edge modes on the side, one has to either (i) break mirror symmetries by external perturbation such as strain or (ii) look at a sample where the side surface consists of a high-index plane [e.g., (221)-surface] and its $C_4$ equivalents.

1D helical modes are well known to be free from back-scattering due to time-reversal symmetry, and here, the back-scattering between two helical modes is also suppressed by the spatial separation between the lines. This unique property allows the design of a helical nanorod made from these new materials, a nanorod symmetrically fabricated along the rotation axis. A helical nanorod has exactly $n$-channels of ballistic transport, independent of its radius, each contributing $e^2/h$ to the longitudinal conductance. One should note that, here, each helical mode itself only requires time-reversal symmetry for protection, and the role of rotation symmetry is to make sure that the $n$ helical modes do not cross each other in real space and gap out. Therefore, as long as the rotation symmetry is not considerably broken, these helical edge modes would remain stable, but no longer related to each other by a rotation.

**MATERIALS AND METHODS**

Anomalous surface states protected by $C_{4v}$-symmetry and time reversal

We show how the anomalous surface states in Fig. 1 (B and C) can be constructed from two Dirac cones from $\Gamma_8$, belonging to two different representations of $C_4$ and $C_6$, respectively. First, look at the case of $C_4$. In the presence of time reversal and the absence of SU(2) spin rotation symmetry, the symmetry group is then generated by $C_4$ and $T$, satisfying $C_4 = -1$, $T = -1$ and $[C_4, T] = 0$. These conditions give two distinct irreducible representations

$$C_{4\pm} = \pm e^{i\sigma_z\pi/2}$$

For the $T$ case, we have

$$T = i\sigma_y K$$

Considering putting these two representations together, one has a reducible 4D representation

$$C_4 = \tau_z e^{i\sigma_z\pi/2}$$

$$T = i\tau_z\sigma_y K$$

The minimal 2D theory compatible with this symmetry group is

$$h(k_x,k_y) = k \cos \theta \tau_z \sigma_x + k \sin \theta \tau_z \sigma_y$$

where $(k, \theta)$ are the polar coordinates of $k$. The only time-reversal invariant mass term is proportional to $\tau_z\sigma_x$, but this matrix anti-commutes with $C_4$. Therefore, the theory cannot be symmetrically gapped. We can add symmetry-allowed terms

$$\delta h(k_x,k_y) = m_1 \tau_z \sigma_0 + m_2 k^2 \tau_z \sin [2(\theta - \alpha)] \sigma_0$$

where $\alpha$ is some arbitrary number. The dispersion is gapless at $k = |m_1|$ and $\theta = \alpha , \alpha + \pi/2, \alpha + \pi$, and $\alpha + 3\pi/2$, that is, four points as shown in Fig. 1B.

Then, we look at the case of $C_6$ and $T$, satisfying $C_6^4 = T^2 = -1$ and $[C_6, T] = 0$. There are three distinct irreducible representations of this symmetry group.
\[ C_0 = \pm e^{i\alpha \pi/6}, i\sigma_z \]  
(13)

\[ T = i\sigma_y K \]  
(14)

For \( C_0 = e^{i\alpha \pi/6} \), the minimal Dirac theory is

\[ h_1(k,\theta) = k \cos \theta s_x + k \sin \theta s_y \]  
(15)

and for \( C_0 = -e^{i\alpha \pi/6} \), the minimal theory is the same

\[ h_2(k,\theta) = h_1(k,\theta) \]  
(16)

For \( C_0 = i\sigma_z \), the minimal theory is

\[ h_{3\pm} = k^3 \cos 3\theta s_x \pm k^3 \sin 3\theta s_y \]  
(17)

Now, we consider superimposing two of the four different theories and ask whether the resultant theory can be symmetrically gapped. We first consider the superposition of \( h_1 \) and \( h_{3+} \)

\[ H_{1,3+} \equiv h_1 \oplus h_{3+} \]  
(18)

We can add the following terms

\[ \delta H_{1,3+} = m_1 \tau_0 s_0 + km_2 (\cos \theta \tau_x s_z + \sin \theta \tau_y) \]  
(19)

and the dispersion becomes fully gapped and also \( \theta \) independent

\[ E(k) = \pm \sqrt{(k \pm m_1)^2 + m_2^2 k^2} \]  
(20)

Similarly, we find that \( H_{1,3-} \equiv h_1 \oplus h_{3-} \) and \( H_{2,3\pm} \equiv h_2 \oplus h_{3\pm} \) can also be symmetrically gapped. Now, we focus on \( H_{1,2} \equiv h_1 \oplus h_2 \) and add the following terms

\[ \delta H_{1,2} = m_1 \tau_0 s_0 + m_2 k^3 \sin 3(\theta - \alpha) \tau_x s_z \]  
(21)

to obtain the dispersion

\[ E_{1,2}(k,\theta) = \pm \sqrt{\left(k^2 + m_1^2 + m_2^2 k^6 \right) \sin^2 \left[3(\theta - \alpha)\right]} \]  
(22)

The dispersion has six Dirac points at \( k = |m_1| \) and \( \theta = m\pi/3 + \alpha \) for \( m = 0, 1, 2, 3, 4, \) and 5, arranged in a configuration shown in Fig. 1C. Last, we study the case

\[ H_{3+,3-}(k,\theta) \equiv k^3 \cos 3\theta \tau_0 s_x + k^3 \sin 3\theta \tau_0 s_y \]  
(23)

and we add terms

\[ \delta H_{3+,3-}(k,\theta) = m_1 \tau_0 s_0 + m_2 \sin (3(\theta - \alpha)) \tau_x s_z \]  
(24)

There are six Dirac points at the same positions as in the case of \( H_{1,2} \). To summarize, for the \( C_0 \)-case, the anomalous configuration of Dirac cones shown in Fig. 1C can be realized by superimposing two combinations of two Dirac theories: (i) \( h_1 \) and \( h_2 \) and (ii) \( h_{3+} \) and \( h_{3-} \), while all other combinations can be gapped by symmetric perturbations.

**Proof of Eq. 1**

Here, we explicitly prove the first equation in Eq. 1. For the other two equations, the readers are referred to (17).

The Berry phase associated with the loop in Fig. 1A is defined as the determinant of the parallel transport operator of the occupied bands along the loop

\[ e^{i\theta_2} = \det \left[ U_{X\rightarrow Y\rightarrow Z\rightarrow X} U_{M\rightarrow M'} U_{M'\rightarrow M} \right] \]  
(25)

\[ = \det \left[ U_{X\rightarrow Y\rightarrow Z} \right] \det \left[ U_{M\rightarrow M'} \right] \det \left[ U_{M'\rightarrow M} \right] \]  
(26)

where \( \Gamma = (0,0), X = (\pi,0), Y = (0, \pi), M = (\pi, \pi), \) and \( M' = (-\pi, \pi) \). One should keep in mind, however, that we picked a gauge such that the Hamiltonian is periodic on the torus, such that \( H(X) = H(-X) \) and \( H(M) = H(M') \). Therefore, we have

\[ \det[U_{X\rightarrow M}] \det[U_{M\rightarrow X}] = \det[U_{X\rightarrow M}] = 1 \]  
(27)

Then, we use \( C_2 \)-rotation symmetry and find

\[ U_{X\rightarrow Y} = C_2^{-1}(X)U_{X\rightarrow Y}C_2(X) \]  
(28)

Plugging in Eqs. 26 to 28 into Eq. 25, we obtain

\[ e^{i\theta_2} = \det[C_2^{-1}(X)C_2(X)^{-1}C_2^{-1}(M)C_2(Y)] = \prod_{n\in occ.} \zeta_n(\Gamma) \zeta_n(\Gamma)^{-1} \zeta_n(Y) \zeta_n(Y)^{-1} \zeta_n(\text{occ}) \]  
(29)

Last, we use \( \zeta^2 = -1 \) to arrive at the result in the first equation in Eq. 1.

**SUPPLEMENTARY MATERIALS**

Supplementary material for this article is available at http://advances.sciencemag.org/cgi/content/full/5/12/eaat2374/DC1

Fig. S1. The definition of Wyckoff positions in simple rectangular, square, and triangular lattices and the nontrivial flows of Wannier centers as \( k \) changes from 0 to \( \pi \).

Fig. S2. Real-space constructions for TCIs protected by \( C_4 \)-rotation and time-reversal symmetries.

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