First Principles Calculations for Topological Quantum Materials

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**ABSTRACT**

Discoveries of topological states and topological materials reshape our understanding of physics and materials in the last one and half decades. First-principles calculations have been playing a significant role in bridging the topology theory and experiments by predicting realistic topological materials. In this article, we overview the first-principles methodology on topological quantum materials and provide a beginner’s guide. First, we unify different concepts of topological states in the same band inversion scenario. Then, we discuss the topology using first-principles band structures and newly-established topological materials databases. We stress challenges in characterizing the symmetry-independent Weyl semimetals and calculating the topological surface states. We outlook the exciting transport and optical phenomena induced by the topology.

**Key points:**

- Heuristically, the simple but intuitive band inversion scenario, which is easily accessible for first-principles calculations, can unify different topological states and rationalize their topological boundary states.
- Quantitatively, topological invariants and symmetry indicators distinguish topological phases from atomic insulators.
- The general first-principles procedures to compute the bulk topology and surface states are demonstrated by representative materials.
- Challenges for topological surface states and Weyl semimetals are addressed. Tutorials are provided for all examples discussed.
- The band structure topology induces interesting anomalous transport and nonlinear optical phenomena.

**Website summary:** First-principles calculations made great success in predicting topological quantum materials. We overview the band topology theory and provide a beginner’s guide in the study of topological materials with the first-principles methods.

1 Introduction

The topological insulator (TI)\(^1\)–\(^4\) and the following topological quantum states were born in a fortunate stage when materials calculations, materials synthesis, and surface-sensitive spectroscopy techniques were readily available. The first-principles materials calculations have been playing a significant role in bridging the fundamental theory and experiments by predicting materials with required topological properties. For example, the last decade witnessed the successful prediction of the Bi\(_2\)Se\(_3\)-family of TIs\(^5,6\), the SnTe-class topological crystalline insulators (TCIs)\(^7\) and the TaAs-family of Weyl semimetals (WSMs)\(^8,9\), stimulating the rapid development of this field. Assisted by the prediction power of first-principles calculations on weakly-interacting systems, the theory usually leads the experimental research in topological materials, which is rare in the field of condensed-matter physics.

Besides the TI, the classification of topology reveals a large family of topological phases including the TCI\(^10\), topological semimetals such as the Dirac semimetal (DSM)\(^11,12\), WSM\(^13–15\) and nodal line semimetal (NLSM)\(^16,17\), and the higher-order topological insulator (HOTI)\(^18–21\), etc. Different criteria and first-principles methods have been developed to identify the topological class from the band structure. Material databases (see TABLE I) were even built to classify tens of thousands of inorganic solids.

Guided by the topological classifications, first-principles calculations identify topological materials by computing the bulk topological invariants (e.g., the \(Z_2\) index characterized by the parity\(^22\) for TIs) and the topological surface states (TSSs). Then related materials can be synthesized and characterized usually by measuring TSSs via angle-resolved photoemission spectroscopy (ARPES)\(^23,24\) or scanning tunneling microscopy (STM)\(^25,26\). The band topology theory, first-principles calculations,
the materials preparation, and the materials measurement cooperate intimately in a back-and-forth way as the materials design. Here, first-principles calculations mainly refer to the density-functional theory (DFT)\textsuperscript{27} and DFT-derived effective models such as the localized Wannier functions.\textsuperscript{28} Studies on topological systems also push today's first-principles calculations to pay more attention to the consequences of the time-reversal symmetry (TRS) and crystalline symmetries on the band structure than before.

There are many excellent reviews on the general topological states, topological materials\textsuperscript{29–46}, and related first-principles (\textit{ab initio}) calculations\textsuperscript{47–52}. This technical review aims to overview the state-of-the-art first-principles methodology and provide a beginner's guide in the study of topological materials. First, we heuristically unify different topological states in the same band inversion scenario and then demonstrate the TSSs by the bulk-boundary correspondence. Second, we introduce the topological invariants and symmetry indicators, which distinguishes a topological state from atomic insulators. Next, we present the general first-principles procedure to extract the bulk topology and compute TSSs by representative topological materials. We address challenges in calculating and characterizing TSSs, and in identifying WSMs. The weak side of first-principles calculations is their limitation to handle strongly correlated systems. We focus on weakly interacting topological materials in the review. In addition, we provide tutorial documents for all examples in supplementary materials.

## 2 Band Inversion and Bulk-Boundary Correspondence

The band theory was a seminal success to apply quantum mechanics in solid materials. After nearly one century, it is incredible to discover qualitatively new phenomena in this field. The TI is such a case, which is characterized by the robust metallic surface states inside the bulk energy gap. The TI band structure is intuitively characterized by a band inversion\textsuperscript{3}, i.e., the order switching between the valence and conduction bands compared to an ordinary insulator. Up to our knowledge, Shockley\textsuperscript{53} first pointed out that the band inversion leads to unique states on the surface by a spinless model. The Shockley surface states represent the charge polarization, which is vulnerable to the surface potential change. Further, a band inversion leads to the gapless bulk phase in the 2D or 3D spinless model without the spin-orbital coupling (SOC). Thus, the Shockley state was debated and ignored as time passed (see REF.\textsuperscript{54} for an overview). However, in the prediction of the first experimentally realized TI, HgTe/CdTe quantum wells\textsuperscript{3}, Benervig, Huges, and Zhang proposed the band inversion as an insightful feature to realize a TI and stressed the role of SOC. In the following, we assume a 3D system with the TRS and include SOC if not specified.

\textit{TIs and the bulk-boundary correspondence.} – Suppose a normal insulator and a TI, which exhibit opposite band orders (see BOX 1a) at the center of the Brillouin zone. As smoothly moving from one material to the other, the band gap needs to be closed at the interface because the valence and conduction bands switch their orders necessarily. Therefore, the interface exhibits metallic surface states. We can naively classify all insulators into two classes, with and without the band inversion, and consider the existence of metallic states at the interface. A normal insulator is not necessarily metallic on the surface, i.e., its interface with the vacuum, if we approximate the vacuum as a normal insulator, too. In contrast, a TI is always metallic on its surfaces. Such an argument only assumes the bulk band inversion and is robust against the surface perturbations such as defects or atomic reconstructions. Therefore, the band inversion in bulk dictates the existence of metallic states, the TSSs, on the boundary, which is usually called the bulk-boundary correspondence\textsuperscript{55, 56}. The TI surface states usually form a single Dirac cone inside the bulk gap and connect the bulk valence and conduction bands. The Dirac point is protected by the TRS, which induces the Kramers degeneracy. Therefore, it is not surprising that TRS also defines the $Z_2$-type topological invariant of the bulk states. To be accurate, the band inversion refers to the order change between two bands with opposite parities\textsuperscript{72}.

\textit{TCIs and HOTIs.} – The bulk-boundary correspondence indicates that one band inversion leads to one surface Dirac cone when projecting the inverted bulk bands to the surface. If an odd number of band inversions occur, the TRS can protect the Dirac states. If an even number of band inversions exist, only the TRS is not enough to preserve them. We may need the crystal symmetries or their combined symmetry with TRS for protection, leading to the topological crystalline insulators (TCIs). Take a mirror-protected TCI for example (see BOX 1b). Double band inversions give rise to double surface Dirac cones that cross with each other. Two Dirac cones thus interact and are gapped out in generic $k$-points except two points (black dots in BOX 1a) in the mirror plane. Only the surfaces that preserve the mirror symmetry are still metallic, while surfaces without mirror symmetry are insulating. On the mirror-breaking surfaces of a TCI, we can further apply the bulk-boundary correspondence. Suppose the mirror plane crosses the hinge between two neighboring surfaces that exhibit opposite signs of surface band gaps (see FIG. 2c). Consequently, the boundary is necessarily gapless. This is an example of the mirror-protected HOTI. The bulk-boundary correspondence for TCIs and HOTIs is illustrated in BOX 1b, which is closely related to the bulk and surface symmetry. Generally, there are seven kinds of topological invariants associated with crystal symmetries, including translation, mirror, glide, rotation, screw, inversion, and $S_4$ in 230 space groups (SGs)\textsuperscript{57, 58}, resulting in the diverse TCI/HOTI phases in BOX 1b.

\textit{Topological semimetals.} – The inverted valence and conduction bands are usually degenerate at the crossing points if SOC is turned off or negligibly small. These degenerate points are called nodal points. If they form lines or rings, they are referred to
as nodal lines or nodal rings. If SOC gaps all crossing points, we obtain topological insulating phases discussed above. Even with SOC, some individual points or lines may remain degenerate. Thus, topological semimetals refer to the gapless bulk states with SOC and mainly include the DSM, WSM, and NLSM. Because of the lack of a bulk gap to isolate the valence bands, topological invariants for topological semimetals are not well defined here. However, we can still expect the existence of TSSs, because topological semimetals usually originate from the band inversion. Unlike the surface Dirac cone, their TSSs exhibit arc-like shapes connecting related nodal points/lines on the Fermi energy contour of the surface.

3 Symmetry indicators

The band inversion is a heuristic scenario to understand the bulk topology and corresponding TSSs. To identify the topological phase accurately, we need the information of the wave functions in the momentum space. Compared to the complex calculation of topological invariants, the symmetry indicator (SI) provides a convenient way to probe the band topology from the wave function symmetry. Because it only requires the information of the band representations at high-symmetry points, and the SI value can be derived based on the coefficients. We provide an example of the \(Z_2\) type indicator in SG #2, which includes both gapped trivial and nontrivial symmetry entries. The SI group is usually generated by several \(Z_2\) type indicators. For a given band structure, we can always express the \(n\) vector by a linear superposition of AI basis. If the coefficients are integral/fractional, the band structure is trivial/nontrivial, and the SI value can be derived based on the coefficients. We provide an example of the \(p2\) wallpaper group in BOX 2 to illustrate the above concepts and procedures. Since SI only relies on the band representation at high-symmetry points, there is an equivalent method to calculate SI by the Fu-Kane like formula. For instance, for the inversion symmetry (SG #2), the SI group is \(Z_2^3 \times Z_4\). Three \(Z_2\) type indicators correspond to the three weak invariants and are expressed as

\[
z_{2w; j=1,2,3} = \sum_{\mathbf{K}, \mathbf{k} \in \text{TRIM}, k_j = \pi} n_{\mathbf{K}^+} - n_{\mathbf{K}^-},
\]

where \(n_{\mathbf{K}^+}\) is the number of occupied odd/even-parity Kramer pairs at \(\mathbf{K}\). The \(Z_4\) type indicator, corresponding to the strong invariant, is expressed as

\[
z_4 = \sum_{\mathbf{K}, \mathbf{k} \in \text{TRIM}} n_{\mathbf{k}^+}^2 - n_{\mathbf{k}^-}^2.
\]

For the 230 SGs, the quantitative Fu-Kane like formula has all been derived.

Technically, some useful tools can analyze the wave functions given by DFT, output band representations, and compute SI. Based on this method, topological materials databases have been established, giving out the SI classification for known materials. For instance, SnTe (SG #225) has the SI group \(Z_8\) and the indicator is \(z_8 = 4\), suggesting a TI/TCI. Except for SG #174 and #187-190, the largest order indicator, like the \(Z_8\) type indicator in SG #225, and \(Z_4\) type in SG #2, is called the strong factor. The odd value indicates a strong TI, while the even value corresponds to a TCI. Therefore, SnTe is a TCI. To understand the nontrivial SI, it relies on the quantitative mapping from SI to topological invariants. There are seven kinds of topological invariants associated with crystal symmetries, including translation, mirror, glide, rotation, screw, inversion, and S4 (BOX 2). Their detailed relation to each SI set in 230 SGs has been established. As shown in BOX 2, the \(z_8 = 4\) in SG #225 corresponds to two possible collections of invariants, because the SI \(z_8 = 4\) alone cannot fully determine the band topology. One set has the nontrivial mirror plane (001) while the other does not. By calculating the mirror Chern number of the (001) plane, the first case can be determined. Another example is Bi with SG #166. The SI group is \(Z_4^3 \times Z_4\), and the indicator is \(z_4 = 4\), belonging to a TCI. The (002) value corresponds to two collections of invariants. By calculating the mirror Chern number of the (210) plane, the nontrivial inversion, rotation \(2^{(001)}\) and screw \(2^{(001)}\) invariant in the first set can be identified. Generally, we can probe the band topology by calculating SI and interpret it by a collection of invariants. Although such mapping is one to many, the mirror Chern number can help to select the correct collection. With the invariants, surface/hinge
states can be further predicted by the bulk-boundary correspondence and demonstrated by first-principles calculations.

The present SI theories and databases also have limitations: they usually work for nonmagnetic topological materials with even electron fillings, and fail to capture the band topology at generic momenta, especially for the WSM phase. Further, the SIs, by definition, are indicators rather than criteria for topological phases. Even if the SI is trivial, it may possess the hidden topology that cannot be discerned by band representations. Additionally, topological classifications of magnetic SGs are recently developed \[^{73-75}\text{, although the related material database is yet to be built up.}\]

### 4 Topological Insulators

Figure 1. Topological Insulators. a I The band structure of the 2D TI graphene, where the red and blue bands are inverted between $\Gamma$ and M. b I The band structure of the 3D TI Bi$_2$Se$_3$ with and without SOC. The blue/green dots are weighted by the projected $p$ orbitals of Bi/Se. c I The surface band structures from the first-principles DFT calculations and the tight-binding calculations. d I The band structure and the Wilson loop of LuBiPt, where the red and blue bands are inverted $\Gamma_8$ and $\Gamma_6$ bands. e I Schematic representation of the slab model and the surface band structures from the first-principles DFT calculations and the tight-binding calculations.

To judge a TI by the band inversion, it is useful to compare band structures with and without SOC. For the presence of SOC, the $\mathbb{Z}_2$ topological invariant can be defined based on the TRS operator $\Theta^2 = -1$ of the spinfull fermion\[^1\]. Without SOC, the TRS operator becomes $\Theta^2 = 1$ in the spinless case, and we only get either trivial insulators or semimetals/metals. For example, Bi$_2$Se$_3$ is a trivial insulator without SOC and exhibits a band inversion as turning the SOC from zero to the correct value, representing a topological phase transition from an ordinary insulator to a TI\[^5\]. In the state-of-art DFT packages, the SOC amplitude can be easily tuned by a scaling parameter (e.g., REF. 76). In addition, the strain can also be applied to examine the band inversion in calculations.

To identify a TI accurately, the parity criteria, based on the first-principles Bloch wave functions, is extensively used for insulators with the inversion symmetry. The $\mathbb{Z}_2$-type topological invariant ($\nu_0$) is calculated by the product of parity eigenvalues ($\sigma = \pm 1$) of all occupied bands at all time-reversal-invariant momenta (TRIM). The TRIM, which satisfy $K = -K + n$ ($n = 0, \pm 1$), include eight points (0/0.5, 0/0.5, 0/0.5) in the units of the reciprocal lattice vectors in the 3D Brillouin zone. $\nu_0$ can be obtained by $(-1)^{\nu_0} = \prod_{K \in \text{TRIM}} \sigma_K$. For an AI described by localized orbitals with no dispersion, the wave functions are identical at all TRIM. The corresponding parity product must be +1, representing a trivial insulator with $\nu_0 = 0$. If the band
inversion occurs once by switching the conduction and valence band at some TRIM, the parity product switches from +1 to –1, generating a TI with $\nu_0 = 1$.

The Bi$_2$Se$_3$ family of TIs is a well-known example to demonstrate the parity criteria. We note that graphene can also be recognized as a TI from the band inversion and parity. The TRIM in the 2D Brillouin zone are $\Gamma$ and $M$ points. Although it was extensively studied with the Dirac model near the $K$-point, between the $\Gamma$ and $M$ points (see FIG. 1a), we can find a clear order switching of two bands with opposite parities, also resulting in a TI. In addition, such a band inversion generates the Dirac cone at $K$.

The TSS of a TI is characterized by an odd number of Dirac cones at the surface TRIM. The TSS calculation is usually based on two schemes: first-principles DFT calculations and tight-binding calculations. The former simulates the surface with a slab model, which is compatible with the periodic boundary condition. The slab model should be thick enough to separate interactions between the top and bottom surfaces, which increases the computational cost dramatically. The latter, which usually uses Wannier function parameters extracted from DFT bulk calculations, can efficiently calculate the half-infinite surface with the iterative Green’s functions. However, the first-principles calculations can capture the surface relaxation, especially the charge redistribution, and are usually more realistic to compare with experiments. Anyhow, the surface states from different methods should provide the same topology. For instance, the surface Dirac cones from two methods are almost identical for Bi$_2$Se$_3$ (FIG. 1c) because Bi$_2$Se$_3$ exhibits the smooth van der Waals type termination with negligible reconstruction.

Materials without inversion symmetry and van der Waals layered structures are more complicated. We take the half-Heusler compound LuPtBi$^{80,81}$. As shown in Fig. 1d, Pt and Bi form a zincblende lattice, and Lu fills the center position of the zincblende cube. Thus, LuPtBi exhibits strong chemical bonds and breaks the inversion symmetry. Around the $\Gamma$ point, there is an inversion between the $\Gamma_8$ and $\Gamma_6$ bands (similar to the case of HgTe$^{8,22}$). Because $\Gamma_8$ is four-fold degenerate, the band structure is gapless (even with SOC) at the Fermi level. However, there is a direct energy gap above $\Gamma_6$, which is relevant to the band inversion. This gap enables us to use a more general method, the Wannier charge center evolution or Wilson loop$^{87–89}$, to determine the topology. The Wilson loop method traces the Wannier charge center (Berry phase) evolution of valence wave functions between TRIM.

FIG. 1d presents the Wilson loop when taking $\Gamma_6$ band and below as valance bands. From $\Gamma$ to $L$ ($k_z$ from 0 to 0.5), the Wannier centers $\theta$ with respect to the integration loop $k_1$ from 0 to 1 exhibit a nontrivial pattern, where $k_{1,2}$ are the reciprocal lattice vectors. At $\Gamma$ and $L$, the Wannier centers are doubly degenerate because of TRS. However, Wannier centers change their partners between $\Gamma$ and $L$, as a consequence of the band inversion. For a trivial insulator, the Wannier centers still recombine with their partners between TRIM (see the case in FIG. 3c(ii)). The Wilson loop also has the same topology as the dispersion of TSSs$^{84}$. Results in FIG. 1d thus dictates the existence of Dirac surface states inside the gap between $\Gamma_6$ and $\Gamma_8$.

To calculate the TSS of LuPtBi, the (111) surface is cleaved and has two possible terminations by Lu or Bi atoms. Both DFT and tight-binding calculations demonstrate the Dirac-cone-type TSSs at –0.5 eV in the inverted gap for both terminations. The tight-binding results are easier to show the topology since they ignore the trivial states. However, when comparing with experiments, first-principles results are more reliable to reveal the detailed dispersion of TSSs and other surface states$^{85}$. The example of LuPtBi thus indicates that metallic bulk materials can also exhibit the nontrivial topology, and TSSs may appear far from the charge neutral point. For instance, TSSs were recognized on the surfaces of noble metals (known as Shockley states)$^{86}$, grey arsenic$^{87}$, and in the empty states of BaBiO$_3$$^{88}$.

### 5 Topological Crystalline Insulators and Higher-Order Topological insulators

TCIs including HOTIs refer to topological phases with even band inversions protected by crystalline symmetries. The bulk topology only features topological surface/hinge states on suitable terminations. We assume the TRS in the following discussions, although some TCIs and HOTIs break TRS. The first TCI is SnTe, protected by the mirror symmetry$^7$. Driven by SOC, band inversions happen four times at four $L$ points, where the Sn-$p$ and Te-$p$ states are inverted, as shown in FIG. 2a. The (110) and each equivalent mirror plane host two $L$ points and the double band inversion inside gives the nontrivial mirror Chern number $C_m = 2$. $C_m$ is defined as $C_m = (C_{\pm i} - C_{-i})/2$, where $C_{\pm i}$ is the Chern number of the mirror eigenstate with eigenvalue $\pm i$. The mirror protection can be intuitively interpreted as two copies of Chern insulators in the $\pm i$ subspace of the mirror, whose surface states can never be hybridized. Furthermore, $C_m = 2$ means two pairs of helical edge states on the boundary of {110} mirror planes. In contrast, {001} mirror planes are trivial with $C_m = 0$, since there is no band inversion inside.

The Wilson loop can demonstrate the nontrivial mirror plane. For the (110) mirror, [001] direction is chosen as the integration loop, and the Wilson loop evolves along [110]. Results in FIG. 2b show two pairs of connected Wilson loop flows. Since $\pm i$ eigenstates are related by TRS, the Wilson loop for only one mirror eigenstate corresponds to two connected upwards/downwards flows with the Chern number $\pm 2$. Therefore, it gives $C_m = 2$. In the language of SIs, SnTe has the indicator $z_8 = 4$, which is mapped into the first collection of invariants in BOX 2. It also gives $C_m = 2$ for {110} mirror planes and other compatible invariants associated with the rotation and screw symmetry.
Figure 2. Topological Crystalline Insulators and Higher-Order Topological Insulators. a | The SnTe crystal structure and the bulk/surface Brillouin zone. The band structure of SnTe is presented on the right, where the blue and green dots are weighted by the projected $p$ orbitals of Sn and Te. b | The Wilson loop of (110) and (110) mirror planes and the corresponding (001) and (111) surface states. Schematic representation of surface Dirac cones is shown in the inset. c | Schematic representation of hinge states for the mirror TCI and [001] hinge states for the strained SnTe. d | The Bi crystal structure and the bulk/surface Brillouin zone. The $C_2$ rotation is along the [100] direction, i.e., the $a$-axis in the hexagonal plane. The mirror plane is normal to the $C_2$ rotation and denoted as $\bar{1}210$ in the hexagonal coordinates. For the $\bar{1}210$ surface, it respects the $C_2$ rotation but breaks the mirror. The corresponding bulk band structure of Bi is presented on the right. e | The bulk Wilson loop and the $\bar{1}210$ surface states. Schematic representation of surface Dirac cones is shown in the inset. f | The $C_2$ hinge states along the [100] direction.

With the bulk topology, the TSS on suitable terminations can be expected. For the (001) surface, it is normal to (110) and (110) mirror planes, which are projected into $\bar{\Gamma}$-$X_1$ and $\bar{\Gamma}$-$X_2$ in the surface Brillouin zone, as shown in FIG. 2a. For the (110) mirror, two L points ($L_2$ and $L_3$) inside are projected into same $X_1$ point. Thus, two surface Dirac cones interact with each other and only remain gapless along the (110) mirror projected line. Such surface topology is reflected in the (110) Wilson loop: the [001] integration loop corresponds to the (001) surface termination and the dispersion along $[110]$ (i.e., $\bar{\Gamma}$-$X_1$-$\bar{\Gamma}$ in the surface Brillouin Zone) shares the similar topology with the TSS. Overall, the (001) surface hosts four Dirac cones on the four equivalent $\bar{\Gamma}$-$X$ lines. Since Dirac cones are related by $C_4$, this scenario further satisfies the nontrivial [001] $C_4$ rotation invariant. Generally, the surface states of each invariant are compatible with each other. Similarly, for the (111) surface, it is normal to three mirror planes (110), (101) and (011), which are projected into three equivalent $\bar{\Gamma}$-$M$ lines. For each mirror plane, two L points inside are projected into $\bar{\Gamma}$ and $\bar{M}$ (FIG. 2a). Therefore, the scenario for the (111) surface is four Dirac cones sitting at one $\bar{\Gamma}$ and three $\bar{M}$ points, respectively. This is consistent with the bulk (110) Wilson loop. If the integration loop is along [111] and the acquired Berry phase disperses in the [112] direction (i.e., $\bar{\Gamma}$-$\bar{M}$-$\bar{\Gamma}$ line in the surface Brillouin Zone), the Wilson loop can correspond to the (111) TSSs (FIG. 2b).

If the nontrivial mirror plane is not normal to side surfaces but passes through the hinge, surface states are all gapped out. However, helical hinge states arise in the mirror-projected lines, as shown in FIG. 2c. This type of TCI belongs to the HOTI phase. To realize the scenario, we choose the [001] as the hinge direction and (100) and (010) as side surfaces. By using the tight-binding model with the uniaxial [110] strain, as suggested in REF. 21, side surfaces are gapped out while two
nontrivial mirror planes (110) and \((\overline{1}10)\) survive, passing through two hinges. The Green’s function method is applied, and the system is considered as finite in the [100] direction, half-infinite in the [010] direction while periodic in the [001] direction (the hinge direction). Two hinge states can be observed in FIG. 2c, protected by (110) and \((\overline{1}10)\) mirror planes. It also satisfies the relation \(C_m = 2n\) for the mirror protected hinge with TRS, where \(n\) is the number of Kramers pairs of hinge states and \(C_m\) is the corresponding mirror Chern number\(^{21}\).

Another TCI/HOTI example is the element Bi\(^{89,90}\). To reveal the band inversions, the parity eigenvalues at the TRIM points are shown in FIG. 2d. At \(\Gamma\), all parity eigenvalues are “+” for the top three valence bands. In contrast, all other TRIM \((F, L, T)\) have two “-” and one “+”. Thus, Bi has double band inversions at the \(\Gamma\) point\(^{90}\). The crystal symmetries, including the inversion and the [100] \(C_2\) rotation (along the \(a\)-axis in the hexagonal plane), define the topology of the double band inversion. Unlike mirror Chern number, topological invariants associated with rotation symmetries are difficult to calculate\(^{91,92}\). Fortunately, the SIs greatly simplify this process. As mentioned in Section 3, Bi possesses the nontrivial \(\delta_{100}, \delta_{4100}\) and \(\delta\), and we focus on the rotation invariant \(\delta_{2100}\) in the following. For the \(C_2\) protection, the double band inversion can be intuitively interpreted as two copies of TIs in the two subspaces of \(C_2\) rotation. Thus, TSSs with different rotation eigenvalues cannot be gapped out. Additionally, similar double band inversion also leads to the HOTI and related TSSs in \(\beta\)-MoTe\(_2\)\(^{68,93}\).

To identify the TSS of \(\delta_{100}\), we cleave the \((\overline{2}10)\) surface that respects the \(C_2\) rotation and search the surface Brillouin zone based on the tight-binding calculations. Two Dirac cones are found in FIG. 2e, which are located at generic \(k\)-points and related by \(C_2\). The corresponding Wilson loop shows the same topology. The \(\delta_{100}\) also dictates two helical hinge states on side surfaces, which connect double Dirac cones on top and bottom. Unlike the mirror HOTI, the \(C_2\) hinge states are unpinched and depend on the geometry of the sample\(^{90,92}\). Using the same method as that in SnTe, we calculated the hinge states in FIG. 2f, which are further compatible with the inversion invariant \(\delta_{2100}\) and the screw rotation invariant \(\delta_{2100}\). However, it is technically challenging to unambiguously address the hinge states of Bi\(^{89,94}\), because both the bulk and side surfaces do not exhibit a global band gap, as indicated in FIG. 2f.

6 Weyl Semimetals

The WSM is a 3D topological semimetal phase without requiring any symmetry protection. Instead, it needs to break either the TRS or inversion symmetry (or both) to lift the spin degeneracy. Thus, the SI method usually cannot be applied to WSMs. A WSM features the two-fold degenerate Weyl points by crossing valence and conduction bands. Weyl points exhibit \(\delta\) which are further compatible with the inversion invariant \(\delta\). Additionally, similar double band inversion also leads to the HOTI and related TSSs in \(\beta\)-MoTe\(_2\)\(^{68,93}\). The crystal symmetries, including the inversion \(\delta\) and screw rotation \(\delta\) invariance, define the topology of the double band inversion. Unlike mirror Chern number, topological invariants associated with rotation symmetries are difficult to calculate\(^{91,92}\). Fortunately, the SIs greatly simplify this process. As mentioned in Section 3, Bi possesses the nontrivial \(\delta_{100}, \delta_{4100}\) and \(\delta\), and we focus on the rotation invariant \(\delta_{2100}\) in the following. For the \(C_2\) protection, the double band inversion can be intuitively interpreted as two copies of TIs in the two subspaces of \(C_2\) rotation. Thus, TSSs with different rotation eigenvalues cannot be gapped out. Additionally, similar double band inversion also leads to the HOTI and related TSSs in \(\beta\)-MoTe\(_2\)\(^{68,93}\). The crystal symmetries, including the inversion \(\delta\) and screw rotation \(\delta\) invariance, define the topology of the double band inversion. Unlike mirror Chern number, topological invariants associated with rotation symmetries are difficult to calculate\(^{91,92}\). Fortunately, the SIs greatly simplify this process. As mentioned in Section 3, Bi possesses the nontrivial \(\delta_{100}, \delta_{4100}\) and \(\delta\), and we focus on the rotation invariant \(\delta_{2100}\) in the following. For the \(C_2\) protection, the double band inversion can be intuitively interpreted as two copies of TIs in the two subspaces of \(C_2\) rotation. Thus, TSSs with different rotation eigenvalues cannot be gapped out. Additionally, similar double band inversion also leads to the HOTI and related TSSs in \(\beta\)-MoTe\(_2\)\(^{68,93}\).
**Figure 3. Weyl Semimetals.** a) The band structure of TaP with and without SOC. The nodal rings and k-path in the Brillouin zone are presented on the top. b) Schematic representation of the nodal line structures (without SOC) and Weyl points (with SOC) in the Brillouin zone. The local band structure connecting a pair of W1 and W2 Weyl points is presented on the right. The Wilson loop of one W2 Weyl point is shown on the bottom, which is summed among all valence bands. c) The Wilson loop of the nontrivial mirror plane $M_y$ and the trivial glide mirror plane $M_{xy}$. d) The (001) surface band structure based on the first-principles DFT calculations (with the P atom termination). e) The (001) surface projected Fermi surfaces around $\bar{X}$ and $\bar{Y}$. Black dots are crossing points in d. While red and blue points are projected Weyl points with opposite chiralities. Panel d and e are adapted from REF. 95 with permission.

The $M_y$ and $M_{xy}$ planes are further projected to the surface $\bar{\Gamma} - \bar{X}$ and $\bar{\Gamma} - \bar{M}$ lines, respectively. The 2D TI of $M_y$ leads to odd pairs of helical edge states along the $\bar{\Gamma} - \bar{X}$ line. In contrast, the trivial TI of $M_{xy}$ leads to even pairs of helical edge states along the $\bar{\Gamma} - \bar{M}$. Therefore, there might be odd pairs of Fermi arcs crossing the $\bar{\Gamma} - \bar{X}$ but stopping somewhere before the $\bar{\Gamma} - \bar{M}$. Indeed, FIG. 3d shows three surface states (point 1-3) between $\bar{\Gamma}$ and $\bar{X}$ but no state between $\bar{\Gamma}$ and $\bar{M}$ at the Fermi surface. In other words, the Fermi arcs can be considered as the extended edge states of the 2D TI (TRS-preserving) or the Chern insulator (TRS-breaking), as demonstrated in BOX 3.

Since Fermi arcs connect Weyl points with opposite chiralities, we can also choose a closed loop in the surface Brillouin zone to identify the topology. If the closed loop contains the net odd chirality, there must be odd times of Fermi cuts across the loop. Otherwise, there must be even cuts. For instance, for the closed $\bar{\Gamma} - \bar{X} - \bar{M} - \bar{\Gamma}$ loop in FIG. 3e, it contains two positive W2 (projected into the same point on the (001) surface) and one negative W1, with the net chirality $-1$. Fermi cuts across this loop are calculated to be five times (point 1-5), as expected. The situation is also similar for the $\bar{\Gamma} - \bar{Y} - \bar{M} - \bar{\Gamma}$ loop. As changing the surface boundary conditions, the Fermi arcs may evolve dramatically\textsuperscript{95,101}. Despite the complexity, the surface topology can still be identified by applying the bulk-boundary correspondence.

WSMs have also attracted extensive studies in magento-transport on the extremely large magnetoresistance\textsuperscript{102} and the chiral anomaly effect\textsuperscript{103} characterized by the negative magnetoresistance\textsuperscript{104–106}. The 3D Fermi surface, especially the Weyl point distance to the Fermi energy, is essential to interpret experiments and exclude other effects like the current jetting\textsuperscript{107–109}. The Fermi surface can be directly calculated from the first-principles or related tight-binding calculations. The extreme cross-section ($A$) of the Fermi surface corresponds to the basic frequency ($F$) of the quantum oscillations in experiments, by
the Onsager’s relation $F = (\phi_0/2\pi^2)A$, where $\phi_0 = h/2e$ is the magnetic flux quantum. We can compare the angle-dependent quantum oscillations and the angle-dependent Fermi surface cross-sections, to determine the exact Fermi surface topology of WSMs.\textsuperscript{107, 110, 111}

7 Dirac Semimetals, Multifold-Degenerate Nodal Points, and Nodal Line Semimetals

DSM can be classified into band inversion-induced\textsuperscript{12, 112} and symmetry-enforced DSM.\textsuperscript{11} The first type is unified in the band inversion scenario and can be viewed as two pairs of WSM: two Weyl points with opposite chiralities overlap and form the four-fold degenerate Dirac point. To maintain the band crossing, it requires the rotation symmetry ($C_n$, $n = 3, 4, 6$) protection. Two Dirac points sit on the rotation axis, and they cannot be gapped due to different symmetry representations of inverted bands. Generally, to check the symmetry protected band crossings, we can calculate the band representations of crossing bands from first-principles. If they belong to different representations, their hybridization is forbidden. To identify the topology of DSM, we can similarly calculate the $Z_2$ number of the 2D plane ($e.g., k_z = 0/0.5$) between Dirac points, in which the band gap is inverted. On the surface, the helical edge states of the 2D TI layer evolve into a pair of Fermi arcs. Two arcs meet each other at the projected Dirac points. The DSM can also transform into other phases by symmetry breaking. If Dirac points pick up a mass term, it becomes a TI or normal insulator. If TRS/inversion symmetry is broken, it becomes a nonmagnetic/magnetic WSM. The other type of DSM is enforced by the nonsymmorphic space symmetry. Such a space group has the four-dimensional irreps of the little group at the high-symmetry momenta of the Brillouin zone boundary. The symmetry requirement pins the Dirac points there and does not necessarily feature surface states.

The symmetry-enforced Dirac points can be generalized to multifold-degenerate nodal points, where the three-, six-, and eight-fold band crossings may occur.\textsuperscript{113–115} The multi-dimensional band representations of nonsymmorphic space symmetries can admit such unconventional fermions in solids. Since they cannot be described by the Dirac or Weyl equation, the general form of the Hamiltonian is formulated in REF. \textsuperscript{115} and further indicates that some band crossings possess the higher monopole charge\textsuperscript{116, 117}.

Triple-point semimetals are another type of semimetal with multifold band crossings, but are induced by the band inversion and protected by the $C_{3v}$ symmetry.\textsuperscript{113, 118–122} Along the $C_{3v}$ rotation axis, the high-symmetry line admits one- and two-dimensional representations. When bands that belong to these two different representations are inverted, the crossing points on the rotation axis are triply degenerate and cannot be gapped out. Such a triple-point carries two monopole charges. It will split into two Weyl points with the same chirality if the rotation symmetry is slightly broken. As projecting to the surface, a pair of triple-points induces two Fermi arcs.

Besides nodal points, the nodal line structure can also occur and lead to the NLSM, which is usually the precursor of other topological phases. With the TRS and inversion symmetry but no SOC, band inversion leads to the nodal line structure in the bulk and the corresponding drumhead-like states on the surface,\textsuperscript{123} as shown in BOX 1b. The topology of NLSM can be identified by the Berry phase of a loop passing through the nodal line ($Z_2$ Berry phase NLSM) or the Wilson loop of the sphere containing the nodal line structure ($Z_2$ monopole NLSM)\textsuperscript{17, 41, 124}. Heuristically, the single band inversion induces the former nodal line structure, and the double inversion may lead to the latter one.\textsuperscript{91} For systems with mirror/glide symmetry, the mirror/glide planes can also host nodal lines if two bands with different mirror/glide eigenvalues are inverted, like the above example of TaP without SOC. However, when switching on SOC, nodal lines can only be maintained in some special conditions, where TRS, inversion, and nonsymmorphic symmetry coexist to protect it\textsuperscript{17, 125, 126}.

Compared to WSM, other topological semimetals generally require the symmetry protection or are enforced by crystal symmetries. Therefore, band crossings are located at high-symmetry points/lines/planes, and can be detected by band representations. DSM, multifold-degenerate nodal points, and NLSM are thus incorporated into the SI theory, and have been similarly identified in the topological materials databases from the symmetry perspective.\textsuperscript{64–66}

8 Topology-Induced Anomalous Transport and Nonlinear Optical Phenomena

Topological materials generally exhibit large SOC and large Berry curvature in the band structure. As demonstrated in BOX 3, we can understand the Fermi arcs of a WSM/DSM from the edge states of stacking the quantum anomalous Hall insulators or 2D TIs (quantum spin Hall insulators). It is natural to expect the anomalous Hall effect (AHE)\textsuperscript{127, 128} in magnetic topological materials and the spin Hall effect (SHE)\textsuperscript{129} in nonmagnetic topological materials.\textsuperscript{130} From the Wannier function based tight-binding Hamiltonian ($H$), the Berry curvature and the anomalous Hall conductivity ($\sigma_Y^A$) can be calculated in the
Kubo-formula scheme\textsuperscript{97},
\begin{equation}
\Omega_{ij}^{\mu}(\mathbf{k}) = 2 \sum_{m \neq n} \text{Im} \left( \langle u_{mk} | dH/dk_j | u_{mk} \rangle \langle u_{mk} | dH/dk_i | u_{mk} \rangle \right) \frac{1}{(E_m - E_n)^2}
\end{equation}
\begin{equation}
\sigma_{ij}^{\mu} = -\frac{e^2}{h} \sum_{n} \int_{BZ} \frac{d^3 \mathbf{k}}{2\pi^3} f(E_n(\mathbf{k})) \Omega_{ij}^{\mu}(\mathbf{k})
\end{equation}

where $E_n$ and $|u_{mk}\rangle$ are the energy and Bloch wave function, respectively, $i,j = x,y,z$, and $f$ is the Fermi-Dirac distribution function. Equation 1 does not involve any differentiation on the wave function and thus can be evaluated under any gauge choice. It is particularly useful for numerical calculations. Usually an infinitesimal number is included in the denominator to avoid the division by zero.

Magnetic WSMs and NLSMs indeed display strong AHE, as observed in Mn$_3$Sn and Mn$_3$Ge\textsuperscript{131–133}, Co$_3$Sn$_2$S$_2$\textsuperscript{134,135}, Co$_2$MnGa\textsuperscript{136} and Co$_2$MnAl\textsuperscript{137}. In these systems, the intrinsic, giant AHE usually dominates the anomalous transport. Thus, the first-principles calculations and experiments usually obtain quantitatively consistent results. In contrast, the calculated SHE sometimes deviates from the experimental value, possibly because of the overwhelming extrinsic contributions. The strong AHE also indicates the large anomalous thermoelectric coupling (i.e., the Nernst effect) and the thermal Hall effect. The anomalous Nernst coefficient ($\alpha_{xy}^\mu$) can be estimated from the Mott’s relation\textsuperscript{138,139},
\[ \frac{\alpha_{xy}^{\mu}}{T} \bigg|_{T \rightarrow 0} = -\frac{x^2}{3|\mu|} \frac{d\sigma_{xy}^{\mu}}{d\mu} , \]
where $\mu$ is the chemical potential. Here, $\alpha_{xy}^{\mu}$ comes from the Berry curvature on the Fermi surface, while $\sigma_{xy}^{\mu}$ corresponds to the Berry curvature summed over all the Fermi sea (Eq. 2). The thermal Hall conductivity ($\kappa_{xy}^{\mu}$) can also be estimated from the Wiedemann-Franz law\textsuperscript{140},
\[ \frac{\kappa_{xy}^{\mu}}{T} \bigg|_{T \rightarrow 0} = L_0 \sigma_{xy}^{\mu} , \]
where $L_0 = \frac{\pi^2 k_B^2}{3} (\frac{2}{3})^2$ is the Lorenz ratio.

Further, noncentrosymmetric topological materials like WSMs attracts increasing interest in the nonlinear electric and optical phenomena, for example, the nonlinear AHE in the presence of TRS\textsuperscript{141–145}, the second harmonic generation\textsuperscript{146}, the generation of dc photocurrents (shift current and injection currents) under light irradiation\textsuperscript{147–151}. Topological materials trigger revival interest in the fundamental understanding of the photocurrent based on the quantum geometric phases (e.g., the Berry curvature and quantum metric) in the band structure\textsuperscript{152–156}. In this direction, first-principles methods are being actively developed to investigate nonlinear phenomena in topological materials\textsuperscript{157–168}.

9 Summary

Table 1. Some useful methods, tools and databases for the first-principles calculations on topological quantum materials.

| Types of tools | Resources |
|----------------|-----------|
| Topological materials databases | Materiade\textsuperscript{66,70}, Topological Materials Database\textsuperscript{60,64}, Topological Materials Arsenal\textsuperscript{65} |
| Wannier function methods and tools | Wannier90\textsuperscript{169}, WannierTools\textsuperscript{170}, ZZPack\textsuperscript{171}, WannierBerri\textsuperscript{172} |
| Band representations tools | Bilbao Crystallographic Server\textsuperscript{173}, SymTopo\textsuperscript{70}, Irvsp\textsuperscript{71}, IrRep\textsuperscript{174} |
| Materials databases | ICSD\textsuperscript{175}, Springer Materials, Materials Project\textsuperscript{176} |
| Visualization tools | VESTA\textsuperscript{177}, Xcrysden\textsuperscript{178} |

The topological classification of solid materials (especially nonmagnetic materials) is to some extent established with the assistance of first-principles calculations. From the material perspective, we still search for the perfect topological materials with negligible bulk carriers, for example, the real-bulk-insulating TIs and the real-bulk-semimetallic WSMs that have all bulk Fermi pockets vanishing at the Weyl point. For new materials, the bulk topology can easily be evaluated based on the available calculations tools and databases (see TABLE 1). However, it usually deserves more effort and attention to compute measurable quantities (e.g., TSSs and bulk quantum oscillations) to predict or interpret experiments. Given that the topology refreshes our understanding of solid-state materials, there is an increasing interest in exploring the more significant consequences of topology in the transport and optical phenomena beyond measuring TSSs. To this goal, more computational methods and tools are being developed based on the first-principles band structure and wave functions.
1 Box 1

a. Band inversion, gapless boundary states, and the bulk boundary correspondence. The black curves represent the surface states, and red curves represent the hinge states. The filled black circles indicate the protected band crossings.

b. Illustration of the bulk and surface states for different topological phases.
We construct a tight-binding model with three orbitals all belong to the $C_{2v}$ with irreps A and B. For a given band structure, the representation data is written as: $\mathbf{n} = (n_1^A, n_1^B, n_2^A, n_2^B, n_3, n_4^A, n_4^B, \nu)$. $\nu$ is the number of valence bands. The element $n_i^A$ is the number of valence bands that belong to the A representation of the little group $C_{2v}$ at $\Gamma$ point.

We consider two valence bands, and the $\mathbf{n}$ vectors are written as: $\mathbf{n}_1 = (0,2,0,2,0,2,0,2,2)$ and $\mathbf{n}_2 = (0,2,0,2,0,2,1,1,2)$. The second band structure is inverted at M and the irrep changes from B to A.

### b. Diagnosing topology by symmetry indicators

The $\{BS\}$ and $\{AI\}$ have already been derived for all space groups. For the p2 group, the $\{BS\}$ and $\{AI\}$ basis is 62,69:

\[
\{BS\} = \left\{ \sum_{i=1}^{5} m_i \mathbf{b}_i : m_i \in \mathbb{Z} \right\}
\]

\[
\{AI\} = \left\{ \sum_{i=1}^{5} m_i \mathbf{a}_i : m_i \in \mathbb{Z} \right\}
\]

\[
\mathbf{b}_1 = (1,0,1,0,1,0,1,1) \quad \mathbf{a}_1 = (1,0,1,0,1,0,1,1)
\]

\[
\mathbf{b}_2 = (0,1,0,1,0,1,1,1) \quad \mathbf{a}_2 = (0,1,0,1,0,1,1,1)
\]

\[
\mathbf{b}_3 = (1,0,0,1,0,1,1,1) \quad \mathbf{a}_3 = (1,0,0,1,0,1,1,1)
\]

\[
\mathbf{b}_4 = (0,1,0,1,0,1,1,1) \quad \mathbf{a}_4 = (0,1,0,0,1,0,1,1)
\]

\[
\mathbf{b}_5 = (0,0,0,0,0,1,1,1) \quad \mathbf{a}_5 = (0,0,0,0,0,2,2,0)
\]

Therefore, the SI group is $\{BS\}/\{AI\} = \mathbb{Z}_2$. To diagnose the topology of a given band, the $\mathbf{n}$ vector is expressed as $\mathbf{n} = \sum_{i=1}^{5} q_i \mathbf{a}_i + \frac{1}{2} \mathbf{a}_5$. If $q_5$ is even, $\mathbf{n}$ belongs to $\{AI\}$. If $q_5$ is odd, it indicates the necessary topology. The odd/even choice of $q_5$ also indicates the $\mathbb{Z}_2$ valued SI group. For the two examples above, $\mathbf{n}_1 = 2\mathbf{a}_2$ and $\mathbf{n}_2 = 2\mathbf{a}_2 + \frac{\mathbf{a}_5}{2}$, corresponding to the $z_2 = 0$ and $z_2 = 1$ case. There is also an equivalent Fu-Kane like formula: $z_2 = \sum_{k=\Gamma,X,Y,M} n_k^B = 1$.

### c. From symmetry indicators to topological invariants

Symmetry indicator is determined by seven topological invariants: weak invariants $\delta_{m_i}, i = 1,2,3$, mirror Chern number $C_m$, hourglass invariant $\delta_h$, rotation invariant $\delta_r$, screw invariant $\delta_s$, inversion invariant $\delta_i$ and $S_4$ invariant $\delta_{s4}$. For rotation/screw, only $C_2$, $C_4$ and $C_5$ feature the corresponding invariants. Except the $\mathbb{Z}_n$ valued mirror Chern number, other invariants are $\mathbb{Z}_2$ valued. Corresponding surface/hinge states are shown in the below 57,58.

### d. Examples of materials

SnTe, SG#225, has the indicator group $\mathbb{Z}_8$. The SI is $z_8 = 4$, corresponding to two collections of invariants:

\[
\begin{array}{cccccccc}
\text{weak} & m^{001} & m^{110} & 2^{011} & 4^{001} & 2^{011} & 4^{001} & 4^{001} \\
000 & 0 & 2 & 1 & 1 & 1 & 1 & 1 \\
004 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

Bi, SG#166, has the indicator group $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$. The SI is (0002), corresponding to two collections of invariants:

\[
\begin{array}{ccccccc}
\text{weak} & m^{110} & 2^{100} & i & 2^{100} \\
000 & 0 & 1 & 1 & 1 \\
002 & 0 & 1 & 0 & 0 \\
\end{array}
\]

Here invariants are denoted by the corresponding symmetries, for instance: $m^{110}$ represents the mirror Chern number $C_m$ of the $\{\bar{1} \bar{1} 0\}$ mirror plane; $2^{100}$ is the rotation invariant $\delta_r$ of the $\{100\} C_2$ rotation; $i$ is the inversion invariant $\delta_i$; $2^{100}$ is the screw invariant $\delta_s$ of the $\{100\} C_2$ screw rotation.
3 Box 3

a. 2D Topological layers. Here we use the BHZ model\textsuperscript{3} to demonstrate the topology of Chern insulators and 2D TIs. For the Chern insulator with broken TRS, we adopt half of the BHZ model in only one spin subspace. The bulk Wilson loop in \textit{a} demonstrates the nontrivial $C=1$. It further dictates the chiral edge states and quantum anomalous Hall effect in \textit{b} and \textit{c}. For the 2D TI protected by TRS, the bulk Wilson loop in \textit{d} demonstrates the nontrivial $Z_2=1$. The corresponding helical edge states and quantum spin Hall effect are presented in \textit{e} and \textit{f}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig.png}
\caption{Wilson loop, Edge states, and Transport}
\end{figure}

b. 3D topological phases from the stacking of 2D topological layers. 3D topological phases can be understood from the stacking of 2D Chern insulators/TIs. The chiral/helical edge states of 2D layers form the surface states. Without the interlayer coupling, it belongs to a 3D Chern insulator/weak TI. Surface states appear on side surfaces, with no dispersion along $k_z$. With the increasing interlayer coupling, the $k_z$ dispersion is enhanced, and the fully inverted band gap starts to close. Depending on the crystal symmetries and dispersion strength, 3D topological states such as the weak TI, strong TI, WSM, and DSM can emerge in this process\textsuperscript{179, 180}. This layer construction scheme can also lead to the TCI and HOTI\textsuperscript{57, 181}. For example, the monolayer of MoTe\textsubscript{2} is a 2D TI\textsuperscript{182} and the corresponding 3D material forms a WSM in the noncentrosymmetric phase ($T_d$)\textsuperscript{183, 184} and a HOTI in the centrosymmetric phase\textsuperscript{68, 93}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig.png}
\caption{3D topological phases from the stacking of 2D topological layers}
\end{figure}
Acknowledgements

B.Y. acknowledges the financial support by the Willner Family Leadership Institute for the Weizmann Institute of Science, the Benoziyo Endowment Fund for the Advancement of Science, Ruth and Herman Albert Scholars Program for New Scientists and the European Research Council (ERC) (ERC Consolidator Grant No. 815869, “NonlinearTopo”).

Competing interests

The authors declare no competing interests.

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