Topological crystalline Kondo insulators and universal topological surface states of SmB$_6$

Mengxing Ye, J. W. Allen, and Kai Sun
Department of Physics, University of Michigan, Ann Arbor, MI 48109, USA
(Dated: May 11, 2014)

We prove theoretically that certain strongly correlated Kondo insulators are topological crystalline insulators with nontrivial topology protected by crystal symmetries. In particular, we find that SmB$_6$ is such a material. In addition to a nontrivial $Z_2$ topological index protected by time reversal symmetry, SmB$_6$ also has nontrivial mirror Chern numbers protected by mirror symmetries. On the (100) surface of SmB$_6$, the nontrivial mirror Chern numbers do not generate additional surface states beyond those predicted by the $Z_2$ topological index. However, on the (110) surface, two more surface Dirac points are predicted. Remarkably, we find that for SmB$_6$ both the $Z_2$ topological index and the mirror Chern numbers are independent of microscopic details, which enables us to obtain surface state properties that are universal.

Introduction— In many strongly correlated heavy fermion or mixed valent insulators, hybridization between bands with opposite parities plays a very important role in the formation of the insulating gap. It has been shown that this mechanism can result in strongly correlated time-reversal-invariant topological insulators (i.e. topological Kondo insulators). Several candidate materials have been predicted theoretically including SmB$_6$ and CeNiSn$_2$, CeOs$_4$As$_{12}$ and CeOs$_4$Sb$_{12}$, and SmS under pressure.

Strong supporting evidence has been obtained in recent experimental studies of SmB$_6$. Transport data reveals that this material has an insulating bulk with a very robust metallic surface. Quantum oscillations find Fermi surfaces and Dirac points on the (100) and (110) surfaces, indicating that the metallic surface states are not due to trivial mechanisms such as band bending. Fermi pockets on the (100) surface have also been observed in angle-resolved photoemission spectroscopy (ARPES) and the locations of these pockets follow exactly the prediction of the topological theory and band structure calculations. Disorder effects have also been investigated. While transport properties show little response to nonmagnetic impurities, magnetic impurities greatly suppress the surface conductivity, consistent with the topological theory. Weak-antilocalization has also been reported in the study of magnetoconductance.

Despite their strong coupling nature, the low-energy physics of mixed valent materials (e.g. SmB$_6$) can often be described by a band structure theory. However, it is worthwhile to emphasize that this is a low-energy effective theory with fermions that emerge from many-body correlations in the f-shell. For SmB$_6$, the bulk band structure has not yet been fully understood. For example it is known that near the Fermi energy ($E_F$) there are three nearly degenerate f-bands. However they have not been resolved experimentally and it is still unclear which of them is responsible for opening the insulating gap and the nontrivial topology.

In this letter, instead of assuming a specific band structure, we focus on universal properties that are independent of the yet unknown microscopic details. We find that on the surface of SmB$_6$, there are two different types of Dirac points, some of which are protected by the time-reversal symmetry, while the others are due to lattice symmetries, i.e. SmB$_6$ is not only a topological insulator, but is also a topological crystalline insulator with nontrivial mirror Chern numbers. The mirror Chern number is a topological index protected by the point group symmetry of the crystal and it has been used in the study of the surface states of various weakly correlated materials e.g., Bi$_{12}$Sb$_{31}$. It is important to note that in topological insulators with mirror symmetry, it is pretty common to have nontrivial mirror Chern numbers and these topological indices don’t necessarily result in any additional surface states beyond the prediction of the $Z_2$ topological indices. However, for SmB$_6$, the nontrivial mirror Chern number indeed plays a very important role in understanding the surface states and it predicts for the (110) surface two additional surface Dirac points, beyond those predicted by the $Z_2$ topological index. Because these two surface Dirac points are protected by the point group symmetry of the crystal, materials of this type are known as topological crystalline insulators.

It is also worthwhile to emphasize that although we use SmB$_6$ as an example, our techniques and conclusions can easily be generalized to other Kondo insulators, as well as other strongly- or weakly-correlated insulators. In general, for systems with two-fold rotational symmetries, our technique shows that the parity of the mirror Chern number always coincides with the $Z_2$ weak topological index and so does not provide any additional information beyond the $Z_2$ topological indices. However, for systems with higher rotational symmetries (e.g. four-fold), our technique can be used to identify additional surface states beyond those protected by time-reversal symmetry.

Band structure of SmB$_6$— In SmB$_6$, the Sm atoms form a simple cubic lattice and inside each cube there is a tetrahedron of six B atoms. From band calculations and spectroscopic experiments it has long been known that the relevant bands near $E_F$ come from the 4$f$ and 5$d$ states of Sm. Over most of the Brillouin zone the 5$d$-bands are above $E_F$ while the 4$f$-bands stay below. However, around the X points $[(\pi, 0, 0), (0, \pi, 0) \text{ and } (0, 0, \pi)]$, the surface states beyond those predicted by the $Z_2$ topological index and the mirror Chern numbers are independent of microscopic details, which enables us to obtain surface state properties that are universal.
the energy of one of the 5d bands goes below $E_F$ and in order to maintain the number of valance bands below $E_F$, which is necessary for an insulator, one of the 4f band must go above. Hybridization between these two bands opens an insulating gap as shown in Fig. 1. This phenomenon is known as a band inversion, which played a very important role in the discovery of the quantum spin Hall insulators. Because d-states (f-states) have even (odd) parity, if we choose Sm as the inversion center, the two inverted bands must have opposite parities at $X$. In this Letter, all our conclusions rely on only two assumptions: (1) two bands with opposite parities are inverted at $X$ and (2) the material has an insulating bulk.

**Time-reversal symmetry and the $Z_2$ topological index—**

The $Z_2$ topological index for Kondo insulators (including SmB$_6$) has been computed before by one of the authors and coworkers. Here we obtain this topological index using a different approach in order to demonstrate a construction which will be used later to compute the mirror Chern number. In Ref. 33 it was proved that in a material with time reversal and space inversion symmetries, the $Z_2$ topological index can be computed using parity eigenvalues of the valence bands at high symmetry points.

$$(-1)^\nu = \prod_{m=1}^{N} \prod_{i=1}^{8} \xi_m(\Gamma_i),$$  

(1)

where $\nu$ is the strong topological index; $m$ is the band index for the valence bands, each of which is required by symmetry to be doubly-degenerate; $\Gamma_i$ represents the eight high symmetry points in the Brillouin zone ($\Gamma$, $X$, $M$ and $R$ for a cubic lattice); and $\xi_m(\Gamma_i) = \pm 1$ is the parity eigenvalue of band $m$ at $\Gamma_i$.

Instead of computing the product directly, here we obtain the topological index $\nu$ by comparing the band structure of SmB$_6$ with that of a trivial insulator, which is obtained by raising (lowering) the energy of the $d$ ($f$) bands such that the band inversion is eliminated. By putting the Fermi energy between the $f$ and $d$ bands, the system is obviously a trivial insulator (analogous to the insulating state of single valent SmS at ambient pressure). For both SmB$_6$ and this trivial insulator the $Z_2$ topological indices ($\nu_{\text{SmB}_6}$ and $\nu_{\text{trivial}}$) can be formulated using Eq. (1). Here we focus on the ratio

$$\frac{(-1)^\nu_{\text{SmB}_6}}{(-1)^\nu_{\text{trivial}}} = \prod_{i=1}^{8} \prod_{m=1}^{N} \frac{\xi_m(\Gamma_i)^{\text{SmB}_6}}{\xi_m(\Gamma_i)^{\text{trivial}}}$$  

(2)

On the l.h.s., the denominator is the identity ($\nu_{\text{trivial}} = 0$). For the r.h.s., it is easy to see that because these two insulators have exactly the same (conduction and valence) bands except for those involved in band inversions, only the parity eigenvalues of the inverted bands fail to cancel. After these simplifications, we get

$$(-1)^{\nu_{\text{SmB}_6}} = \left[ \frac{\xi_{\text{SmB}_6}^{IV}(X)}{\xi_{\text{IV}}^{\text{trivial}}(X)} \right]^3 = \left[ \frac{\xi_{\text{SmB}_6}^{X}}{\xi_{\text{IC}}^{\text{trivial}}(X)} \right]^3 = -1.$$  

(3)

The power three arises because there are three $X$ points. $\xi_{\text{SmB}_6}^{IV}(X) = +1$ and $\xi_{\text{IC}}^{\text{trivial}}(X) = -1$ are the parity eigenvalues of the inverted-valence (IV) and inverted-conduction (IC) bands in SmB$_6$ at $X$ respectively, where the former comes from parity even (+1) 5d-states and the latter are due to parity odd ($-1$) 4f-states. $\xi_{\text{IV}}^{\text{trivial}}(X)$ is the parity eigenvalue of the corresponding valence band in the trivial insulator. Here we used the fact that at $X$ the inverted conduction band in SmB$_6$ is identical to the corresponding valence band in the trivial insulator: $\xi_{\text{SmB}_6}^{IV}(X) = \xi_{\text{trivial}}^{IV}(X)$, which enables us to substitute the denominator into $\xi_{\text{IC}}^{\text{trivial}}(X)$. The final result $(-1)$ indicates that SmB$_6$ is a strong topological insulator.

This technique can be easily generalized to other materials with time-reversal and space-inversion symmetries and can also be utilized to compute the weak topological indices (See SI for details).

**Mirror Chern number—**

For insulators with a mirror symmetry we can define another topological index, the mirror Chern number. We start our discussion by considering 2D insulators with D$_{nh}$ symmetry. The mirror symmetry that protects the nontrivial topological structure is horizontal reflection in a plane parallel to the 2D surface. For particles with half-integer spins, we can use the mirror eigenvalues of the horizontal mirror plane to classify all Bloch waves into two groups: $|\psi_m^+(\mathbf{k})\rangle$ and $|\psi_m^-(-\mathbf{k})\rangle$, where the “$+$” (“$-$”) states have mirror eigenvalue $+i$ ($-i$). The subscript $m$ is the band index and $\mathbf{k}$ is the momentum. Using either $|\psi_m^+(\mathbf{k})\rangle$ or $|\psi_m^-(-\mathbf{k})\rangle$, we can define the mirror Chern number $C^+$ or $C^-$ as

$$C^\pm = i\epsilon_{ab} \sum_{m=1}^{N} \int_{BZ} \frac{d\mathbf{k}}{2\pi} \langle \partial_a \psi_m^\pm(\mathbf{k}) | \partial_b \psi_m^\pm(\mathbf{k}) \rangle.$$  

(4)

Here, we sum over all valence bands ($m = 1, \ldots, N$) and integrate over the whole Brillouin zone. $\epsilon_{ab}$ is the 2D Levi-Civita symbol with $a$ and $b$ being $k_x$ and $k_y$. The sum $C = C^+ + C^-$ is the (first) Chern number. Because
C is odd under the mirror reflection, the point group
symmetry requires $C = 0$, i.e. $C^+ = -C^-$. The mirror Chern number has properties similar to
the first Chern numbers. If the mirror symmetry is
preserved both in the bulk and on the edge, a nonzero
mirror Chern number implies the existence of (left- or
right-moving) edge modes, and the mirror Chern num-
ber $C^+ (C^-)$ is the difference between the numbers
of left-moving and right-moving edge modes with mirror
eigenvalue $+i (-i)$. Because modes with opposite mirror
eigenvalues cannot hybridize, these edge states cross each
other and form Dirac points on the edge. These Dirac
points are protected by the mirror symmetry, without
which $|\psi_{m}^+(k)|$ will hybridize with $|\psi_{m}(k)|$ and gap out
the Dirac points.

In a 3D insulator, the mirror Chern number can be de-
finite for any 2D planes with horizontal mirror symmetry
in the 3D Brillouin zone. For example, the $k_z = 0$ plane
of SmB$_6$ has symmetry D$_{4h}$ (Here, the main axis direc-
tions are chosen to be along the three four-fold-rotational
axes of the cubic lattice). In Ref. [34], it is proved that
for a system with $n$-fold rotational symmetry ($C_n$), the
Chern number can be computed (up to modulo $n$) as
a product of eigenvalues of the rotational operators at
high symmetry points. Here we use the same principle
to compute the mirror Chern number $C^+$

$$
(i)C^+ = \prod_{m=1}^{N} (-1)^{\eta_m(\Gamma)}\eta_m(M)\zeta_m(X), \tag{5}
$$

where $\eta_m(\Gamma)$ and $\eta_m(M)$ are eigenvalues of the 90°-
rotation along the normal direction of the 2D plane (z) for
band $|\psi_{m}^+(k)|$ at $\Gamma$ and $M$ respectively. $\zeta_m(X)$ is the eigenvalue of the 180°-rotation along the same axis at
$X$. The band index $m$ runs over all valence bands. It is
important to notice that we require $|\psi_{m}^+(k)|$ to be eigen-
states of the mirror operator (about the $x - y$ plane),
as well as the four-fold and two-fold rotational operators
(along $z$). This can always be achieved because these
operators commute with one another.

We compute this mirror Chern number by comparing
SmB$_6$ with the trivial insulator discussed above

$$
\frac{(i)C^+}{(i)C^{\text{trivial}}} = \prod_{m=1}^{N} \frac{\eta_m^{\text{SmB}_6}(\Gamma)\eta_m^{\text{SmB}_6}(M)\zeta_m^{\text{SmB}_6}(X)}{\eta_m^{\text{trivial}}(\Gamma)\eta_m^{\text{trivial}}(M)\zeta_m^{\text{trivial}}(X)}. \tag{6}
$$

Similar to the $Z_2$ topological index, most of the eigen-
values on the r.h.s. cancel out, except for those of the
inverted bands at $X$,

$$
(i)C^+ = \frac{\zeta_{\text{IV}}^{\text{SmB}_6}(X)}{\zeta_{\text{trivial}}^{\text{IV}}(X)} \cdot \frac{\zeta_{\text{IV}}^{\text{SmB}_6}(X)}{\zeta_{\text{IC}}^{\text{SmB}_6}(X)} = -1. \tag{7}
$$

Here we use the fact that $C^+_{\text{trivial}} = 0$ and IC and IV repre-
sent inverted-conduction and inverted-valence bands re-
spectively. Same as in Eq. (5), we substitute the denomi-
ator using the fact $\zeta_{\text{IV}}^{\text{trivial}}(X) = \zeta_{\text{IC}}^{\text{SmB}_6}(X)$.

The ratio in Eq. (7) can be easily determined using the
representations of the space group. At a momentum
point, all the bands can be labeled according to their
symmetry properties using double group representations
of the little group at this momentum point. For $X$, the
little group is D$_{4h}$, and the group theory requires that
all the parity even (odd) d- (f-) bands must have either
the symmetry of $\Gamma_6^+ \text{ or } \Gamma_6^-$ ($\Gamma_6^+ \text{ or } \Gamma_6^-$). Here, the $+/-$
sign represents even/odd parity. As proved in the Sup-
plementary Information (SI), for the two inverted bands,
because the hybridization between them opens up a full
gap, they must belong to the same representation up to
their differing parities. This conclusion is enough to
determine the ratio in Eq. (7) using eigenvalues provided
by the group representations, which is $-1$ as shown in
SI. This result tells us that the mirror Chern number
$C^+_{\text{SmB}_6} = 2$ up to modulo 4, and therefore SmB$_6$ is a
topological crystalline insulator.

Using the same technique, we find that the mirror
Chern number of the $k_z = \pi$ plane is 1. For mirror planes
with D$_{2h}$ symmetry (e.g. the $k_z = k_y$ plane), our tech-
nique can be used to show that the parity of the mirror
Chern number always coincides with the weak topologi-
ical index, implying no new insight beyond the $Z_2$ indices
(See SI for details).

Surface states— The topological indices discussed
above have direct impacts on the surface states. For the
$Z_2$ topological index, if nonzero, it predicts Dirac points
at certain high symmetry points of the surface Brillouin
zone. For a nontrivial mirror Chern number, it results in
Dirac points along certain high symmetry line in the
surface Brillouin zone.

For the $Z_2$ index, the surface Dirac cone can be found
by projecting the bulk high symmetry points with band
inversions ($X$ for SmB$_6$) onto the surface. If an odd
number of the bulk $X$ points are projected to a surface
high symmetry point, there must be a surface Dirac point
at this location. For the (100) surface of SmB$_6$, this
technique predicts three Dirac points at $\Gamma$, $X$ and $X'$. On
the (110) surface, one of the bulk $X$ points is projected
to $Y$, while the other two are both projected to $\bar{X}$. As
a result, time-reversal symmetry only protects one Dirac
point on the (110) surface located at $Y$ (Fig. 2).

For the mirror Chern number defined on a 2D plane
in the 3D Brillouin zone, if this 2D plane is perpendicu-
lar to the surface, its projection on the surface Brillouin zone forms a 1D line, along which there should be (at least) $|C^+|$ surface Dirac points. On the (100) surface of SmB$_6$, mirror Chern numbers give us no additional Dirac points. For example, the bulk $k_z = 0$ plane (with mirror Chern number 2) is projected to the $k_z = 0$ line onto the (100) surface. The mirror Chern number 2 implies that there should be two left-moving modes with parity $+i$ and two right-moving modes with parity $-i$ along this surface high symmetry line, and the intersections between these modes will form two surface Dirac points. By comparing with Fig. 2(a), it is easy to notice that these two surface Dirac points are just the Dirac points at $\Gamma$ and $X$ which are required by time-reversal symmetry. The bulk $k_z = \pi$ plane with mirror Chern number 1 is projected to the $k_z = \pi$ line on the (100) surface. The mirror Chern number requires this surface line to have one Dirac point, which is just the Dirac point at $\bar{\Gamma}$. The bulk $k_z = k_y$ plane also has mirror Chern number 1, and therefore the surface $k_z = k_y$ plane should have one Dirac point, which is the $\bar{\Gamma}$ Dirac point.

For the (110) plane [Fig. 2(b)], however, the mirror Chern number of the bulk $k_z = 0$ plane predicts two additional surface Dirac points. By projecting this plane onto the (110) surface, we obtain the $k_z = 0$ line and the mirror Chern number requires that there should be two Dirac points along this line. In the same time, the $Z_2$ topological index generates no surface Dirac points along this line, which implies that these two Dirac points are beyond the prediction of the $Z_2$ topological index and are not protected by time-reversal symmetry (but by the mirror symmetry). The two-fold rotational symmetry requires these two Dirac points to be located at $(k, 0)$ and $(-k, 0)$ on the surface $k'_{z-k_z}$ plane, as marked in Fig. 2(b). These two Dirac points are the direct prediction of the topological crystalline Kondo insulator and can be verified directly in experiments.

For other surfaces, e.g. (111), if the mirror planes perpendicular to the surface only have $D_{2h}$ (or lower) symmetry, this technique of computing mirror Chern numbers doesn’t offer any new insight beyond the $Z_2$ topological indices. It is also worthwhile to emphasize that in addition to the universal part of the surface states predicted above, other mechanism could induce extra pockets on the surface, e.g. band bending, which relies on microscopic details and is beyond the scope of this investigation.

**Model calculation**—To properly model the band structure of SmB$_6$, we need to take into account three nearly degenerate $f$-bands around $E_F$, which form a $j = 5/2$ representation of the $SU(2)$ group. The space group theory tells us that at the $X$ point, two of these three band shall have $\Gamma_{7}^-$ symmetry, while the other has $\Gamma_6^-$. Experimentally, because they are very close in energy, these three bands have not been clearly resolved and thus we don’t know exactly which band gets inverted. Knowledge of the $d$-band is relatively clear because there is only one $d$-band near $E_F$. Early band calculations without spin-orbit coupling show that in similar materials the relevant 5$d$-band has $\Gamma_3^+$ symmetry at $X$. If we include spin-orbit coupling, the symmetry for this band is $\Gamma_{16}^+ \otimes \Gamma_6^+ = \Gamma_7^+ \oplus \Gamma_3^+$ consistent with later numerical studies. Because SmB$_6$ has a full gap, as described above, the space group symmetry requires the inverted $f$-band to have the symmetry of $\Gamma_7^-$ at $X$, in order to match the symmetry of the $d$-band. However, which one of the two $\Gamma_7^-$ bands is inverted is unclear. One additional complication comes from the cubic symmetry, which distinguishes these two $\Gamma_7^-$ $f$-bands. If we follow the three $f$-bands from $X$ to $\Gamma$, the group theory requires one of the $\Gamma_7$ band to merge with the $\Gamma_6$ band at $\Gamma$ forming a quartet ($\Gamma_8^-$), whereas the other $\Gamma_7$ band remains a doublet ($\Gamma_7^-$). Whether the inverted $\Gamma_7$ band is part of the quartet at $\Gamma$ or it comes from the doublet at $\Gamma$ is still unclear.

Because we have proved that all the topological properties are independent of these microscopic details, the topological surface states of SmB$_6$ can be obtained (qualitatively) using a minimum two-band model. The minimal model we constructed here is a tight-binding model on a cubic lattice with two orbitals per site with opposite parities. By choosing parameters such that the two bands formed by these two orbitals are inverted at $X$, all the necessary ingredients are captured and the surface states of this model as shown in Fig. 3 are in perfect agreement with the universal conclusions proved above. In addition, we also computed surfaces states on the (100) and (111) surfaces (not shown), which also agree with our universal theory.

**Discussion**—According to the classification of topological band-insulators in Ref. 38, SmB$_6$ belongs to the $T-p3(4)_X$ (XYZ) class. For other insulators in this class, they shall share the same qualitative surface states and our technique can be generalized to obtain the topological surfaces states for insulators in other symmetry classes discussed therein. In recent quantum oscillation measurement, a Dirac point on the (110) surface of SmB$_6$ is observed, but it is still unclear which of the three Dirac points in Fig. 2(b) is responsible for the observed quantum oscillations. To fully understand the (110) surface, experimental techniques with momentum resolution are required.
necessary (e.g. ARPES).

Acknowledgment—K.S. thanks Liang Fu for constructive comments. The work was supported in part by the MCubed program at the University of Michigan.

Appendix A: Symmetry of the inverted bands

For SmB\textsubscript{6}, at the X point where the band inversion takes place, the two inverted bands can be labeled according to the group representations of the little group at X (D\textsubscript{4h}). For spin-1/2 particles, the representation must be one of the four double group representations $\Gamma^+_6$, $\Gamma^-_6$, $\Gamma^+_7$, or $\Gamma^-_7$.

As shown in Fig.1, it is the hybridization between the two inverted bands that opens up the insulating gap. This hybridization has strong dependence on the symmetry of the inverted bands. Most importantly, the symmetry of the two bands along $\Delta$ (i.e. the line connecting $\Gamma$ and X along the main axis direction) dictates whether the hybridization can open a full gap or not, i.e. whether or not the band crossing points located between $\Gamma$ and $X$ shown in Fig.1(a) can be gapped out (Band crossings away from $\Delta$ don’t provide additional information on the symmetry of the bands and thus will not be discussed).

The compatibility relation of the space group\textsuperscript{22} tells us that if a band has symmetry $\Gamma^+_6$ or $\Gamma^-_6$ at $X$, along the $\Delta$ line, this band shall corresponds to the $\Gamma_6$ representation of the little group at $\Delta$ (C\textsubscript{4v}). Similarly, for a band with symmetry $\Gamma^+_7$ or $\Gamma^-_7$ at $X$, the symmetry of this band along $\Delta$ is $\Gamma^-_7$. The parity eigenvalues play no role along $\Delta$, because space inversion is not part of the C\textsubscript{4v} group.

If one of the two inverted bands belongs to the $\Gamma^+_6$ representation at $X$, while the other one is a $\Gamma^+_7$ band, these two bands will have different symmetries along $\Delta$ (i.e. a $\Gamma_6$ band and a $\Gamma^-_7$ band along $\Delta$). This symmetry difference prohibits hybridization between these two bands along $\Delta$. As a result, band crossing point shown in Fig.1(a) between $\Gamma$ and $X$ cannot be gapped out, i.e. the bulk contains symmetry-protected 3D Dirac states somewhere along $\Delta$, and therefore we cannot have a fully insulating bulk.

To open an insulating gap in the bulk, the two inverted bands must have the same symmetry at $X$ (up to different parities). For example, if one of the inverted bands has symmetry $\Gamma^+_7$ at $X$, while the other has $\Gamma^-_7$, these two bands along $\Delta$ has the same symmetry $\Gamma^-_7$ and thus a hybridization gap becomes allowed. Same is true if the two bands have are $\Gamma^+_6$ and $\Gamma^-_6$ bands at $X$.

For SmB\textsubscript{6}, band structure calculations suggest that the two inverted bands have symmetries $\Gamma^+_7$ and $\Gamma^-_7$ at $X$, but our conclusions remain valid even if the two bands are $\Gamma^+_6$ and $\Gamma^-_6$.

Appendix B: $Z_2$ topological indices

Here, we generalize the formula that we used to compute the $Z_2$ topological index of SmB\textsubscript{6}. For an arbitrary insulator with time-reversal and space-inversion symmetries, the strong topological index $\nu$ can be computed using the following formula, where $(-1)^\nu$ equals the ratio between total parity of the inverted valence bands and that of the inverted conduction bands at all high symmetry points.

$$ (-1)^\nu = \prod_{\nu = 1}^{8} \prod_{m_i} \xi_{m_i}^\text{IV}(\Gamma_i), $$(B1)

where $\Gamma_i$ represents the eight high symmetry points in the 3D Brillouin zone ($i = 1, \ldots, 8$) and the product $\prod_{m_i}$ runs over all the inverted bands at the high symmetry point $\Gamma_i$. The superscript IV (IC) represents the inverted-valence (inverted-conduction) bands and $\xi$ is the parity eigenvalue for the corresponding band at a high symmetry point.

The same technique can be used to compute the weak topological index, if we only use the eigenvalues at four high symmetry points on a high symmetry plane.

$$ (-1)^\nu_{\text{weak}} = \prod_{i = 1}^{4} \prod_{m_i} \xi_{m_i}^\text{IV}(\Gamma_i). $$(B2)

Appendix C: 2D planes with $D_{2h}$ symmetry

For a 2D system with two-fold rotational symmetry $C_2$, the parity of the Chern number can be determined using eigenvalues of rotational operators at high symmetry points as shown in Ref.\textsuperscript{[34]}. For a 2D system with $D_{2h}$ symmetry, the mirror Chern number (up to modulo 2) can be determined using a similar technique.

$$ (-1)^{C^+} = \prod_{i=1}^{4} \prod_{m=1}^{N} (-1) \zeta_{m}(\Gamma_i), $$

(C1)

where $\Gamma_i$ are the four high-symmetry points of the 2D Brillouin zone. $\zeta_{m}(\Gamma_i)$ is the eigenvalue of the 180°rotation along the direction normal to the plane for the Bloch state $|\psi_m^\text{h}(k = \Gamma_i)\rangle$.

If we compute the mirror Chern number by comparing with a trivial insulator with no band inversion, we find that

$$ (-1)^{C^+} = \prod_{i=1}^{4} \prod_{m} \xi_{m}^\text{IV}(\Gamma_i), $$

(C2)

where $\Gamma_i$ represents four high symmetry points of the 2D Brillouin zone ($i = 1, \ldots, 4$). The product $\prod_{m}$ runs over all the inverted bands at the high symmetry points $\Gamma_i$. $\zeta_{m}(\Gamma_i)$ and $\zeta_{m}(\Gamma_i)$ are the eigenvalues of the
180°-rotation for the inverted-valence (IV) and inverted-conduction (IC) bands respectively at the high symmetry point \( \Gamma \). Same as in the main text, we use the eigenvalues of the inverted conduction bands in the topological material to substitute the eigenvalues of the corresponding valence bands in the trivial insulator in the denominator. As will be proved below, this ratio coincides with Eq. (B2) and thus the parity of this mirror Chern number is identical to the weak topological index.

For a 2D system with \( D_{2h} \) symmetry, the horizontal mirror reflection \( \sigma \) is the product of the 180°-rotation along the normal direction \((C_2)\) and the space inversion \((I)\)

\[
\sigma = C_2 \otimes I. \tag{C3}
\]

For bands with positive parities \((I = E \text{ where } E \text{ is the identity matrix})\), we find that \(\sigma = C_2\) and thus \( C_2 \) and \(\sigma\) have the same eigenvalues and eigenstates. This implies that at a high symmetry point \( \Gamma \), for the Bloch wave \(|\psi_m^+ (k)\rangle\), which has mirror eigenvalue \(+i\), it is also an eigenstate of \( C_2 \) with the same eigenvalue \(\zeta = +i\). For bands with negative parity \((I = -E)\), we have \(\sigma = -C_2\) and thus \(|\psi_m^-(k)\rangle\) has rotation eigenvalue \(\zeta = -i\), opposite to the eigenvalue of the mirror reflection. In summary, the ratio between \(\zeta\) for different bands at a high symmetry point is exactly the same as the ratio between parity eigenvalues \((\xi)\) of the same bands. Therefore, we get

\[
(-1)^{C^+} = \prod_{i=1}^{4} \frac{\xi_{\text{IC}}^m (\Gamma_1)}{\xi_{\text{IV}}^m (\Gamma_1)} \cdot \prod_{i=1}^{4} \frac{\xi_{\text{IC}}^m (\Gamma_1)}{\xi_{\text{IV}}^m (\Gamma_1)}. \tag{C4}
\]

By comparing with Eq. (B2), we find that

\[
(-1)^{C^+} = (-1)^{\epsilon_{\text{weak}}}. \tag{C5}
\]

Therefore, we proved that for the \( D_{2h} \) symmetry, the parity of the mirror Chern number obtained by the technique we use coincides with the weak \( Z_2 \) topological index, and thus it offers no additional insight beyond the \( Z_2 \) topological indices.

If we apply this technique to \( \text{SmB}_6 \), it is easy to notice that for the \( k_z = k_y \) plane, which has \( D_{2h} \) symmetry, the mirror Chern number is

\[
(-1)^{C^+} = \frac{\xi_{\text{IV}}^{\text{SmB}_6} (X)}{\xi_{\text{IC}}^{\text{SmB}_6} (X)} = \frac{\xi_{\text{IV}}^{\text{SmB}_6} (X)}{\xi_{\text{IC}}^{\text{SmB}_6} (X)} = -1. \tag{C6}
\]

Here we used the fact that in \( \text{SmB}_6 \) at \( X \) point, there is only one pair of inverted bands, which have opposite parities \(\xi_{\text{IV}}^{\text{SmB}_6} (X) = +1\) and \(\xi_{\text{IC}}^{\text{SmB}_6} (X) = -1\).

**Appendix D: The \( k_z = 0 \) plane**

For the \( k_z = 0 \) plane (with \( D_{4h} \) symmetry), as shown in the main text,

\[
\xi_{\text{IV}}^{\text{SmB}_6} (X) \xi_{\text{IC}}^{\text{SmB}_6} (X). \tag{D1}
\]

Utilizing the same arguments as we used in Eq. (C4), we find

\[
\binom{C^+}{\text{SmB}_6} = \frac{\xi_{\text{IV}}^{\text{SmB}_6} (X)}{\xi_{\text{IC}}^{\text{SmB}_6} (X)} = -1. \tag{D2}
\]

This conclusion implies that \(C^+_{\text{SmB}_6} = 2\) up to modulo 4.

**Appendix E: The \( k_z = \pi \) plane**

For the \( k_z = \pi \) plane, the high symmetry points are \( X, R\) and \( M \). The first two have four-fold rotational symmetry along the normal direction \((z)\) while \( M \) has two-fold. Because of the \( D_{4h} \) symmetry, the mirror Chern number of this plane is

\[
\xi_{\text{IV}}^{\text{SmB}_6} (X) \xi_{\text{IC}}^{\text{SmB}_6} (X). \tag{E1}
\]

By comparing with the trivial insulator with no band inversion, we find

\[
\xi_{\text{IV}}^{\text{SmB}_6} (X) \xi_{\text{IC}}^{\text{SmB}_6} (X). \tag{E2}
\]

Here, \( \eta_\text{IV}^{\text{SmB}_6} (X) \) and \( \eta_\text{IC}^{\text{SmB}_6} (X) \) are the eigenvalues of the 90°-rotation (along \( z \)) for the inverted-valence (IV) and inverted-conduction (IC) bands at the momentum point \((0, 0, \pi)\) respectively. As will be proved below, this ratio is \(+i\), and therefore the mirror Chern number is \(+1\).

The eigenvalues of the 90°-rotation can be determined utilizing the representation of the space group, which can be easily constructed using the character table and bases provided in group theory literature (e.g. Ref. [36]). At \( X, (0, 0, \pi) \), possible representations for spin-1/2 particles are \( \Gamma_{\pm}^2 \) and \( \Gamma_{\pm 6}^2 \), which are the double-group representation of the little group at \( X (D_{4h}) \). All these four representations are two-dimensional representations and thus all the group elements can be written as \( 2 \times 2 \) matrices. The matrices of the relevant operators are listed below. Here, we choose the basis such that the matrix of the mirror reflection is diagonalized.

\[
U_{C_4}^{\pm} = \begin{pmatrix} -\sqrt{2}/2 + i\sqrt{2}/2 & 0 \\ 0 & -\sqrt{2}/2 - i\sqrt{2}/2 \end{pmatrix} \tag{E3}
\]

\[
U_{C_4}^{\mp} = \begin{pmatrix} -\sqrt{2}/2 - i\sqrt{2}/2 & 0 \\ 0 & -\sqrt{2}/2 + i\sqrt{2}/2 \end{pmatrix} \tag{E4}
\]

\[
U_{\sigma_h}^{+} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \tag{E5}
\]

\[
U_{\sigma_h}^{-} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \tag{E6}
\]
\[ U_{\sigma h}^{-} = \left( \begin{array}{cc} i & 0 \\ 0 & -i \end{array} \right) \]  
(E7)

\[ U_{\sigma h}^{0} = \left( \begin{array}{cc} i & 0 \\ 0 & -i \end{array} \right) \]  
(E8)

The subscripts \( C_4 \) and \( \sigma \) represent the 90°-rotation (along \( z \)) and the horizontal mirror reflection (about the \( x-y \) plane) operators respectively. The superscripts \( 6^+, \ 6^-, \ 7^+, \ 7^- \) mark the representations.

Using these matrices, it is easy to notice that if the two inverted bands have \( \Gamma^\pm_7 \) symmetry (as in \( \text{SmB}_6 \)), the inverted valence band (\( \Gamma^+_7 \)) has

\[ \eta_{\text{IV}}^{\text{SmB}_6}(X) = -\frac{\sqrt{2}}{2} - i\frac{\sqrt{2}}{2}, \]  
(E9)

and the inverted conduction band (\( \Gamma^-_7 \)) has

\[ \eta_{\text{IC}}^{\text{SmB}_6}(X) = -\frac{\sqrt{2}}{2} + i\frac{\sqrt{2}}{2}. \]  
(E10)

As a result,

\[ (i)^{C^{+}_{\text{SmB}_6, k_z = \pi}} = \eta_{\text{IV}}^{\text{SmB}_6}(X)/\eta_{\text{IC}}^{\text{SmB}_6}(X) = +i. \]  
(E11)

If the two inverted bands are \( \Gamma^+_6 \) bands, the inverted valence band (\( \Gamma^+_6 \)) has

\[ \eta_{\text{IV}}(X) = \frac{\sqrt{2}}{2} + i\frac{\sqrt{2}}{2}, \]  
(E12)

and the inverted conduction band (\( \Gamma^-_6 \)) has

\[ \eta_{\text{IC}}(X) = \frac{\sqrt{2}}{2} - i\frac{\sqrt{2}}{2}. \]  
(E13)

As a results,

\[ (i)^{C^{+}_{\text{SmB}_6, k_z = \pi}} = \eta_{\text{IV}}^{\text{SmB}_6}(X)/\eta_{\text{IC}}^{\text{SmB}_6}(X) = +i. \]  
(E14)
27 L. Fu and C. L. Kane, Phys. Rev. Lett. 109, 246605 (2012).
28 Y. J. Wang, W.-F. Tsai, H. Lin, S.-Y. Xu, M. Neupane, M. Hasan, and A. Bansil, ArXiv e-prints arXiv:1304.8119 (2013).
29 J. Liu, W. Duan, and L. Fu, ArXiv e-prints arXiv:1304.0430 (2013).
30 Y. Okada, M. Serbyn, H. Lin, D. Walkup, W. Zhou, C. Dhital, M. Neupane, S. Xu, Y. J. Wang, R. Sankar, F. Chou, A. Bansil, M. Z. Hasan, S. D. Wilson, L. Fu, and V. Madhavan, ArXiv e-prints arXiv:1305.2823 (2013).
31 J. C. Y. Teo, L. Fu, and C. L. Kane, Phys. Rev. B 78, 045426 (2008).
32 B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science 314, 1757 (2006).
33 L. Fu and C. L. Kane, Phys. Rev. B 76, 045302 (2007).
34 C. Fang, M. J. Gilbert, and B. A. Bernevig, Phys. Rev. B 86, 115112 (2012).
35 M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, Group Theory: Application to the Physics of Condensed Matter (Springer, 2010).
36 G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, The Properties of the Thirty-Two Point Groups (The MIT Press, 1963).
37 A. Hasegawa and A. Yanase, Journal of Physics F: Metal Physics 7, 1245 (1977).
38 R.-J. Slager, A. Mesaros, V. Juricic, and J. Zaanen, Nat. Phys. 9, 98 (2013).