

Stable real-space invariants and topology beyond symmetry indicators

Received: 16 May 2025

Accepted: 15 June 2026

Published online: 11 July 2026

Yoonseok Hwang^{1,2,3}, Vaibhav Gupta^{1,2}, Frank Schindler³, Luis Elcoro^{4,5}, Zhida Song⁶, B. Andrei Bernevig^{7,8,9} & Barry Bradlyn^{1,2} 

We introduce stable real-space invariants (SRSIs), topological invariants defined from adiabatic deformations between Wannier states, generalizing previously discovered local and composite real-space invariants. SRSIs are $\mathbb{Z}$ - and $\mathbb{Z}_n$ -valued ($n = 2, 4$) linear combinations of Wannier state multiplicities characterizing the stable equivalence of atomic insulators. We enumerate all SRSIs in nonmagnetic space groups with and without spin-orbit coupling. $\mathbb{Z}$ SRSIs are in one-to-one correspondence with momentum-space symmetry data and thus determine symmetry indicators of topology (SIs). $\mathbb{Z}_n$ SRSIs capture real-space information beyond momentum-space symmetry data and SIs. Applying SRSIs to split elementary band representations (EBRs) whose symmetry data decomposes into positive sums of other EBR symmetry data, we diagnose the topology of all 211 cases across 51 space groups except for 8 exceptions in 5 space groups. Our results solidify Topological Quantum Chemistry beyond SIs and momentum-space symmetry data. Finally, we use SRSIs to diagnose an obstructed atomic insulator in a realistic material.

In topological quantum chemistry (TQC)^{1–9}, bands that cannot be expressed as a positive-integer linear combination of atomic limits, also known as elementary band representations (EBRs), are considered topological. Such bands are often characterized by nontrivial symmetry indicators (SIs) calculated from momentum-space symmetry data, which include the representation of bands at high-symmetry momenta in the Brillouin zone (BZ)^{10–21}. The combination of TQC and SIs with first-principles calculations has enabled the discovery of numerous topological material candidates^{22–28}. One corollary of TQC is that when an EBR splits into disconnected bands, some of these bands must be topological. Refs. 29–32 highlighted that, in specific cases, one group of bands in a split EBR may appear trivial—sharing identical SI with an atomic limit—while the other group of bands is indicated as topological, both by TQC and by SIs, as its momentum-space symmetry data is inconsistent with that of sums of atomic limits. While

TQC provides a conceptually more general real-space framework, many known examples suggest that SIs often reproduce the same diagnosis in practice, including but not limited to the case of split EBRs. This raises the question of whether TQC and SIs yield identical results, and more importantly, when TQC can, in principle, distinguish a broader class of topological phases beyond SIs alone. It is known, for instance, that SIs do not capture all aspects of band topology, especially in cases involving fragile or non-symmetry-indicated stable topological phases. Moreover, SIs do not distinguish between distinct trivial atomic insulators that cannot be deformed into each other, despite their topological inequivalence^{9,33}.

In this work, we introduce stable real-space invariants (SRSIs) to address these limitations. By generalizing the previously discovered real-space invariants (RSIs)^{34–36}, SRSIs provide a comprehensive classification that accounts for the (stable) adiabatic equivalence of bands.

¹Department of Physics, University of Illinois Urbana-Champaign, Urbana, IL, USA. ²Anthony J. Leggett Institute for Condensed Matter Theory, University of Illinois Urbana-Champaign, Urbana, IL, USA. ³Blackett Laboratory, Imperial College London, London, United Kingdom. ⁴Department of Physics, University of the Basque Country UPV/EHU, Apartado 644, Bilbao, Spain. ⁵EHU Quantum Center, University of the Basque Country UPV/EHU, Apartado 644, Bilbao, Spain. ⁶International Center for Quantum Materials, School of Physics, Peking University, Beijing, China. ⁷Department of Physics, Princeton University, Princeton, NJ, USA. ⁸Donostia International Physics Center, P. Manuel de Lardizabal 4, Donostia-San Sebastian, Spain. ⁹IKERBASQUE, Basque Foundation for Science, Bilbao, Spain. ✉e-mail: bbradlyn@illinois.edu

SRSIs enable the identification and characterization of both trivial and topological phases beyond the information contained in momentum-space symmetry data or SIs. We systematically derive and tabulate all SRSIs, which are of two types: $\mathbb{Z}$ - and $\mathbb{Z}_n$ -valued SRSIs ($\mathbb{Z}$ SRSIs and $\mathbb{Z}_n$ SRSIs, where $n = 2, 4$) in the 230 space groups (SGs) with and without spin-orbit coupling (SOC). Notably, $\mathbb{Z}$ SRSIs determine the full set of SIs, and $\mathbb{Z}_n$ SRSIs provide additional information about band structures not captured by momentum-space symmetry data and SIs. Hence, the formalism of TQC with SRSIs contains, but goes beyond, that of SIs.

After introducing the general framework, we demonstrate the application of SRSIs to band topology. For atomic insulators, we show that SRSIs provide both a classification and a diagnostic of stable equivalence. Specifically, we prove that if two atomic insulators have the same values for all $\mathbb{Z}$ and $\mathbb{Z}_n$ SRSIs, then they can be adiabatically deformed into each other in the presence of auxiliary trivial bands. For topological insulators, we demonstrate that $\mathbb{Z}$ SRSIs can be assigned based on the mapping between momentum-space symmetry data and $\mathbb{Z}$ SRSIs, with their fractional (i.e., rational numbers that are not integers) values implying nontrivial SIs. While $\mathbb{Z}_n$ SRSIs cannot be directly assigned to topological bands, they can still serve as indicators of topological gaps that cannot be diagnosed using SIs. Specifically, we investigate the situation where disconnected parts of a split EBR appear indistinguishable from atomic limits based on momentum-space symmetry data (SIs) alone. Even in such cases, the real-space framework of TQC reveals an obstruction to both split parts being atomic limits^{5,31,32,37,38}. Using SRSIs, we analyze all 211 split EBRs in 51 SGs where TQC implies band topology beyond SIs^{33,39–45}. Notably, we show that constraints arising from $\mathbb{Z}_n$ SRSIs can be used to diagnose band topology in all split EBR cases except for only 8 cases across 5 SGs, highlighting the power of SRSIs in capturing band topology beyond the scope of SIs. This demonstrates the existence of many topological-only systems where at least some bands have to be topological (either stable or fragile), regardless of the model parameters. Finally, we illustrate our results using simple tight-binding models, where we use the Wilson loop to confirm the band topology. In addition, we demonstrate the material-level applicability of SRSIs by presenting a concrete example of the symmetry-based diagnosis of an obstructed atomic insulator in Y_3Al_2 .

Results

Real-space invariants

Before we introduce the SRSIs, let us review the local RSIs derived in refs. 34,35. To define RSIs, let us consider topologically trivial, atomic bands, which transform under a representation of a space group induced from site-symmetry representations (or exponentially localized and symmetric Wannier orbitals) at WPs within a unit cell. Recall from refs. 2,6,30,46 that for each WP W , the site-symmetry group G_W consists of symmetries that leave W invariant, and the site-symmetry irreducible representations (irreps) ρ_W^i ($i = 1, \dots, N_W^p$) are defined for G_W .

Local RSIs are defined locally at each WP W in the unit cell, in terms of the multiplicities $m(\rho_W^i)$ of site-symmetry irreps at W for a given set of bands. For a WP W , we first consider all WPs connected to W , meaning those WPs with coordinates that can be continuously tuned to those of W while preserving all crystal symmetries^{2,6}. The local RSIs remain invariant under adiabatic processes that deform occupied site-symmetry irreps between W and the connected lower-symmetry WPs without breaking the symmetries of the SG G and without closing a gap to other bands.

The full set of local RSIs in the 1651 magnetic SGs was computed in ref. 36, where it was found that there are both $\mathbb{Z}$ - and $\mathbb{Z}_n$ -valued ($n = 2$) local RSIs. Earlier works^{47,48} identified related local RSIs for specific point-group settings, such as rotation and (roto)inversion symmetries. These works provide early examples of local RSIs in restricted

symmetry settings. To compute the local RSIs at a WP W , we first analyze the induction relations between the site-symmetry group G_W of W and the site symmetry groups of all connected lower-symmetry WPs. These relations determine how direct sums of irreps of G_W decompose into irreps at lower-symmetry WPs, corresponding to possible adiabatic processes. As detailed in Section 2 of the Supplementary Note (SN 2), local RSIs can be systematically derived using the Smith decomposition of the matrix enumerating these adiabatic processes.

Local RSIs fall into two distinct categories: those defined at maximal Wyckoff positions (WPs) and those defined at non-maximal WPs. A WP W is maximal if all connected WPs have lower site-symmetry groups than G_W ; otherwise, W is non-maximal. The local RSIs at maximal WPs are topological invariants under all adiabatic processes, whereas the local RSIs at non-maximal WPs are invariant only under a subset of adiabatic processes. That is, local RSIs associated with non-maximal WPs are not strictly topological invariants when arbitrary adiabatic processes are considered. In contrast, we will demonstrate that SRSIs are robust topological invariants under all adiabatic processes, addressing these subtleties comprehensively. This motivates the need for SRSIs as a comprehensive framework for real-space topology.

As an example, let us consider the SG $Pmm21'$ (No. 25) with spin-orbit coupling (SOC) in two dimensions (2D). This SG is generated by x - and y -flipping mirror symmetries, $M_{x,y} = \{m_{x,y}|\mathbf{0}\}$, time-reversal symmetry T , and two translations $\{E|1, 0\}$ and $\{E|0, 1\}$. Here, m_x (m_y) flips the x (y) coordinate, and E is the trivial point-group element. (Note that while $Pmm21'$ is a 3D SG, it can be viewed as the trivial direct product of the 2D wallpaper group $p2mm1'$ with translations along the z -direction. As such, in what follows we suppress the z -translations for simplicity.) See Fig. 1a for the unit cell structure. The WPs and site-symmetry irreps are summarized in Table 1. In this SG, the direct sum of two $(\bar{E})_{1d}$ irreps at maximal WP $1d$ can be adiabatically deformed to $(^1\bar{E}^2\bar{E})_{2f}$ or $(^1\bar{E}^2\bar{E})_{2h}$ at connected non-maximal WP $2f$ or $2h$, as shown in Fig. 1b, c. Thus, we define the equivalence relation, $2(\bar{E})_{1d} \iff (^1\bar{E}^2\bar{E})_{2f/2h}$. For these adiabatic processes, $m[(\bar{E})_{1d}] \bmod 2$ remains invariant and serves as a local RSI at WP $1d$. Similarly, by considering the adiabatic deformation between $(^1\bar{E}^2\bar{E})_{2f} \oplus (^1\bar{E}^2\bar{E})_{2f}$ and $(\bar{A}\bar{A})_{4i}$, the local RSI at WP $2f$ is defined as $m[(^1\bar{E}^2\bar{E})_{2f}] \bmod 2$. In the same way, the local RSI at WP $2h$ is defined as $m[(^1\bar{E}^2\bar{E})_{2h}] \bmod 2$.

There is a crucial difference between the local RSIs at maximal and non-maximal WPs. Local RSIs at maximal WPs remain invariant under all adiabatic processes and are thus topological invariants. In contrast, local RSIs at non-maximal WPs W' may change when site-symmetry irreps are moved from W' to another connected maximal WP W . The irreps at WP W may further be moved to another non-maximal WP W' connected to W . For example, $(^1\bar{E}^2\bar{E})_{2f}$ at $2f(x, 1/2)$ can be moved to $1d(1/2, 1/2)$ by tuning the free real parameter x without breaking any symmetry, as shown in Fig. 1c. Then, this irrep can be deformed to $2(\bar{E})_{1d}$. Moreover, $2(\bar{E})_{1d}$ can be further deformed to $(^1\bar{E}^2\bar{E})_{2h}$ as the WP $2h$ is connected to WP $1d$ (see Fig. 1c). During this adiabatic process, the local RSI at WP $2f(2h)$, $m[(^1\bar{E}^2\bar{E})_{2f}]$ ($m[(^1\bar{E}^2\bar{E})_{2h}]$) $\bmod 2$, changes from 1 (0) to 0 (1).

The above example demonstrates why local RSIs at non-maximal WPs cannot serve as topological invariants. Below, we introduce the SRSIs that address this issue. For a detailed review of local RSIs, see SN 2.

Stable real-space invariants

To define true topological invariants, we introduce and calculate SRSIs that remain invariant under all adiabatic processes in an SG. SRSIs fully contain the local RSIs at maximal WPs and also include additional topological invariants formed as linear combinations of site-symmetry-irrep multiplicities at multiple WPs, including both maximal and non-maximal positions. Similar to local RSIs, both $\mathbb{Z}$ - and

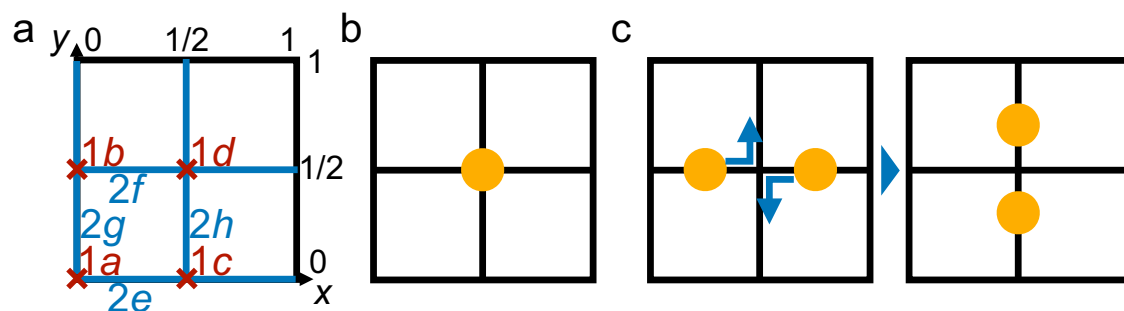


Fig. 1 | Real-space invariants (RSIs) in the SG $Pmm21'$ (No. 25). **a** Unit cell structure in 2D. There are four maximal WPs (1a, 1b, 1c, 1d), four non-maximal WPs (2e, 2f, 2g, 2h), and non-maximal, general WP 4i (not shown). **b** A single Kramers pair of site-symmetry irreps forms the irrep $(\bar{E})_{1d}$ at the maximal WP 1d²⁸, which cannot be

moved away from 1d. This is encoded in a nonzero local RSI, $\delta_{1d} = m[(\bar{E})_{1d}] \bmod 2 = 1$, which is also an SRSI. **c** A pair of Kramers pairs forms the irrep $1\bar{E}2\bar{E}$ at the WP 2f, which can be adiabatically moved to the WP 2h. This process changes the local RSIs at WPs 2f and 2h, $\{m[(1\bar{E}2\bar{E})_{2f}], m[(1\bar{E}2\bar{E})_{2h}]\} \bmod 2$, from (1, 0) to (0, 1).

Table 1 | Wyckoff positions (WPs) and site-symmetry irreps in the SG $Pmm21'$ (No. 25) in 2D

WP W	G_W	ρ_W
1a(0, 0)	$\{m_x 0\}, \{m_y 0\}$	$(\bar{E})_{1a}$
1b(0, 1/2)	$\{m_x 0\}, \{m_y 0, 1\}$	$(\bar{E})_{1b}$
1c(1/2, 0)	$\{m_x 1, 0\}, \{m_y 0\}$	$(\bar{E})_{1c}$
1d(1/2, 1/2)	$\{m_x 1, 0\}, \{m_y 0, 1\}$	$(\bar{E})_{1d}$
2e(x, 0)	$\{m_y 0\}$	$(1\bar{E}2\bar{E})_{2e}$
2f(x, 1/2)	$\{m_y 0, 1\}$	$(1\bar{E}2\bar{E})_{2f}$
2g(0, y)	$\{m_x 0\}$	$(1\bar{E}2\bar{E})_{2g}$
2h(1/2, y)	$\{m_x 1, 0\}$	$(1\bar{E}2\bar{E})_{2h}$
4i(x, y)	$\{E 0, 0\}$	$(\bar{A}\bar{A})_{4i}$

The first column indicates the type of WP and its representative position for each WP W . When W has a multiplicity larger than 1, other positions are generated by the full symmetry group. The second and third columns denote the site-symmetry group generators at the representative position and the site-symmetry irreps, respectively. For the second column, nontrivial generators are provided. The WPs 1a, 1b, 1c, 1d are maximal. For non-maximal WPs 2e, 2f, 2g, 2h, 4i, x and y are free real parameters.

$\mathbb{Z}_n$ -valued SRSIs exist. However, while $\mathbb{Z}_n$ -valued local RSIs exist only for $n = 2$ both with and without SOC, $\mathbb{Z}_n$ -valued SRSIs exist for $n = 2, 4$. Notably, $\mathbb{Z}_4$ -valued SRSIs appear in only 4 SGs, all with SOC. While $\mathbb{Z}_2$ -valued local RSIs arise due to either time-reversal symmetry (protecting Kramers pairs if SOC exists) or the presence multiple adiabatic processes (that hinder the emergence of $\mathbb{Z}$ -valued RSIs)^{35,36}, $\mathbb{Z}_4$ -valued SRSIs require both (though their presence is not guaranteed even when both conditions are met). For a detailed examination on $\mathbb{Z}_4$ -valued SRSIs, see SN 3C. In what follows, we define SRSIs, establish their relation to other RSIs, and derive their key properties. Figure 2 provides a schematic overview of this framework.

To calculate the SRSIs, we first define the symmetry-representation vector p associated with a set of trivial (atomic limit) bands. The vector p lists all site-symmetry irrep multiplicities at all WPs:

$$p = [m(\rho_{W_1}^1), m(\rho_{W_1}^2), \dots, m(\rho_{W_2}^1), \dots]^T, \quad (1)$$

where the irrep multiplicity $m(\rho_{W_j}^j)$ ($j = 1, \dots, N_{UC}^p$) is the multiplicity of the j -th irrep of the site-symmetry group at the WP W , and $m(\rho_{W_j}^j)$ is a non-negative integer. The total length of p is $\sum_W N_W^p = N_{UC}^p$, which is the total number of distinct site-symmetry irreps defined within a unit cell (UC). Adiabatic processes can be characterized by changes in the

irrep multiplicities by $\Delta m(\rho_{W_j}^j)$ associated with moving orbitals, consistent with the symmetries; collecting the $\Delta m(\rho_{W_j}^j)$, we can associate to each adiabatic process a column vector q_m which represents the change to p under the adiabatic process m , i.e. $p \rightarrow p + q_m$.

For any SG (either with and without SOC), we can find a finite basis set that generates all adiabatic processes. Such a basis is constructed as follows: site-symmetry irreps at non-maximal WPs W' can always be deformed into direct sums of irreps at the WPs connected to W' with larger site-symmetry groups. For all site-symmetry irreps at all non-maximal WPs W' , we list the adiabatic processes that deform the irrep from W' to all connected high-symmetry WPs. Then, we define a matrix of adiabatic processes q , whose component $(q)_{im}$ represents the change to the i -th entry of the symmetry-representation vector p by the m -th basis of the adiabatic process. Here, $i = 1, \dots, N_{UC}^p$ runs over all site-symmetry irreps for every WP in the unit cell (including the general WP), and $m = 1, \dots, N_{adia}$ runs over all adiabatic processes. The entries of the columns of q are integers that specify the change in irrep multiplicities under the adiabatic process: when an adiabatic process deforms an irrep at W' into a linear combination of irreps at a connected high-symmetry WP W , the corresponding column of q contains a negative integer reflecting the decrease of irrep multiplicity at W' and positive integers indicating the increases of irrep multiplicities at W . Note that only integer multiples of the columns of q correspond to valid adiabatic processes.

To extract meaningful invariants that remain unchanged under adiabatic processes, we perform the Smith decomposition:

$$q = L \cdot \Lambda \cdot R, \quad (2)$$

where L and R are $N_{UC}^p \times N_{UC}^p$ and $N_{adia} \times N_{adia}$ unimodular matrices, respectively. Λ is an $N_{UC}^p \times N_{adia}$ matrix with non-negative integers on the diagonal and zeros for all entries off the diagonal. We will always choose L and R such that the distinct diagonal entries $\lambda, \lambda', \lambda'', \dots$ of Λ are sorted in decreasing order, $\lambda > \lambda' > \lambda'' \dots \geq 0$. The nonzero diagonal entries of Λ are known as the elementary divisors of q . Notably, the number of elementary divisors of q is equal to the rank(q).

A linear combination of adiabatic processes changes the symmetry-representation vector p by $\Delta p = q \cdot z$ with $z \in \mathbb{Z}^{N_{adia}}$ a vector of integers specifying the adiabatic process. It follows that under any adiabatic process the quantities

$$\theta_i = \begin{cases} (L^{-1} \cdot p)_i \bmod \Lambda_{ii} & \text{for } i \leq \text{rank}(q) \\ (L^{-1} \cdot p)_i & \text{for } i > \text{rank}(q), \end{cases} \quad (3)$$

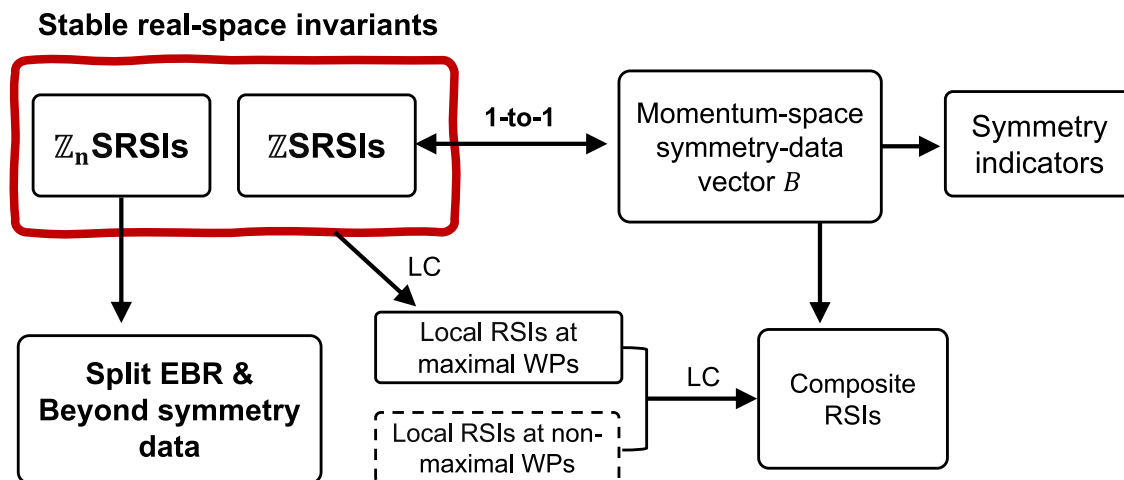


Fig. 2 | Schematic relationship between SRSIs, local RSIs, composite RSIs, symmetry indicators (SIs), and symmetry-data vectors. $\mathbb{Z}$ SRSIs are in one-to-one correspondence with the symmetry-data vector and therefore fully determine all SIs. $\mathbb{Z}$ SRSIs also encode information that can be further processed into indicators for quantities such as fragile topology^{35,48,79} or filling anomaly^{80,81}. $\mathbb{Z}_n$ SRSIs may

capture additional topological information that is invisible to momentum-space data, including topology associated with split EBRs and other non-symmetry-indicated phases. Both local RSIs at maximal and non-maximal WPs, as well as composite RSIs formed from them, can be obtained as linear combinations (LCs) of SRSIs.

are invariant under all adiabatic processes, i.e., $\Delta\theta_i = 0$. This follows from the fact that

$$\Delta\theta_i = (L^{-1} \cdot q \cdot z)_i = \Lambda_{ii}(R \cdot z)_i. \quad (4)$$

Since R is unimodular, $(R \cdot z)_i \in \mathbb{Z}$ and thus $\Delta\theta_i \in \Lambda_{ii}\mathbb{Z}$, which vanishes for all i according to Eq. (3). Eq. (3) constitute our definition for the SRSIs. The first and second cases in Eq. (3) correspond to $\mathbb{Z}_{\Lambda_{ii}}$ SRSIs and $\mathbb{Z}$ SRSIs, respectively. We refer to $\mathbb{Z}_{\Lambda_{ii}}$ SRSIs collectively as $\mathbb{Z}_n$ SRSIs. Practically, for $\mathbb{Z}_n$ SRSIs, we only consider i with $\Lambda_{ii} > 1$, as $\mathbb{Z}_1$ SRSIs are trivial. For further details on the algorithm obtaining SRSIs and the exhaustive listing of SRSIs in all SGs with and without SOC, see SN 3 and SN 7A, respectively.

In the example of SG $Pmm21'$, the algorithm described above yields one $\mathbb{Z}$ SRSI and three $\mathbb{Z}_2$ SRSIs. (For a step-by-step procedure, see Constructing SRSIs from adiabatic processes in “Methods” and SN 3C.) These SRSIs are given by

$$\begin{aligned} \theta_1 &= m[(\bar{E})_{1a}] + m[(\bar{E})_{1b}] + m[(\bar{E})_{1c}] + m[(\bar{E})_{1d}] \\ &\quad + 2m[(\bar{E})_{2e}] + 2m[(\bar{E})_{2f}] + 2m[(\bar{E})_{2g}] \\ &\quad + 2m[(\bar{E})_{2h}] + 4m[(\bar{A})_{4i}], \\ \theta_2 &= m[(\bar{E})_{1b}] \bmod 2, \quad \theta_3 = m[(\bar{E})_{1c}] \bmod 2, \\ \theta_4 &= m[(\bar{E})_{1d}] \bmod 2. \end{aligned} \quad (5)$$

A unique $\mathbb{Z}$ SRSI, θ_1 , corresponds to half the total number of electrons per unit cell, which is invariant under any adiabatic process and fixed by the number of bands. In other SGs, multiple $\mathbb{Z}$ SRSIs may exist, providing information beyond this physical invariant. More generally, SRSIs are linear combinations of site-symmetry irrep multiplicities that can involve contributions from multiple WPs, including both maximal and non-maximal ones.

Finally, let us comment that local RSIs at maximal WPs are a subset of SRSIs. In the case of SG $Pmm21'$, the $\mathbb{Z}_2$ SRSIs θ_2 , θ_3 and θ_4 are identical to the local RSIs at the maximal WPs $1b$, $1c$ and $1d$, respectively. The local RSI at the maximal WP $1a$ can be obtained from the linear combination,

$$\theta_1 + \theta_2 + \theta_3 + \theta_4 \bmod 2 = m[(\bar{E})_{1a}] \bmod 2. \quad (6)$$

While a local RSI at a non-maximal WP is not a topological invariant, the multiplicities of irreps at non-maximal WPs appear in the definition of SRSIs (such as θ_1), reflecting the consideration of all adiabatic processes that involve multiple WPs.

Stable equivalence of band topology

We will now argue that the SRSIs are intimately connected to the notion of stable equivalence of bands. We will start by considering atomic insulators induced from localized orbitals that transform as direct sums of site-symmetry irreps. Consider two site symmetry representations, ρ_1 and ρ_2 , and their corresponding (E)BRs, $\rho_1 \uparrow G$ and $\rho_2 \uparrow G$. These BRs are stably equivalent if they can be adiabatically deformed into each other in the presence of auxiliary trivial bands corresponding to the (E)BR $\rho_{aux} \uparrow G$. Importantly, $\rho_1 \uparrow G$ and $\rho_2 \uparrow G$ can be stably equivalent even if they are inequivalent, i.e., even if they cannot be deformed into each other (and are therefore topologically distinct). The stable equivalence between $\rho_1 \uparrow G$ and $\rho_2 \uparrow G$ can be denoted as $\rho_1 \uparrow G \oplus \rho_{aux} \uparrow G \equiv \rho_2 \uparrow G \oplus \rho_{aux} \uparrow G$.

One crucial property of SRSIs is their ability to indicate the stable equivalence between atomic insulators. We prove in SN 3B that two atomic insulators are stably equivalent if and only if they have matching $\mathbb{Z}$ SRSIs and $\mathbb{Z}_n$ SRSIs. This property justifies the name of SRSIs: if $\rho_1 \uparrow G$ and $\rho_2 \uparrow G$ are two atomic insulators that are not equivalent but have matching SRSIs, then they are (adiabatically and hence topologically) equivalent in the presence of additional trivial bands. This is analogous to the case of fragile topology, which becomes equivalent to trivial bands in the presence of additional (trivial) bands. Topologically trivial bands in the same stable equivalence class must have the same SRSIs.

To illustrate the idea of stable equivalence, we will consider two examples. Let us first consider the simplest case where the adiabatic deformation between two sets of site-symmetry irreps with matching SRSIs does not require auxiliary bands. In the SG $Pmm21'$ with SOC, let us focus on the two band representations induced from distinct site-symmetry irreps, $(\bar{E})_{1a}$ and $(\bar{E})_{1b}$. Their $\mathbb{Z}$ SRSI and $\mathbb{Z}_2$ SRSIs, computable from Eq. (5), are given as

$$\begin{aligned} (\bar{E})_{1a} \uparrow G : & \quad (\theta_1, \theta_2, \theta_3, \theta_4) = (1, 0, 0, 0), \\ (\bar{E})_{1b} \uparrow G : & \quad (\theta_1, \theta_2, \theta_3, \theta_4) = (1, 1, 0, 0). \end{aligned} \quad (7)$$

Since the SRSI vectors differ, we know that these irreps cannot be deformed into one another, even with the addition of auxiliary irreps ρ_{aux} , i.e., $(\bar{E})_{1a} \oplus \rho_{aux} \not\cong (\bar{E})_{1b} \oplus \rho_{aux}$ for any ρ_{aux} . Physically, a single $(\bar{E})_{1a}$ irrep corresponds to a Kramers pair of two orbitals with opposite mirror (M_x or M_y) eigenvalues located at (0, 0). At any position, time-reversal symmetry imposes that orbitals form Kramers pairs. Thus, moving orbitals at (0, 0) to another position while preserving SG symmetries requires at least two Kramers pairs to move together, such as to WP 2g with positions (0, y) and (0, -y) (see also Fig. 1a). Hence, a single Kramers pair at WP 1a cannot move to any other position. The same argument applies to the irrep $(\bar{E})_{1b}$. However, because θ_2 is a $\mathbb{Z}_2$ SRSIs, the SRSIs of $2(\bar{E})_{1a}$ and $2(\bar{E})_{1b}$ are same, meaning that they can be deformed to each other. For example, $2(\bar{E})_{1a}$ at (0,0) can be deformed to $(\bar{E}^2\bar{E})_{2h}$ at (0, y) and (0, -y), and further deformed to $2(\bar{E})_{1b}$ at (0, 1/2) by tuning y from 0 to 1/2.

Now, we consider a case with two distinct band representations that are inequivalent but stably equivalent, requiring auxiliary irrep(s) for deformation between them. Such band representations can be induced from either the same WP or different WPs. For simplicity, we focus on the case where they are induced from the same WP, specifically in SG I432. (For cases where stably equivalent band representations are induced from different WPs, see SN 4D.)

Specifically, consider the two band representations induced from the irreps $(B_2)_{12d}$ and $(B_3)_{12d}$ at the maximal WP 12d(1/4, 1/2, 0). As distinct irreps at the same maximal WP, they cannot be deformed into each other, making them topologically inequivalent. In SG I432, we can define seven $\mathbb{Z}$ SRSIs (θ_z) and three $\mathbb{Z}_2$ SRSIs (θ_{z_2}) (see also SN 3C).

Table 2 | WPs 12d and 24i and site-symmetry irreps in the SG I432 (No. 211)

WP W	G_W	ρ_W
12d(1/4, 1/2, 0)	$C_{2x}, C_{2,y+z}, C_{2,y-z}$	$(A_1)_{12d}, (B_1)_{12d},$ $(B_2)_{12d}, (B_3)_{12d}$
24i(1/4, z + 1/2, z)	$C_{2,y+z}$	$(A)_{24i}, (B)_{24i}$

The second and third columns denote the generators of the site-symmetry group and site-symmetry irreps at the representative position, respectively. Note that, $C_{2x} = \{2_{100}|0, 1, 0\}$, $C_{2,y+z} = \{2_{011}|1/2, 1/2, -1/2\}$, $C_{2,y-z} = \{2_{0\bar{1}1}|1/2, 1/2, 1/2\}$, which transform the coordinates (x, y, z) to (x, -y + 1, -z), (-x + 1/2, z + 1/2, y - 1/2), and (-x + 1/2, -z + 1/2, -y + 1/2), respectively. z is a free real parameter.

Notably, the band representations induced from both $(B_2)_{12d}$ and $(B_3)_{12d}$ have matching SRSIs:

$$\theta_z = (1, 0, 1, 1, 1, -1, 0)^T, \quad \theta_{z_2} = (0, 0, 0)^T, \quad (8)$$

indicating their stable equivalence.

The stable equivalence can be understood through the connectivity between the maximal WP 12d and the non-maximal WP 24i. (For the site-symmetry groups and irreps at these WPs, see Table 2.) For the WP 12d, with representative position $\mathbf{x}_{12d} = (1/4, 1/2, 0)$, there are four points in the WP 24i that are connected to $\mathbf{x}_{12d}$, explicitly given as $\mathbf{x}_{24i,1,\dots,4} = (1/4, z + 1/2, z), (1/4, -z + 1/2, -z), (1/4, z, -z + 1/2), (1/4, -z + 1, z - 1/2)$, where z is a free real parameter. (See Fig. 3a.) A pair of site-symmetry irreps (A) at $\mathbf{x}_{24i,1}$ and $\mathbf{x}_{24i,2}$ can be deformed to the linear combination of (A_1) and (B_3) irreps at $\mathbf{x}_{12d}$, as shown in Fig. 3b. Alternatively, as shown in Fig. 3c, a pair of (A) irreps at $\mathbf{x}_{24i,3}$ and $\mathbf{x}_{24i,4}$ can be deformed to the (A_1) and (B_2) irreps at $\mathbf{x}_{12d}$. Thus, the two different deformation processes considered involving the $(A)_{24i}$ irrep imply the following equivalence relation,

$$(B_2)_{12d} \oplus \rho_{aux} \iff (B_3)_{12d} \oplus \rho_{aux}, \quad (9)$$

where $\rho_{aux} = (A)_{12d}$. This establishes the stable equivalence between the EBRs $(B_2)_{12d} \uparrow G$ and $(B_3)_{12d} \uparrow G$ in the presence of bands $\rho_{aux} \uparrow G$ induced from the auxiliary site-symmetry irrep ρ_{aux} . This example demonstrates how SRSIs capture subtle aspects of band topology, such as stable equivalence, that go beyond simple adiabatic deformation arguments. We note that this I432 example was tabulated in refs. 3,33 as a case where distinct site-symmetry irreps at the same WP induce band representations with matching momentum space little group representations, i.e., they are irrep equivalent in the language of ref. 33. Here we see that the physical origin of the irrep equivalence comes from the stable equivalence of the band representations.

$\mathbb{Z}$ SRSIs are determined by symmetry-data vector

We now establish a crucial property of SRSIs: the $\mathbb{Z}$ SRSIs are in one-to-one correspondence with the momentum-space symmetry data of bands in every non-magnetic space group. We first explain this mapping for atomic insulators and then extend this concept to show how $\mathbb{Z}$ SRSIs can also be assigned to topological phases. To construct the mapping explicitly, let us define the symmetry-data vector B . The symmetry-data vector B is composed of the multiplicities of little-

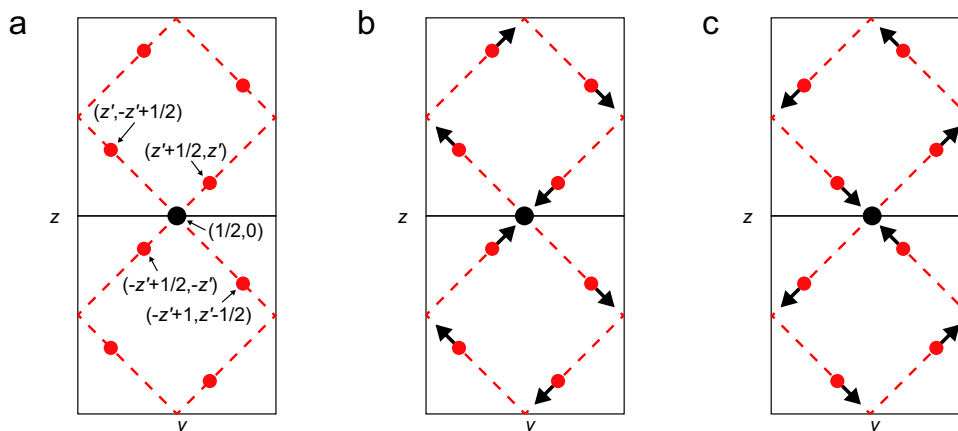


Fig. 3 | Stable equivalence in SG I432 (No. 211). The site-symmetry irreps at WP 12d and 24i are shown on the (y, z) plane with a fixed x-coordinate, x = 1/4. Unit cells are indicated by the solid black lines. The schematic is depicted in reduced coordinates, where the length in both the x- and y-directions is 1. **a** A representative position $\mathbf{x}_{12d} = (1/2, 0)$ of WP 12d (marked as a black dot) is connected to four

positions of WP 24i (marked by red dots with black arrows). **b** A pair of (A) irreps at $(y, z) = (z' + 1/2, z')$ and $(-z' + 1/2, -z')$ are deformed to a sum of (A_1) and (B_3) irreps at $\mathbf{x}_{12d}$, by tuning z' to 0. **c** A pair of (A) irreps at $(z', -z' + 1/2)$ and $(-z' + 1, z' - 1/2)$ are deformed to a sum of (A_1) and (B_2) irreps at $\mathbf{x}_{12d}$, by tuning z' to 1/2.

group irreps at all high-symmetry momenta in the BZ, which we write as

$$B = [m(\rho_{k_1}^1), m(\rho_{k_1}^2), \dots, m(\rho_{k_2}^1), m(\rho_{k_2}^2), \dots]^T, \quad (10)$$

where the nonnegative integers $m(\rho_k^\alpha)$ denote the multiplicity of the irrep ρ_k^α ($\alpha = 1, \dots, N_k^\rho$). The length of B is $N_{\text{BZ}}^\rho = \sum_k N_k^\rho$. The vector B is determined by the symmetry-representation vector p in Eq. (1) as $B = BR \cdot p$, where BR is $N_{\text{BZ}}^\rho \times N_{\text{UC}}^\rho$ band-representation (BR) matrix. The columns of BR are indexed by each irrep ρ_W^i of the site-symmetry group of every WP W , and the corresponding column vectors give the symmetry-data vector for the BR induced from ρ_W^i . By introducing a pseudoinverse $BR^\dagger$ of BR , we find

$$p = BR^\dagger \cdot B + p_{\ker, BR}, \quad (11)$$

where $p_{\ker, BR}$ is a general vector in $\ker BR$, i.e., $BR \cdot p_{\ker, BR} = \mathbf{0}$. By expressing the $\mathbb{Z}$ SRSIs in the second line of Eq. (3) as $\theta_Z = \Theta^{(0)} \cdot p$, collectively, we have

$$\theta_Z = \Theta^{(0)} \cdot BR^\dagger \cdot B + \Theta^{(0)} \cdot p_{\ker, BR}. \quad (12)$$

In a similar way, we represent B as

$$B = BR \cdot [\Theta^{(0)}]^\dagger \cdot \theta_Z + BR \cdot p_{\ker, \Theta^{(0)}}. \quad (13)$$

In all SGs with and without SOC, $\Theta^{(0)} \cdot p_{\ker, BR} = \mathbf{0}$ and $BR \cdot p_{\ker, \Theta^{(0)}} = \mathbf{0}$ (see SN 3B). This establishes a one-to-one mapping between symmetry-data vector B and $\mathbb{Z}$ SRSIs for atomic insulators. We give further details of the construction and explicit examples of the one-to-one mapping between $\mathbb{Z}$ SRSIs and symmetry data vectors in SN 3B and SN 3C.

Let us comment on three key implications of this one-to-one mapping. First, for any atomic insulators AI_1 and AI_2 with the same symmetry-data vector, there exists some integer $\mathcal{N}$ such that $\mathcal{N}AI_1$ and $\mathcal{N}AI_2$ are stably equivalent. We can choose $\mathcal{N}$ by demanding that $\mathcal{N}\theta_{Z_n} = \mathbf{0}$ for all the $\mathbb{Z}_n$ SRSIs in the space group.

Second, all composite RSIs are determined by $\mathbb{Z}$ SRSIs. Local RSIs, particularly at non-maximal WPs, are not mapped uniquely to symmetry-data vectors due to their failure as topological invariants. To address this, ref. 36 introduced composite RSIs, which are linear combinations of local RSIs across multiple WPs that can be determined from the symmetry-data vector. However, the definitions of composite RSIs rely on ad hoc methods, leaving their organizing principles still to be found. By contrast, $\mathbb{Z}$ SRSIs incorporate composite RSIs as a subset, providing a systematic framework based on the one-to-one mapping.

Finally, while our discussion so far has focused on atomic insulators with symmetry-representation vectors composed of non-negative integers, the linear nature of the one-to-one mapping ensures that $\mathbb{Z}$ SRSIs can be assigned to topological phases. This includes symmetry-indicated fragile or stable topological phases, where Eq. (11) yields a symmetry-representation vector p having negative integers or rational fractions for a given symmetry-data vector, respectively. As $\mathbb{Z}$ SRSIs are directly calculable from symmetry-data vectors, they remain well-defined even for symmetry-indicated topological phases.

SRSIs determine SIs

The SIs determine whether a given set of bands is necessarily (symmetry-indicated) stable topological bands. They are expressed in terms of the symmetry-data vector B as

$$\kappa = A \cdot B \bmod w, \quad (14)$$

where κ is the N_k -dimensional vector of SIs, A is a $N_k \times N_{\text{BZ}}^\rho$ matrix defining the SIs (as derived in ref. 18), and $w \in \mathbb{N}$ is a N_k -dimensional

vector. A non-zero κ indicates that the corresponding bands must be stably topologically nontrivial. For symmetry-indicated stable topological phases, where the symmetry-representation vector p takes fractional values, the $\mathbb{Z}$ SRSIs calculated from B , take fractional values^{35,48}. Since $\mathbb{Z}$ SRSIs are in one-to-one correspondence with symmetry-data vectors, the fractional values of $\mathbb{Z}$ SRSIs fully specify all nontrivial SIs. In general, using Eq. (13) combined with $BR \cdot p_{\ker, \Theta^{(0)}} = \mathbf{0}$, we can write

$$\kappa = A \cdot BR \cdot [\Theta^{(0)}]^\dagger \cdot \theta_Z \bmod w. \quad (15)$$

In SN 7B, we provide a comprehensive list of the quantitative relationship between $\mathbb{Z}$ SRSIs and SIs in all 230 SGs with and without SOC.

Topological band splitting indicated by $\mathbb{Z}_n$ SRSIs

In contrast to $\mathbb{Z}$ SRSIs, there is no straightforward way to extend $\mathbb{Z}_n$ SRSIs to topological bands since they are not determined by momentum space symmetry data. Despite this, we demonstrate that $\mathbb{Z}_n$ SRSIs provide a sufficient criterion for band topology, even in cases where symmetry-data vectors or SIs fail to diagnose nontrivial topology. The key idea is as follows: Suppose we assume that a given set of bands is topologically trivial, allowing the assignment of position space orbital multiplicities and $\mathbb{Z}_n$ SRSIs. If the assigned $\mathbb{Z}_n$ SRSIs violate certain consistency conditions, this assumption of trivial topology is invalidated, indicating that the bands must exhibit nontrivial topology.

As a concrete illustration, let us consider a set of valence and conduction bands separated by a band gap. Denote the Hilbert spaces spanned by the valence and conduction bands as V and C , respectively. We assume that the full Hilbert space $\mathcal{H}_{\text{Lat}} = V \oplus C$ is topologically trivial, and so induced from orbitals at some WPs. However, the valence and conduction bands corresponding to V and C can individually be atomic, fragile topological, or stable topological. (If either of V or C is stable topological, then both must be stable topological.)

Now, let us compare the symmetry data vectors of the full, valence, and conduction bands. They must satisfy

$$B[\mathcal{H}_{\text{Lat}}] = B[V] + B[C]. \quad (16)$$

Similarly, let us denote the SRSIs of a set of bands X by $\theta[X]$ ($X = C, V, \mathcal{H}_{\text{Lat}}$). The $\mathbb{Z}$ SRSIs $\theta_Z[X]$ can be computed from the symmetry-data vector of X . If at least one of $\theta_Z[X]$ ($X = C, V$) takes a fractional value, the corresponding bands must be stable topological and have nontrivial SIs. Otherwise, the band splitting is either trivial or non-symmetry-indicated topological (NSIT), implying that either V or C is topological, but its topology is not indicated by the symmetry-data vector.

We now show how $\mathbb{Z}_n$ SRSIs can provide sufficient conditions to detect NSIT band splittings. Suppose that V and C have integer-valued $\mathbb{Z}$ SRSIs. Let us temporarily assume that both V and C correspond to atomic insulators with well-defined $\mathbb{Z}_n$ SRSIs. Under this assumption, the full set of SRSIs is well-defined for V , C , and $\mathcal{H}_{\text{Lat}}$, and must satisfy

$$\theta_{Z_n}[\mathcal{H}_{\text{Lat}}] = \theta_{Z_n}[V] + \theta_{Z_n}[C] \bmod n. \quad (17)$$

If Eq. (17) is not satisfied, it indicates that our initial assumption—that both V and C are trivial—is incorrect. Instead, the gap between V and C must result in band topology not captured by SIs, implying that either V or C must be fragile or NSIT. Below, we explicitly demonstrate how $\mathbb{Z}_n$ SRSIs can identify a topological band gap using a tight-binding model in the SG $P41'$.

$\mathbb{Z}_n$ RSIs and split EBRs

A central result of ref. 1 is that when any EBR is separated into multiple sets of bands by band gap(s), at least one of these sets must be

topological. This holds true even if the symmetry-data vector of the gapped sets of bands can be decomposed into those of other EBRs. Previous works^{1,30–32} have studied cases where the bands constituting an EBR are split by a band gap, and the (stable or fragile) SIs of each resulting gapped sets of bands are nontrivial.

However, there are instances where an EBR (denoted as *EBR*) has a symmetry data vector that is identical to the symmetry data vector for a sum of other EBRs. This is expressed as

$$B[EBR] = B[EBR_1] + B[EBR_2] + \dots \quad (18)$$

Nontrivial solutions to Eq. (18) exist in 51 SGs. In such cases, the splitting of *EBR* is NSIT since symmetry-data vectors fail to capture the nontrivial topology of gapped band sets of split EBRs. In SN 7C, a detailed list of all 211 split EBRs with NSIT band splitting (with and without SOC) is provided, occurring in 51 of the 230 SGs.

Since $\mathbb{Z}_n$ SRSIs provide a sufficient criterion even for NSIT band splitting, it is natural to ask how effectively $\mathbb{Z}_n$ SRSIs can diagnose all split EBR cases. For this, we generalize Eq. (17) for the putative EBR decomposition implied by Eq. (18) as

$$\theta_{\mathbb{Z}_n}[EBR] \equiv \theta_{\mathbb{Z}_n}[EBR_1] + \theta_{\mathbb{Z}_n}[EBR_2] \dots \text{mod } n. \quad (19)$$

We find that violations of this condition are sufficient to diagnose NSIT in all but 8 solutions to Eq. (18) in 5 SGs (all in the presence of SOC). That is, except for these 8 exceptions, violation of Eq. (19) implies that the splitting Eq. (18) cannot imply an (adiabatic) equivalence of band representations. The eight exceptional cases arise in cases where *EBR* is stably equivalent (but not equivalent) to a sum of EBRs. In these cases, the fact that the split EBR [*EBR* in Eq. (18)] and its hypothetical EBR decompositions, $EBR_1 \oplus EBR_2 \oplus \dots$, have matching SRSIs, including $\mathbb{Z}_n$ SRSIs, means that there exists some auxiliary band representation BR_{aux} such that $EBR \oplus BR_{\text{aux}} \equiv EBR_1 \oplus EBR_2 \oplus \dots \oplus BR_{\text{aux}}$ could be true (see SN 4D). Nonetheless, the ability of $\mathbb{Z}_n$ SRSIs to diagnose almost all split EBR cases—except 8 exceptions—underscores the power of SRSIs in capturing band topology beyond the limitations of symmetry-data vectors and SIs. Note, however, that while SRSIs allow us to exclude the existence of an adiabatic equivalence of split EBRs (in all but 8 cases), they alone do not rule out the theoretical possibility of rewriting an EBR as a sum of other EBRs through a large gauge transformation (i.e., a non-trivial change of basis that cannot be carried out adiabatically). In many cases, Wilson loop techniques such as those employed in ref. 33 can be used to rule out the existence of such large gauge transformations. We currently know of no cases where a pair of EBRs is equivalent under such a large gauge transformation, and we conjecture that no such cases exist. We defer a more thorough investigation of this point to future work.

Tight-binding model in SG P41'

We now discuss an example of a split EBR with NSIT and demonstrate how $\mathbb{Z}_n$ SRSIs diagnose this case. Specifically, we consider the SG P41' (No. 75) with SOC and time-reversal symmetry (TRS) in 2D. The spatial symmetries of this SG include twofold and fourfold rotations, C_{2z} and C_{4z} , as well as two translations, $\{E|\hat{x}\}$ and $\{E|\hat{y}\}$. Note that C_{2z} and C_{4z} transform (x, y) to $(-x, -y)$ and $(-y, x)$, respectively. We focus on the maximal WP 1a and the non-maximal WP 2c. The WP 1a is located at $(0, 0)$, and its site-symmetry group, generated by C_{4z} , has two irreps: $(^1\bar{E}_1^2\bar{E}_1)_{1a}$ and $(^1\bar{E}_2^2\bar{E}_2)_{1a}$. The WP 2c consists of the positions $(0, 1/2)$ and $(1/2, 0)$. At these positions, the site-symmetry group are generated by $\{E|\hat{y}\}C_{2z}$ and $\{E|\hat{x}\}C_{2z}$, respectively. This group has a unique irrep $(^1\bar{E}^2\bar{E})_{2c}$.

For a split EBR with NSIT band splitting, let us consider a putative EBR decomposition:

$$(^1\bar{E}^2\bar{E})_{2c} \uparrow G \equiv (^1\bar{E}_1^2\bar{E}_1)_{1a} \uparrow G \oplus (^1\bar{E}_2^2\bar{E}_2)_{1a} \uparrow G. \quad (20)$$

This decomposition satisfies the symmetry-data vector condition in Eq. (16). However, a unique $\mathbb{Z}_2$ SRSI (see SN 7A), $\theta_5 = m[(^1\bar{E}^2\bar{E})_{2c}] \text{mod } 2$, reveals that the decomposition in Eq. (20) is invalid. Specifically, we find

$$\begin{aligned} \theta_5[(^1\bar{E}^2\bar{E})_{2c}] &= 1, & \theta_5[(^1\bar{E}_1^2\bar{E}_1)_{1a}] &= 0, \\ \theta_5[(^1\bar{E}_2^2\bar{E}_2)_{1a}] &= 0, \end{aligned} \quad (21)$$

contradicting Eq. (17). Consequently, a gap separating the two sets of bands identified as $(^1\bar{E}_1^2\bar{E}_1)_{1a} \uparrow G$ and $(^1\bar{E}_2^2\bar{E}_2)_{1a} \uparrow G$ requires at least one set of bands to be either fragile or non-symmetry-indicated stable topological. Physically, the decomposition in Eq. (20) is impossible because two $(^1\bar{E}^2\bar{E})_{2c}$ irreps can be symmetrically moved away from the WP 2c; however, a single $(^1\bar{E}^2\bar{E})_{2c}$ irrep alone cannot.

As a concrete example, consider a tight-binding Hamiltonian where the full Hilbert space $\mathcal{H}_{\text{Lat}}$ is spanned by the irrep $(^1\bar{E}^2\bar{E})_{2c}$. The basis orbitals for this irrep consist of two Kramers pairs of *s*-like orbitals possessing opposite spins, located at $\hat{x}/2 = (1/2, 0)$ and $\hat{y}/2 = (0, 1/2)$ of WP 2c in each unit cell. Denoting the unit cells by Bravais lattice vectors $\mathbf{R}$, we label the basis orbitals in each unit cell as $|\mathbf{R}, \alpha\rangle = (|\mathbf{R} + \hat{x}/2, \uparrow\rangle, |\mathbf{R} + \hat{x}/2, \downarrow\rangle, |\mathbf{R} + \hat{y}/2, \uparrow\rangle, |\mathbf{R} + \hat{y}/2, \downarrow\rangle)_\alpha$ ($\alpha = 1, \dots, 4$). To achieve a band splitting described in Eq. (20), we construct trial Wannier states transforming under the EBR $(^1\bar{E}_1^2\bar{E}_1)_{1a} \uparrow G$ (see SN 5A). These states can be used to construct a tight-binding Hamiltonian^{38,49,50}. We choose the trial states $|\Phi_{\mathbf{R}}^\pm\rangle$ with the following (unnormalized) Fourier transforms:

$$u_{\mathbf{k}\alpha}^+ = \frac{1}{\sqrt{2}} \left(\cos \frac{k_x}{2}, -i \sin \frac{k_x}{2}, \cos \frac{k_y}{2}, -\sin \frac{k_y}{2} \right)_\alpha, \quad (22)$$

$$u_{\mathbf{k}\alpha}^- = \frac{1}{\sqrt{2}} \left(-i \sin \frac{k_x}{2}, -\cos \frac{k_x}{2}, \sin \frac{k_y}{2}, -\cos \frac{k_y}{2} \right)_\alpha, \quad (23)$$

where $\mathbf{k} = (k_x, k_y)$ lies in the BZ. The tight-binding Hamiltonian is then constructed as

$$[H(\mathbf{k})]_{\alpha\beta} = t(u_{\mathbf{k}\alpha}^+ u_{\mathbf{k}\beta}^{+\dagger} + u_{\mathbf{k}\alpha}^- u_{\mathbf{k}\beta}^{-\dagger}), \quad (24)$$

with the energy scale t .

This model hosts two exact zero-energy flat bands and two dispersive bands, as shown in Fig. 4a. In position space, Eq. (24) represents the hopping processes between trial states, i.e., $[H(\mathbf{R})]_{\alpha\beta} = \sum_{\mathbf{R}'} t(|\Phi_{\mathbf{R}}^\pm\rangle\langle\Phi_{\mathbf{R}'}^\pm| + |\Phi_{\mathbf{R}}^\pm\rangle\langle\Phi_{\mathbf{R}'}^\mp|)$. This means that the bands spanned by these trial states become dispersive. Thus, the dispersive bands correspond to the EBR $(^1\bar{E}_1^2\bar{E}_1)_{1a} \uparrow G$, as determined by the representation of the trial states $|\Phi_{\mathbf{R}}^\pm\rangle$. Since the full Hilbert space corresponds to $(^1\bar{E}^2\bar{E})_{2c} \uparrow G$, the gapped flat bands, which are spanned by the complement of the trial states correspond to $(^1\bar{E}^2\bar{E})_{2c} \uparrow G \ominus (^1\bar{E}_1^2\bar{E}_1)_{1a} \uparrow G$, whose symmetry-data vector matches that of $(^1\bar{E}_2^2\bar{E}_2)_{1a} \uparrow G$. As indicated by Eq. (21), this band must be topological – either with fragile or non-symmetry-indicated stable topology.

The Wilson loop spectrum of the two flat bands exhibits double winding, indicating fragile topology protected by $C_{2z}T$ symmetry^{51–56} (see Fig. 4b). In contrast, the Wilson loop of the dispersive bands is trivial, consistent with the fact that they correspond to an EBR. Notably, a phase transition could subsequently induce stable $\mathbb{Z}_2$ quantum spin hall topology in each of the valence and conduction bands, as shown in Fig. 4d (see SN 5A for more details). However,

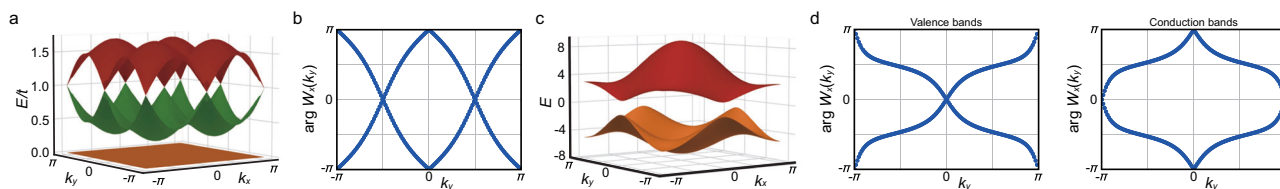


Fig. 4 | Tight-binding models in SG $P41'$. **a** Energy spectrum of $H(\mathbf{k})$ in Eq. (24). There are two degenerate zero-energy flat bands and two dispersive bands. The dispersive bands form the EBR $(^1\bar{E}_1^2\bar{E}_1)_{1a} \uparrow G$. **b** Spectrum of the k_x -directed Wilson loop $W_x(k_y)$ for the two flat bands. The double winding, protected by $C_{2z}T$ symmetry, implies fragile topology. The Wilson loop of the two dispersive bands does

not wind (not shown). **c** Energy spectrum of the model in the $\mathbb{Z}_2$ -odd phase discussed in SN 5A. Each band is doubly-degenerate. **d** k_x -directed Wilson loop spectra of the valence and the conduction bands. The windings indicate the $\mathbb{Z}_2$ -odd topology of both the valence and conduction bands. Wilson loops were computed using the algorithm of ref. 82.

unlike the standard $\mathbb{Z}_2$ models like the Kane-Mele model⁵⁷ and the BHZ model⁵⁸, where both sets of bands can be trivialized via band inversions, it is impossible to remove the windings of both the sets as this model still realizes a split EBR and violates Eq. (19). A hint of this can be seen in the relative π -phase shift between the spectra of the valence and the conduction band Wilson loops, as shown in Fig. 4d. A comprehensive study of this phenomenon is deferred to a future work.

SRSI-based diagnosis of a real material

To illustrate how SRSIs enable the identification of symmetry-protected phases beyond SIs, we consider obstructed atomic insulators (OAI). Although OAIs are characterized by trivial SIs, they can exhibit nontrivial boundary phenomena, which have been linked to enhanced catalytic functionalities^{36,59}. OAIs, therefore, provide a well-defined and physically meaningful class of materials for which SRSI-based indicators can be constructed systematically.

In general, once the atomic WPs of a material are specified, one can construct $\mathbb{Z}$ - or $\mathbb{Z}_m$ -valued ($m \geq 2$) OAI indicators as linear combinations of SRSIs that necessarily vanish for any unobstructed phase in that material. A nonzero value of such an indicator implies that at least one Wannier orbital must reside on a WP not occupied by the constituent atoms, thereby diagnosing an obstructed limit. The general construction of these SRSI-based OAI indicators is described in SN 6.

As a concrete material example, we consider the compound Y_3Al_2 [Inorganic Crystal Structure Database (ICSD)⁶⁰ collection code 609643], crystallizing in SG $P4_2nm$ (No. 102). In a conventional unit cell, the crystal contains twelve Y atoms and eight Al atoms, occupying the $4b$ and $4c$ WPs of this SG. Using the symmetry data for this material, we evaluate the relevant $\mathbb{Z}$ SRSI for SG $P4_2nm$. Combining this $\mathbb{Z}$ SRSI with the information that the atoms occupy the $4b$ and $4c$ WPs, we obtain a $\mathbb{Z}_2$ -valued OAI indicator, which is nonzero for Y_3Al_2 . This establishes that Y_3Al_2 realizes an OAI. See SN 6 for the detailed analysis. We note that Y_3Al_2 has been previously identified as a filling-enforced OAI⁶¹ by exploiting local RSIs along with a set of filling constraints. While such approaches rely on specific filling constraints, the SRSI-based diagnosis presented here does not depend on filling-enforced conditions and applies more generally. Specifically, a main advantage of the SRSI-based diagnosis is that it depends only on symmetry data and the atomic WP configuration of a material within any SG. This highlights the broader applicability of SRSIs as a real-space framework for diagnosing topology beyond SIs.

Discussion

In this work, we introduced SRSIs as a novel framework that extends the capabilities of TQC beyond SIs. While SIs have been instrumental in identifying topological materials using momentum-space symmetry data, SRSIs offer a complementary perspective by incorporating position-space information. Both $\mathbb{Z}$ SRSIs and

$\mathbb{Z}_n$ SRSIs provide more information than SIs; $\mathbb{Z}$ SRSIs are one-to-one mapped to symmetry-data vectors and determine the SIs, while symmetry data cannot determine $\mathbb{Z}_n$ SRSIs, meaning that $\mathbb{Z}_n$ SRSIs have information not encoded in the symmetry-data vector. Moreover, $\mathbb{Z}_n$ SRSIs enable the diagnosis of NSIT band splittings (with only 8 rare exceptions in 5 SGs), which cannot be diagnosed by SIs or symmetry-data vectors.

In addition, SRSIs enrich the TQC framework by highlighting the importance of stable equivalence of band representations and offering a more comprehensive classification of both topological and trivial phases. We demonstrated how distinct EBR can be shown to be adiabatically connected in the presence of auxiliary trivial bands, implying their stable equivalence, based on matching SRSIs. This stable equivalence is important in several situations. For example, when studying the topology of bands, extending the set of bands with additional trivial bands (by considering energetically close bands) necessitates a classification scheme based on stable equivalence, ensuring that the classification remains independent of such extensions. Also, in 3D photonic crystals, Maxwell's equations often give rise to singular band structures for transversely polarized modes^{62–64}. To regularize this singularity, additional auxiliary bands can be introduced^{63–66}. The stable equivalence relation between bands thus naturally arises in the classification of photonic bands, ensuring the independence of the classification from the choice of auxiliary bands. The application of SRSIs provides a framework connecting stable equivalence and topological classification, which is directly applicable to bands in 3D photonic crystals as well⁶⁷. This underscores the practical utility of SRSIs in identifying and classifying topological phases in both electronic and metamaterial systems. Beyond classification, we note that SRSIs are connected to known topological and geometric responses in crystalline systems. Fractional SRSIs are tied to bulk topological response coefficients via nonzero SIs^{13,18}, while local RSIs contained within SRSIs control quantized defect-bound and geometric responses^{68,69}.

We also briefly comment on the relation between our approach and the classification scheme based on K theory^{70,71}. The number of $\mathbb{Z}$ SRSIs and $\mathbb{Z}_n$ SRSIs matches the group structure of the $E_{0,0}^2$ page in the real-space Atiyah-Hirzebruch spectral sequence introduced in ref. 71, where the equivalence classes are defined by adiabatic deformations of site-symmetry orbitals. Thus, the SRSIs provide a systematic way to compute this E^2 -page, and our formulas for the SRSIs in SN 7A give an explicit construction of the elements of the $E_{0,0}^2$ page that was not provided in earlier references.

A further natural follow-up to our work would be the generalization of SRSIs to magnetic space groups^{72–75}. As a concrete example, we analyzed the magnetic SG $F43c$ in SN 3C, demonstrating that our formalism can be directly extended to magnetic systems. More broadly, recent works based on K theory⁷⁶ suggest that magnetic SGs may host new types of adiabatic equivalences beyond those in nonmagnetic cases. Connecting these ideas with

SRSIs may offer an interesting direction. It would also be interesting to develop an efficient algorithm for calculating the SRSIs from density functional theory, enabling high-throughput material searches based on SRSIs and SRSI-derived OAI indicators, as well as the split EBR tables provided in SN 7. Since SRSIs do not distinguish between topologically distinct but stably equivalent (E)BRs with auxiliary trivial bands, the derivation and characterization of fragile RSIs, which address these distinctions, represent an important avenue for future study. Finally, additional research is required to definitively exclude the existence of large gauge transformations that could signify equivalences between split EBRs and a linear combination of EBRs.

Methods

Constructing SRSIs from adiabatic processes

We illustrate the construction of stable real-space invariants (SRSIs) using the space group (SG) $Pmm21'$ with spin-orbit coupling. The Wyckoff positions (WPs) and site-symmetry irreps are summarized in Table 1. The distinct site-symmetry irreps defining the site-symmetry representation vector p are

$$(\bar{E})_{1a}, (\bar{E})_{1b}, (\bar{E})_{1c}, (\bar{E})_{1d}, ({}^1\bar{E}^2\bar{E})_{2e}, ({}^1\bar{E}^2\bar{E})_{2f}, ({}^1\bar{E}^2\bar{E})_{2g}, ({}^1\bar{E}^2\bar{E})_{2h}, (\bar{A}\bar{A})_{4i}, \quad (25)$$

giving $N_{UC}^p = 9$. To construct the adiabatic-process matrix q , we identify 12 adiabatic processes that span the space of all possible adiabatic deformations in this SG. As explained in the main text, for example, two $(\bar{E})_{1d}$ irreps can be adiabatically deformed into either a $({}^1\bar{E}^2\bar{E})_{2f}$ or a $({}^1\bar{E}^2\bar{E})_{2h}$ irrep. Similarly, two $(\bar{E})$ irreps at the maximal WPs $1a, 1b, 1c$ can be adiabatically deformed into a $({}^1\bar{E}^2\bar{E})$ irrep at the connected non-maximal WPs $(2e, 2g), (2f, 2g)$, and $(2e, 2h)$, respectively. The remaining four adiabatic processes deform the $(\bar{A}\bar{A})_{4i}$ irrep at the general WP $4i$ into two copies of the irrep $({}^1\bar{E}^2\bar{E})$ at a WP $2y$ ($y = e, f, g, h$). We therefore find $N_{adia} = 12$. For these 12 processes, the adiabatic-process matrix q is

$$q = \begin{pmatrix} 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 2 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \end{pmatrix}, \quad (26)$$

where the row basis is ordered as in Eq. (25), and each column represents an adiabatic process described above. For instance, the first column of q represents the adiabatic process, $2(\bar{E})_{1a} \iff ({}^1\bar{E}^2\bar{E})_{2e}$, which creates (removes) two $(\bar{E})_{1a}$ irreps while removing (creating) a $({}^1\bar{E}^2\bar{E})_{2e}$ irrep.

The Smith decomposition of the integer matrix q is given by $L \cdot A \cdot R$, where L and R are integer unimodular matrices. In the present

example, the matrices L, A , and R are given by

$$L = \begin{pmatrix} 2 & 2 & 0 & -4 & 2 & -1 & 0 & 2 & -1 \\ 0 & 0 & 2 & 0 & -2 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 4 & -2 & 2 & 0 & -3 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (27)$$

$$R = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 2 & 2 & 2 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & -2 & 0 & 1 & 0 & -1 & 1 & -3 & 1 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 & 0 & 1 & 1 & -1 & 1 & -3 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 2 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 2 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The diagonal entries of A are

$$\text{diag}(A) = (1, 1, 1, 1, 1, 2, 2, 2, 0)^T. \quad (28)$$

From this, we find that $\text{rank}(q) = 8$. According to the definition in Eq. (3), this decomposition yields three $\mathbb{Z}_2$ SRSIs and a single $\mathbb{Z}$ SRSI, since $N_{UC}^p - \text{rank}(q) = 1$. We discard the rows i corresponding to $A_{ii} = 1$, as these generate trivial $\mathbb{Z}_1$ SRSIs and therefore contain no physical information. The remaining three rows, corresponding to $A_{ii} = 2$, imply the existence of three $\mathbb{Z}_2$ SRSIs. To construct the SRSI matrices explicitly, we compute the inverse of L :

$$L^{-1} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 \\ 1 & 0 & 1 & 0 & 2 & 0 & 2 & 1 & 3 \\ 2 & 1 & 1 & 1 & 4 & 2 & 4 & 0 & 6 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & -2 & 0 \\ 2 & 2 & 1 & 2 & 4 & 4 & 4 & 2 & 6 \\ 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 4 \end{pmatrix}. \quad (29)$$

Let us denote the three $\mathbb{Z}_2$ SRSIs $(\theta_1, \theta_2, \theta_3)$ and the $\mathbb{Z}$ SRSI θ_4 as

$$(\theta_1, \theta_2, \theta_3)^T = \Theta^{(2)} \cdot p, \quad \theta_4 = \Theta^{(0)} \cdot p. \quad (30)$$

Then, following the definition of SRSIs in Eq. (3), we obtain

$$\begin{aligned}\Theta^{(2)} &= (L^{-1})_{6,7,8} \bmod 2 = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \\ \Theta^{(0)} &= (L^{-1})_9 = \begin{pmatrix} 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 4 \end{pmatrix}.\end{aligned}\quad (31)$$

Note that the matrices $\Theta^{(0)}$ and $\Theta^{(2)}$ are not unique, since they may always be redefined by unimodular transformations. For example, by performing the Hermite decomposition⁷⁷ of $\Theta^{(2)}$, we obtain the redefined matrix

$$\begin{aligned}\Theta_{\text{new}}^{(2)} &= \begin{pmatrix} 1 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix} \cdot \Theta^{(2)} \\ &= \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.\end{aligned}\quad (32)$$

Using the $\mathbb{Z}$ SRSI together with the $\mathbb{Z}_2$ SRSIs defined by $\Theta^{(0)}$ and $\Theta_{\text{new}}^{(2)}$, we recover the same expressions for the SRSIs in SG $Pmm21'$ as those presented in Eq. (5) of the main text. A more detailed discussion of the algorithm for obtaining SRSIs and their possible redefinitions is provided in SN 3A, and additional examples for other SGs are presented in SN 3C.

Data availability

The data supporting the findings of this study are available from the corresponding author upon request.

Code availability

The code supporting the findings of this study are available from the corresponding author upon request.

References

- Bradlyn, B. et al. Topological quantum chemistry. *Nature* **547**, 298 (2017).
- Cano, J. & Bradlyn, B. Band representations and topological quantum chemistry. *Annu. Rev. Condens. Matter Phys.* **12**, 225 (2021).
- Bacry, H., Michel, L., & Zak, J. Symmetry and classification of energy bands in crystals. in *Group Theoretical Methods in Physics*, edited by H.-D. Doebner, J.-D. Hennig, and T. D. Palev 289–308 (Springer Berlin Heidelberg, Berlin, Heidelberg, 1988).
- Vergniory, M. G. et al. Graph theory data for topological quantum chemistry. *Phys. Rev. E* **96**, 023310 (2017).
- Cano, J. et al. Building blocks of topological quantum chemistry: Elementary band representations. *Phys. Rev. B* **97**, 035139 (2018).
- Elcoro, L. et al. Double crystallographic groups and their representations on the Bilbao Crystallographic Server. *J. Appl. Crystallogr.* **50**, 1457 (2017).
- Evarestov, R. A. & Smirnov, V. P., *Site Symmetry in Crystals*. (Springer, 1997).
- Michel, L. & Zak, J. Connectivity of energy bands in crystals. *Phys. Rev. B* **59**, 5998 (1999).
- Bacry, H., Michel, L. & Zak, J. Symmetry and analyticity of energy bands in solids. *Phys. Rev. Lett.* **61**, 1005 (1988).
- Fu, L. & Kane, C. L. Topological insulators with inversion symmetry. *Phys. Rev. B* **76**, 045302 (2007).
- Hughes, T. L., Prodan, E. & Bernevig, B. A. Inversion-symmetric topological insulators. *Phys. Rev. B* **83**, 245132 (2011).
- Turner, A. M., Zhang, Y., Mong, R. S. K. & Vishwanath, A. Quantized response and topology of magnetic insulators with inversion symmetry. *Phys. Rev. B* **85**, 165120 (2012).
- Fang, C., Gilbert, M. J. & Bernevig, B. A. Bulk topological invariants in noninteracting point group symmetric insulators. *Phys. Rev. B* **86**, 115112 (2012).
- Alexandradinata, A., Dai, X. & Bernevig, B. A. Wilson-loop characterization of inversion-symmetric topological insulators. *Phys. Rev. B* **89**, 155114 (2014).
- Kruthoff, J. et al. Topological classification of crystalline insulators through band structure combinatorics. *Phys. Rev. X* **7**, 041069 (2017).
- Khalaf, E., Po, H. C., Vishwanath, A. & Watanabe, H. Symmetry indicators and anomalous surface states of topological crystalline insulators. *Phys. Rev. X* **8**, 031070 (2018).
- Po, H. C., Vishwanath, A. & Watanabe, H. Symmetry-based indicators of band topology in the 230 space groups. *Nat. Commun.* **8**, 50 (2017).
- Song, Z., Zhang, T., Fang, Z. & Fang, C. Quantitative mappings between symmetry and topology in solids. *Nat. Commun.* **9**, 3530 (2018).
- Ono, S. & Watanabe, H. Unified understanding of symmetry indicators for all internal symmetry classes. *Phys. Rev. B* **98**, 115150 (2018).
- Po, H. C. Symmetry indicators of band topology. *J. Phys.: Condens. Matter* **32**, 263001 (2020).
- Zhang, T. & Murakami, S. Predicting topological materials: symmetry-based indicator theories and beyond. *J. Phys. D: Appl. Phys.* **54**, 414002 (2021).
- Vergniory, M. G. et al. A complete catalogue of high-quality topological materials. *Nature* **566**, 480 (2019).
- Zhang, T. et al. Catalogue of topological electronic materials. *Nature* **566**, 475 (2019).
- Tang, F., Po, H. C., Vishwanath, A. & Wan, X. Comprehensive search for topological materials using symmetry indicators. *Nature* **566**, 486 (2019).
- Wang, D. et al. Two-dimensional topological materials discovery by the symmetry-indicator method. *Phys. Rev. B* **100**, 195108 (2019).
- Xu, Y. et al. High-throughput calculations of magnetic topological materials. *Nature* **586**, 702 (2020).
- Vergniory, M. G. et al. All topological bands of all nonmagnetic stoichiometric materials. *Science* **376**, eabg9094 (2022).
- Wieder, B. J. et al. Topological materials discovery from crystal symmetry. *Nat. Rev. Mater.* **7**, 196 (2022).
- Po, H. C., Watanabe, H. & Vishwanath, A. Fragile topology and Wannier obstructions. *Phys. Rev. Lett.* **121**, 126402 (2018).
- Cano, J. et al. Topology of disconnected elementary band representations. *Phys. Rev. Lett.* **120**, 266401 (2018).
- Bouhon, A., Black-Schaffer, A. M. & Slager, R.-J. Wilson loop approach to fragile topology of split elementary band representations and topological crystalline insulators with time-reversal symmetry. *Phys. Rev. B* **100**, 195135 (2019).
- Bradlyn, B., Wang, Z., Cano, J. & Bernevig, B. A. Disconnected elementary band representations, fragile topology, and Wilson loops as topological indices: An example on the triangular lattice. *Phys. Rev. B* **99**, 045140 (2019).
- Cano, J. et al. Topology invisible to eigenvalues in obstructed atomic insulators. *Phys. Rev. B* **105**, 125115 (2022).
- Peri, V. et al. Experimental characterization of fragile topology in an acoustic metamaterial. *Science* **367**, 797 (2020).
- Song, Z.-D., Elcoro, L. & Bernevig, B. A. Twisted bulk-boundary correspondence of fragile topology. *Science* **367**, 794 (2020).
- Xu, Y. et al. Three-dimensional real space invariants, obstructed atomic insulators and a new principle for active catalytic sites. Preprint at arXiv <https://doi.org/10.48550/arXiv.2111.02433> (2021).

37. Alexandradinata, A., Höller, J., Wang, C., Cheng, H. & Lu, L. Crystallographic splitting theorem for band representations and fragile topological photonic crystals. *Phys. Rev. B* **102**, 115117 (2020).
38. Schindler, F. & Bernevig, B. A. Noncompact atomic insulators. *Phys. Rev. B* **104**, L201114 (2021).
39. Kooi, S. H., van Miert, G. & Ortix, C. Classification of crystalline insulators without symmetry indicators: atomic and fragile topological phases in twofold rotation symmetric systems. *Phys. Rev. B* **100**, 115160 (2019).
40. Li, H. & Sun, K. Pfaffian formalism for higher-order topological insulators. *Phys. Rev. Lett.* **124**, 036401 (2020).
41. Bouhon, A., Bzdušek, T. & Slager, R.-J. Geometric approach to fragile topology beyond symmetry indicators. *Phys. Rev. B* **102**, 115135 (2020).
42. Kooi, S., van Miert, G. & Ortix, C. The bulk-corner correspondence of time-reversal symmetric insulators. *npj Quantum Mater.* **6**, 1 (2021).
43. Henke, J., Kurttutan, M., Kruthoff, J. & van Wezel, J. Topological invariants of rotationally symmetric crystals. *Phys. Rev. B* **104**, L201110 (2021).
44. Li, H. & Wan, S. Homotopy invariant in time-reversal and twofold rotation symmetric systems. *Phys. Rev. B* **104**, 045150 (2021).
45. Chen, Y., Huang, S.-J., Hsu, Y.-T. & Wei, T.-C. Topological invariants beyond symmetry indicators: boundary diagnostics for twofold rotationally symmetric superconductors. *Phys. Rev. B* **105**, 094518 (2022).
46. Bradlyn, B. et al. Band connectivity for topological quantum chemistry: band structures as a graph theory problem. *Phys. Rev. B* **97**, 035138 (2018).
47. van Miert, G. & Ortix, C. Higher-order topological insulators protected by inversion and rotoinversion symmetries. *Phys. Rev. B* **98**, 081110 (2018).
48. Hwang, Y., Ahn, J. & Yang, B.-J. Fragile topology protected by inversion symmetry: diagnosis, bulk-boundary correspondence, and Wilson loop. *Phys. Rev. B* **100**, 205126 (2019).
49. Hwang, Y., Rhim, J.-W. & Yang, B.-J. General construction of flat bands with and without band crossings based on wave function singularity. *Phys. Rev. B* **104**, 085144 (2021).
50. Graf, A. & Piéchon, F. Designing flat-band tight-binding models with tunable multifold band touching points. *Phys. Rev. B* **104**, 195128 (2021).
51. Benalcazar, W. A., Bernevig, B. A. & Hughes, T. L. Electric multipole moments, topological multipole moment pumping, and chiral hinge states in crystalline insulators. *Phys. Rev. B* **96**, 245115 (2017).
52. Wieder, B. J. & Bernevig, B. A. The axion insulator as a pump of fragile topology. Preprint at *arXiv* <https://doi.org/10.48550/arXiv.1810.02373> (2018).
53. Ahn, J., Park, S. & Yang, B.-J. Failure of Nielsen-Ninomiya theorem and fragile topology in two-dimensional systems with space-time inversion symmetry: application to twisted bilayer graphene at magic angle. *Phys. Rev. X* **9**, 021013 (2019).
54. Ahn, J. & Yang, B.-J. Symmetry representation approach to topological invariants in C_{2v} -symmetric systems. *Phys. Rev. B* **99**, 235125 (2019).
55. Ahn, J. et al. Stiefel–Whitney classes and topological phases in band theory. *Chin. Phys. B* **28**, 117101 (2019).
56. Schindler, F., Tsirkin, S. S., Neupert, T., Bernevig, B. A. & Wieder, B. J. Topological zero-dimensional defect and flux states in three-dimensional insulators. *Nat. Commun.* **13**, 5791 (2022).
57. Kane, C. L. & Mele, E. J. $\mathbb{Z}_2$ topological order and the quantum spin Hall effect. *Phys. Rev. Lett.* **95**, 146802 (2005).
58. Bernevig, B. A., Hughes, T. L. & Zhang, S.-C. Quantum spin Hall effect and topological phase transition in HgTe quantum wells. *Science* **314**, 1757 (2006).
59. Li, G. et al. Obstructed surface states as the descriptor for predicting catalytically active sites in inorganic crystalline materials. *Adv. Mater.* **34**, 2201328 (2022).
60. Bergerhoff, G., Hundt, R., Sievers, R. & Brown, I. The inorganic crystal structure database. *J. Chem. Inf. Comput. Sci.* **23**, 66 (1983).
61. Xu, Y. et al. Filling-enforced obstructed atomic insulators. *Phys. Rev. B* **109**, 165139 (2024).
62. Watanabe, H. & Lu, L. Space group theory of photonic bands. *Phys. Rev. Lett.* **121**, 263903 (2018).
63. Christensen, T., Po, H. C., Joannopoulos, J. D. & Soljačić, M. Location and topology of the fundamental gap in photonic crystals. *Phys. Rev. X* **12**, 021066 (2022).
64. Wang, D., Wu, Y., Zhang, Z. & Chan, C. Non-Abelian frame charge flow in photonic media. *Phys. Rev. X* **13**, 021024 (2023).
65. Morales-Pérez, A. et al. Transversality-enforced tight-binding models for three-dimensional photonic crystals aided by topological quantum chemistry. *Phys. Rev. B* **111**, 235206 (2025).
66. Devescovi, C. et al. Axion topology in photonic crystal domain walls. *Nat. Commun.* **15**, 6814 (2024).
67. Hwang, Y. et al. Building blocks of topological band theory for photonic crystals. Preprint at *arXiv* <https://doi.org/10.48550/arXiv.2601.06293> (2026).
68. Herzog-Arbeitman, J., Peri, V., Schindler, F., Huber, S. D. & Bernevig, B. A. Superfluid weight bounds from symmetry and quantum geometry in flat bands. *Phys. Rev. Lett.* **128**, 087002 (2022).
69. Herzog-Arbeitman, J., Bernevig, B. A. & Song, Z.-D. Interacting topological quantum chemistry in 2D with many-body real-space invariants. *Nat. Commun.* **15**, 1171 (2024).
70. Shiozaki, K., Sato, M. & Gomi, K. Atiyah-Hirzebruch spectral sequence in band topology: general formalism and topological invariants for 230 space groups. *Phys. Rev. B* **106**, 165103 (2022).
71. Shiozaki, K. & Ono, S. Atiyah-Hirzebruch spectral sequence for topological insulators and superconductors: E_2 pages for 1651 magnetic space groups. Preprint at *arXiv* <https://doi.org/10.48550/arXiv.2304.01827> (2023).
72. Watanabe, H., Po, H. C. & Vishwanath, A. Structure and topology of band structures in the 1651 magnetic space groups. *Sci. Adv.* **4**, eaat8685 (2018).
73. Ono, S., Po, H. C. & Shiozaki, K. $\mathbb{Z}_2$ -enriched symmetry indicators for topological superconductors in the 1651 magnetic space groups. *Phys. Rev. Res.* **3**, 023086 (2021).
74. Bouhon, A., Lange, G. F. & Slager, R.-J. Topological correspondence between magnetic space group representations and subdimensions. *Phys. Rev. B* **103**, 245127 (2021).
75. Elcoro, L. et al. Magnetic topological quantum chemistry. *Nat. Commun.* **12**, 5965 (2021).
76. Wada, H. et al. General corner charge formulas in various tetrahedral and cubic space groups. *Phys. Rev. B* **109**, 085114 (2024).
77. Cohen, H. A course in computational algebraic number theory. **138**, (Springer Science & Business Media, 2013).
78. Aroyo, M. et al. Crystallography online: Bilbao crystallographic server. *Bulg. Chem. Commun.* **43**, 183 (2011).
79. Song, Z.-D., Elcoro, L., Xu, Y.-F., Regnault, N. & Bernevig, B. A. Fragile phases as Affine monoids: classification and material examples. *Phys. Rev. X* **10**, 031001 (2020).
80. Benalcazar, W. A., Li, T. & Hughes, T. L. Quantization of fractional corner charge in C_n -symmetric higher-order topological crystalline insulators. *Phys. Rev. B* **99**, 245151 (2019).
81. Velury, S., Hwang, Y. & Hughes, T. L. Global and local topological crystalline markers for rotation-symmetric insulators. *Phys. Rev. B* **112**, 094204 (2025).
82. Devescovi, C. et al. Tutorial 2.0: computing topological invariants in 3D photonic crystals. *Opt. Mater. Express* **14**, 2161 (2024).

Acknowledgments

The authors thank Ken Shiozaki for fruitful discussions.

Author contributions

F.S., Z.S., B.B., and B.A.B. conceived of the project. Y.H. and F.S. derived the properties of the SRSIs and analyzed specific examples with input from B.B., B.A.B., Z.S., and L.E. The SRSIs were computed for all space groups by L.E. The SRSI mismatch criteria for band topology were formulated by F.S. and Y.H., and concrete examples were analyzed by Y.H. and V.G. The manuscript was prepared by F.S., Y.H., V.G., and L.E. with input from all authors. B.B. and B.A.B. oversaw the work and were responsible for the overall research direction.

Funding

The initial work of Y.H., V.G., and B.B. was supported by the Air Force Office of Scientific Research under award number FA9550-21-1-0131 and the National Science Foundation under grant No. DMR-1945058. Y.H. received additional support from the US Office of Naval Research (ONR) Multidisciplinary University Research Initiative (MURI) grant N00014-20-1-2325 on Robust Photonic Materials with High-Order Topological Protection. F.S. and Y.H. were supported by a UKRI Future Leaders Fellowship MR/Y017331/1. Z.-D. S. were supported by the National Natural Science Foundation of China (General Program No. 12274005), the National Key Research and Development Program of China (No. 2021YFA1401900), and the Innovation Program for Quantum Science and Technology (No. 2021ZD0302403). L.E. was supported by the Government of the Basque Country (Project IT1458-22) and the Spanish Ministry of Science and Innovation (PID2019-106644GB-I00). B.B. received additional support from the National Science Foundation under grant No. DMR-2510219. B.A.B. was supported by NSF-MRSEC Grant No. DMR-2011750, Simons Investigator Grant Nos. 404513 and SFI-MPS-NFS-00006741-01, ONR Grant No. N00014-20-1-2303, the Schmidt Fund for Innovative Research, the BSF Israel US Foundation Grant No. 2018226, the Gordon and Betty Moore Foundation through Grant No. GBMF8685 towards the Princeton theory program and Grant No. GBMF11070 towards the EPiQS Initiative, and the Princeton Global Network Fund. L.E. and B.A.B. acknowledge additional support through the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant Agreement No. 101020833).

Competing interests

The authors declare no competing interests.

Additional information

Supplementary information The online version contains supplementary material available at <https://doi.org/10.1038/s41467-026-74844-w>.

Correspondence and requests for materials should be addressed to Barry Bradlyn.

Peer review information *Nature Communications* thanks the anonymous reviewers for their contribution to the peer review of this work. A peer review file is available.

Reprints and permissions information is available at <http://www.nature.com/reprints>

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Open Access This article is licensed under a Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International License, which permits any non-commercial use, sharing, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if you modified the licensed material. You do not have permission under this licence to share adapted material derived from this article or parts of it. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by-nc-nd/4.0/>.

© The Author(s) 2026