

Nonsymmorphic Time-Reversal-Doubled Axion Insulators

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The axion insulator exhibits a topological magnetoelectric effect characterized by an axion angle $\theta = \pi$, while the time-reversal-doubled axion insulator (*T*-DAXI) can be viewed as two copies of an axion insulator related by time-reversal symmetry. In this work, we show that a nonsymmorphic topological crystalline insulator with glide (or screw) symmetry can host the nonsymmorphic *T*-DAXI phase, diagnosed by the nontrivial hourglass (screw) invariant $\delta_h = 1$ ($\delta_s = 1$). In this phase, the partial axion angles ($\theta^\pm = \pi$) are quantized by the glide and/or screw symmetry, and the gapped surfaces realize half-quantized quantum spin Hall states. Furthermore, we show that nonsymmorphic *T*-DAXIs also exhibit the spin-magnetoelectric effect. Namely, an external magnetic field can induce a topological nonlocal spin polarization in real space. When the magnetic field is time periodic, this leads to an alternating spin current detectable in experiment. Using *ab initio* calculations, we demonstrate that mixed bismuth monohalides $\text{Bi}_4\text{Br}_x\text{I}_{4-x}$ realize the nonsymmorphic *T*-DAXI. Our findings not only reveal the symmetry-enforced *T*-DAXIs in nonsymmorphic topological crystalline insulators, but also demonstrate the spin-magnetoelectric effect as a detectable topological spin response in nonsymmorphic *T*-DAXIs.

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I. INTRODUCTION

In recent decades, topological phases of matter have attracted sustained interest in condensed matter physics and materials science [1–8]. One of the intriguing properties characteristic of three-dimensional (3D) topological materials is the topological magnetoelectric effect arising from an effective action $S_\theta = (\theta e^2)/(4\pi^2) \int dt d^3\mathbf{x} \mathbf{E} \cdot \mathbf{B}$, where θ is the axion angle defined over a period of 2π [9–13]. An insulator with $\theta = \pi$ quantized by symmetry that reverses odd times of space-time coordinates (e.g., I , $T\tau$, M , and C_2T) is termed a (magnetic) axion insulator (AXI) and exhibits a detectable quantized magnetoelectric effect [14–17]. The AXI can be constructed from weakly coupled alternating Chern-insulator layers with $C = \pm 1$ [18–20]. Materials such as MnBi_2Te_4 [21–24], $\text{Eu}_3\text{In}_2\text{As}_4$ [25], and others [26–33] have been theoretically proposed as candidates for AXIs. Moreover, an AXI features half of a quantum anomalous Hall

state on a surface due to the parity anomaly [34–36]. In fact, the half-quantized surface conductivity is carried by the chiral hinge states [37], which links AXIs to chiral higher-order topological insulators (HOTIs), or magnetic topological crystalline insulators (TCIs) [38–45].

On the other hand, time-reversal (*T*)-invariant TCIs [46–52] host gapless helical boundary states at terminations that preserve protecting crystalline symmetries [53,54]. An example is the helical hinge states in *T*-invariant inversion TCIs with inversion index $Z_4 = 2$ [55–59], also known as helical HOTIs [40–42]. Recent work [60] has shown that, for a chosen spin-resolved direction, an inversion TCI can realize one of the three refined spin-resolved topological phases: a 3D quantum spin Hall insulator (QSHI), a spin Weyl-fermion state, and notably a *T*-invariant doubled axion insulator (*T*-DAXI). The *T*-DAXI can be viewed as two copies of a magnetic AXI related by time-reversal symmetry, with nontrivial π partial axion angles quantized by inversion symmetry. The discovery of *T*-DAXIs has expanded the possible venues for axion physics, e.g., half-quantized 2D surface QSHI. Especially, novel spin-magnetoelectric responses are introduced in those inversion-based HOTIs and/or *T*-DAXIs [54,60,61]. However, both 0 and π of the partial axion angles are allowed for the spin-resolved topology of an inversion TCI, and, thus, whether a *T*-DAXI can be realized depends on the details of the projected spin bands. These facts raise three natural

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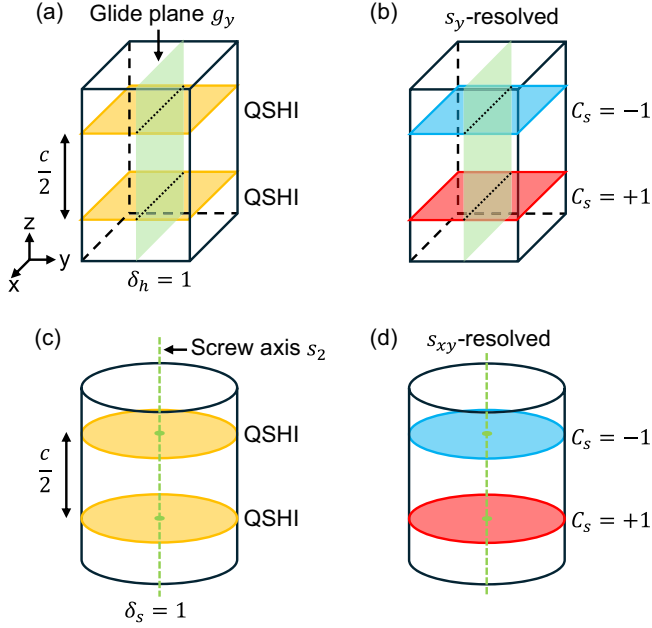


FIG. 1. The layer constructions of the nonsymmorphic TCIs and symmetry-enforced spin-resolved phases of nonsymmorphic T -DAXIs. (a) Layer construction of a gTCI with an hourglass invariant $\delta_h = 1$, where two QSHIs are related by g_y . (b) Symmetry-enforced spin-resolved topology of the glide T -DAXI in the s_y spin direction for a gTCI of (a). (c) Layer construction of a sTCI with a screw invariant $\delta_s = 1$, where two QSHIs are related by s_2 . (d) Symmetry-enforced spin-resolved topology of the screw T -DAXI in the s_{xy} spin direction for a sTCI of (c). In (b) and (d), the two QSHIs carry opposite s_y and s_{xy} spin Chern numbers due to the glide and screw symmetry, respectively, both realizing a nonsymmorphic T -DAXI.

questions: (i) can T -DAXI phases arise with partial axion angles quantized by other crystalline symmetries, instead of inversion, (ii) can the T -DAXI phases be diagnosed by any topological invariants, and (iii) does the spin-magnetoelectric effect still exist in the nonsymmorphic T -DAXI phases?

In this work, we introduce the spin-resolved topological classifications for 3D T -invariant insulators with glide g_y or screw s_2 symmetry, as shown in Table I. In the s_y (s_{xy}) spin-resolved topology, we find that the T -DAXI phases are protected by the nonsymmorphic symmetry in TCIs with a nontrivial hourglass (screw) invariant $\delta_h = 1$ ($\delta_s = 1$). The partial axion angles of a nonsymmorphic T -DAXI defined

in spin subspaces are quantized by the symmetry g_y ($s_2 T$). To illustrate the properties of the nonsymmorphic T -DAXI, we construct a glide TCI model as an example and explicitly reveal the following properties, including the quantized partial axion angles $\theta^\pm = \pi$, surface quantum anomalies with a surface half-quantized spin Chern number plateau $-C_{s,\text{top}} = C_{s,\text{bot}} = 1/2$, and a topological spin-magnetoelectric effect that produces a detectable transport signature. Finally, using *ab initio* calculations, we predict that the mixed bismuth monohalides Bi_4BrI_3 and $\text{Bi}_4\text{Br}_3\text{I}$ can realize the nonsymmorphic T -DAXIs, providing a promising platform for experimental detection.

II. T -DAXIs IN NONSYMMORPHIC TCIs

To investigate the spin-resolved topology, one has to separate the occupied-band space into two spin subspaces by projecting the n -directed spin operator $\hat{s}_n$ [62]:

$$S_n(\mathbf{k}) = P(\mathbf{k})\hat{s}_n P(\mathbf{k}),$$

$$S_n|\psi_{mk}^\pm\rangle = \lambda_{mk}^\pm|\psi_{mk}^\pm\rangle, \quad (1)$$

where $P(\mathbf{k}) = \sum_{m \in \text{occ}} |\psi_{mk}\rangle\langle\psi_{mk}|$ projects onto the occupied-band space and n denotes the spin direction. When a spin gap exists between upper and lower spin bands, labeled by eigenvalues λ_{mk}^+ and λ_{mk}^- , the occupied bands can be separated into two sectors. Thus, in a QSHI, one can define partial Chern numbers $C^\pm$ for the two sectors, with time-reversal symmetry requiring $C^+ = -C^-$. Accordingly, nonzero spin Chern number $C_s \equiv (C^+ - C^-)/2$ indicates the existence of a topological contribution to the intrinsic spin Hall conductivity (SHC) σ_s [63,64]. Provided a system is spin conserved, its intrinsic SHC will strictly equal to a quantized value, $\sigma_s = C_s e / (2\pi)$. When spin conservation is perturbatively broken (normally in real materials), the intrinsic SHC does not instantaneously vanish but deviates from and lies close to such quantized value if the spin-nonconserving spin-orbit coupling (SOC) is relatively weak.

A glide TCI (gTCI) can be constructed in real space by stacking QSHI layers in the z direction, where two QSHIs per unit cell are related by g_y and individually occupy the $(001; d_0)$ and $(001; d_0 + c/2)$ planes [here, $(hkl; d)$ denotes Miller indices hkl and the distance d to the origin], as shown in Fig. 1(a). Meanwhile, a screw TCI (sTCI) is

TABLE I. Spin-resolved topological classifications in spinful 3D nonsymmorphic TCIs. θ^+ is the partial axion angle and C^+ is the partial Chern number in the upper spin subspace. Because of the time-reversal symmetry, $\theta^+ = -\theta^-$ and $C^+ = -C^-$.

Nonsymmorphic TCI	$g_y \equiv \{M_y 0, 0, 0.5\}$		$s_2 \equiv \{C_{2z} 0, 0, 0.5\}$	
Spin direction	y axis	xz plane	xy plane	z axis
Symmetry in a subspace	g_y	$g_y T$	$s_2 T$	s_2
Topological number	$\theta^\pm$	$C^\pm$	$\theta^\pm$	$C^\pm$
Classification and topology	$\mathbb{Z}_2$ (T -DAXI)	$\mathbb{Z}$ (3D QSHI)	$\mathbb{Z}_2$ (T -DAXI)	$\mathbb{Z}$ (3D QSHI)

constructed by simply replacing the glide plane with a twofold screw axis. Such layer construction yields a nontrivial hourglass invariant $\delta_h = 1$ or screw invariant $\delta_s = 1$ with trivial strong and weak time-reversal $\mathbb{Z}_2$ indices $(\nu_0; \nu_1 \nu_2 \nu_3) = (0; 000)$ for the gTCIs or sTCIs [55], which we refer to as nonsymmorphic TCIs in this work. For a gTCI, when the bands are separated by the eigenvalues of $P_{s_y}P$, the g_y symmetry is preserved in each spin sector and can quantize the partial axion angle. Based on spin-resolved bubble-equivalence analysis, the spin-resolved topology is $\mathbb{Z}_2$ classified (see Appendix A). In Fig. 1(b), since the two QSHIs are related by g_y , the s_y spin Chern numbers of them are opposite, consistent with a nontrivial partial axion angle $\theta^\pm = \pi$ in both spin sectors [Fig. 6(b)]. Therefore, the system realizes the spin-resolved topological state of a T -DAXI. For other spin-resolved directions, the T -DAXI phase is not allowed or protected because the partial axion angles are no longer quantized due to the lack of g_y in each set of spin bands. Additionally, when the bands are separated by s_{xz} (we denote s_{ab} for an arbitrary spin direction in the ab plane), the partial Chern numbers for each QSHI layer are identical due to $g_y T$, and the spin-resolved topology is $\mathbb{Z}$ classified, corresponding to a spin-resolved 3D QSHI. Regarding an sTCI with s_2 symmetry, the spin-resolved topology for spin directions in the xy plane yields T -DAXIs, whose partial axion angles are quantized by $s_2 T$ symmetry, while the s_z spin resolution produces an s_2 -protected 3D QSHI. In particular, unlike in inversion-symmetric TCIs that the spin-resolved topology (T -DAXI or 3D QSHI) depends on detailed spin-spectrum diagnosis [60], the s_y (s_{xy}) spin-resolved topology of a nonsymmorphic T -DAXI is protected and indicated by the invariant of gTCIs (sTCIs).

III. MINIMAL MODEL

To study the T -DAXI in nonsymmorphic TCI, we take gTCI as an example and construct an eight-band model:

$$H_g(\mathbf{k}) = \begin{pmatrix} H_+(k_x, k_y) & H_1(k_z) \\ H_1^\dagger(k_z) & H_-(k_x, k_y) \end{pmatrix},$$

$$H_\pm(k_x, k_y) = M_k s_0 \sigma_z + v_x \sin k_x s_z \sigma_x - v_y \sin k_y s_0 \sigma_y \pm A_x \sin k_x s_y \sigma_x \pm A_y \sin k_y s_x \sigma_x,$$

$$M_k = m + t \cos k_x + t \cos k_y,$$

$$H_1(k_z) = e^{ik_z/2} \left(f_1 \cos \frac{k_z}{2} + f_2 \sin \frac{k_z}{2} \right). \quad (2)$$

Here, τ , s , and σ are Pauli matrices for layer, spin, and orbital degrees of freedom, respectively. H_+ and H_- describe the two QSHI layers (with $|m| < |2t|$) in a unit cell, respectively located at $(001; d_0)$ and $(001; d_0 + c/2)$, and related by the glide symmetry g_y . We choose $d_0 = 0$ and $c = 1$ without loss of generality. $H_1(k_z)$ represents the

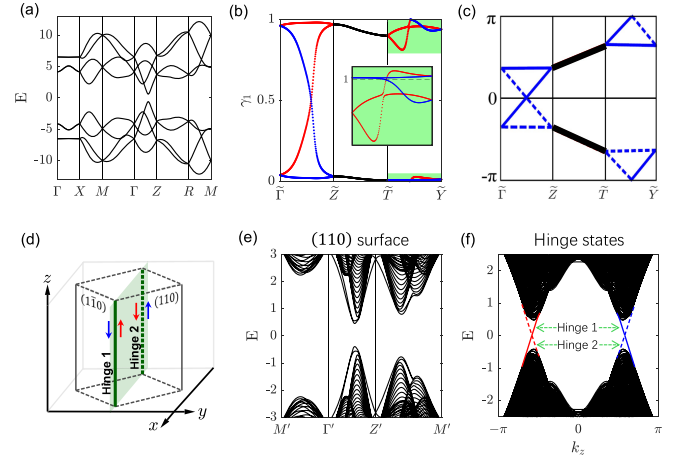


FIG. 2. (a) Bulk energy bands of the gTCI model in Eq. (2). The parameters are $-m = t = 2$, $v_x = v_y = A_x = A_y = 2$, $t_1 = t_4 = 0.5$, $t_5 = t_2 = 2$, and $t_6 = -t_3 = 1.5$. (b) WCCs γ_1 of the k_x -directed Wilson loops for the four occupied bands. Red and blue dots carry different glide eigenvalues $+ie^{-ik_z/2}$ and $-ie^{-ik_z/2}$, respectively. The inset plot shows the enlargement of the WCCs along $\tilde{T}-\tilde{Y}$ highlighted in green, showing the hourglass-type pattern. (c) Schematic plot: the zigzag-connected hourglass-type Wilson bands for a gTCI, adapted from Ref. [48]. Solid and dashed lines carry different glide eigenvalues. (d) Schematic plot of a rod geometry (along the z direction), bounded by the (110) and $(1\bar{1}0)$ surfaces. (e) Surface spectra of the (110) and $(1\bar{1}0)$ surfaces, which are identical due to g_y . (f) k_z -directed spectra of the rod geometry in (d). The topological helical states are located at the hinges.

interlayer coupling with $f_1 = t_1 s_0 \sigma_0 + it_2 s_y \sigma_x + it_3 s_x \sigma_0$ and $f_2 = it_4 s_0 \sigma_x + t_5 s_y \sigma_0 + t_6 s_x \sigma_x$. The energy bands of the gTCI model $H_g(\mathbf{k})$ are shown in Fig. 2(a).

If $H_1(k_z)$ is omitted, based on the real-space layer construction, the model realizes a gTCI with invariants $\delta_h = 1$ and $(\nu_0; \nu_1 \nu_2 \nu_3) = (0; 000)$ [55]. Upon adding $H_1(k_z)$ without closing the bulk gap, these invariants remain unchanged. In addition, the gTCI can also be confirmed by the zigzag pattern of hourglass Wilson bands on a glide-preserving surface. To illustrate this, we compute the glide-protected k_x -directed Wilson loop and plot the Wannier charge centers (WCCs) along the (100) -surface Brillouin-zone path $\tilde{\Gamma}-\tilde{Z}-\tilde{T}-\tilde{Y}$ in Fig. 2(b). One can see that the Wilson bands have the nontrivial zigzag pattern, which is identical to Fig. 2(c) adapted from Ref. [48], confirming a gTCI phase. Meanwhile, the glide-protected Wilson loop carries a glide Z_4 value [65–67] that can be computed as

$$\chi_y = \frac{1}{2\pi} \sum_{j=1}^{n_{\text{occ}}/2} \left[2\gamma_{1,j}^-(\tilde{Z}) - 2\gamma_{1,j}^-(\tilde{T}) + \int_{\tilde{\Gamma}}^{\tilde{Z}} (d\gamma_{1,j}^+ - d\gamma_{1,j}^-) + \int_{\tilde{T}}^{\tilde{Y}} (d\gamma_{1,j}^+ - d\gamma_{1,j}^-) \right] + \frac{1}{2\pi} \sum_{j=1}^{n_{\text{occ}}} \int_{\tilde{Z}}^{\tilde{T}} d\gamma_{1,j} \bmod 4, \quad (3)$$

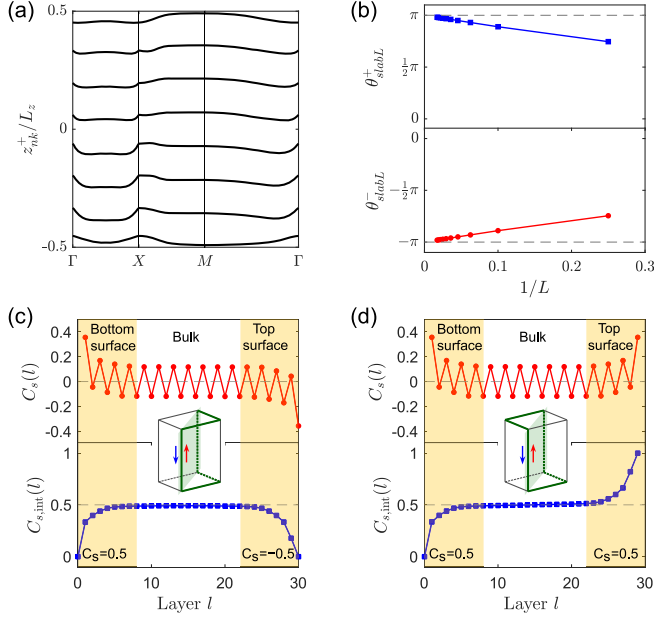


FIG. 3. (a) Partial WCCs z_{nk}^+ for the s_y upper spin bands of a four-unit slab, where eight upper spin Wannier bands are located on eight layers (two QSHI layers per unit cell). (b) Evolution of the slab partial axion terms $\theta_{slabL}^\pm$ in the s_y resolution as a function of $1/L$. $\theta_{slabL}^\pm$ are quantized to $\pm\pi$ as $L \rightarrow \infty$, indicating a T -DAXI phase. (c) Upper panel: layer-dependent spin Chern number $C_s(l)$ for a 15-unit-cell slab (being even QSHI layers). Lower panel: accumulated spin Chern number $C_{s,int}(l)$ up to depth l . (d) Layer-dependent spin Chern number and its accumulation for a modified slab after removing the topmost QSHI layer (being odd QSHI layers). Insets in (c) and (d): helical hinge states configurations (green lines) for even- and odd-layer-QSHI geometry, respectively, which serve as conducting channels for the surface SHC.

with $\gamma_1^\pm$ being the WCCs of the k_x -directed Wilson loops in the $\pm$ glide sectors, respectively. The glide Z_4 invariant is obtained to be $\chi_y = 2$, further confirming the gTCI phase.

On glide-preserved surfaces, the hourglasslike surface states are expected in a gTCI. However, on the (110) surface without glide symmetry, a glide-breaking perturbation introduces a mass term that gaps the surface spectrum. Meanwhile, due to the glide symmetry, the (1 $\bar{1}$ 0) and (110) surfaces have the same spectrum but with opposite mass terms. Consequently, helical hinge states emerge at the interface between the two surfaces, as shown in Fig. 2(f). The presence of the topological helical hinge states demonstrates that a glide TCI also manifests itself as a helical HOTI. We further find that the helical hinge states extend to propagate through the top and bottom surfaces, encircling the entire sample of a glide TCI. The position of the top and bottom helical hinge states is related to the even or odd number of total QSHI layers of the sample, as shown in the insets in Figs. 3(c) and 3(d). We note that the helical hinge modes

that encircle the whole sample of a glide TCI require nearly perfect glide symmetry of the real sample.

IV. PROPERTIES OF A T -DAXI

The spin-resolved topology of our gTCI model in the s_y direction, thus, yields a T -DAXI as discussed above. In this section, we study the properties of the T -DAXI in three aspects using the gTCI model, including partial axion angles, surface partial quantum anomalies, and spin-magnetoelectric effect.

A. Partial axion angles

As viewed as two T -related copies of a magnetic AXI, the T -DAXI can be characterized by partial axion angles $\theta^\pm$, which can be evaluated from partial Wannier functions constructed in separated spin subspaces [19]. In this scenario, for an L -unit-cell slab along the z direction, we define an auxiliary slab partial axion term

$$\theta_{slabL}^\pm = -\frac{1}{L} \int d^2\mathbf{k} \sum_{n=1}^{L \times N_{occ}/2} [z_{nk}^\pm \tilde{\Omega}_{kn}^{xy,\pm}], \quad (4)$$

where $z_{nk}^\pm$ are the eigenvalues of z -directed position operator defined in the spin subspaces $P_k^\pm \hat{z} P_k^\pm$, where $P_k^\pm = \sum_n |\psi_{nk}^\pm\rangle \langle \psi_{nk}^\pm|$ project onto the two spin subspaces. $\tilde{\Omega}_{kn}^{xy,\pm}$ is the corresponding partial non-Abelian Berry curvature [68–71] defined in the eigenstates of $P_k^\pm \hat{z} P_k^\pm$. N_{occ} is the number of occupied bands. In the infinite thickness limit, the slab partial axion terms in Eq. (4) converge to the partial axion angles defined by the Chern-Simons three-form [19] in the two spin subspaces, i.e., $\theta^\pm = \lim_{L \rightarrow \infty} \theta_{slabL}^\pm$.

For illustration, in the s_y resolution, we show z_{nk}^+ for the upper spin bands of a four-unit-cell slab of our gTCI model in Fig. 3(a). Eight separated partial WCCs correspond to the eight weakly coupled QSHI layers. In Fig. 3(b), the upper (lower) panel shows the evolution of θ_{slabL}^+ (θ_{slabL}^-) as a function of the inverse of L . The intercepts on the y axis indicate $\theta^\pm = \pm\pi$, confirming the T -DAXI phase. Here, the signs “ $\pm$ ” before π are still well defined by means of the asymptotic convergence behavior together with time-reversal symmetry.

B. Layer-dependent spin Chern numbers

We now discuss the surface anomaly implied by the partial axion angles. In a magnetic AXI, the surface anomalous Hall conductivity (AHC) is half-quantized as $\sigma^{AHC} = e^2/(2h)$ [11,14,34,35]. Regarding a T -DAXI, the net surface AHC vanishes because of the time-reversal symmetry. However, with spin conservation, the topological contribution to the surface SHC should be nontrivial and half-quantized as $\sigma^{SHC} = e/(4\pi)$ [60]. This half-quantized surface SHC feature can be captured

using the layer-dependent spin Chern number $C_s(l) = \frac{1}{2}[C^+(l) - C^-(l)]$, where $C^\pm(l)$ resolve the Thouless-Kohmoto-Nightingale-Nijs integer into contributions from individual layers [14]:

$$C^\pm(l) = \frac{i}{2\pi} \int d^2k \text{Tr}[P_k^\pm \epsilon_{ij} (\partial_i P_k^\pm) P_l (\partial_j P_k^\pm)]. \quad (5)$$

Here, ϵ_{ij} is the antisymmetric tensor with $i, j \in \{k_x, k_y\}$. P_l projects onto the l th layer of a slab ($l \in [1, 2L]$). In the upper panel in Fig. 3(c), we plot the layer-dependent spin Chern number $C_s(l)$ in the s_y resolution for an L -unit-cell slab of the gTCI model. $C_s(l)$ is primarily localized on the surfaces and decays to zero in the bulk in an oscillatory manner. We then accumulate the layer-dependent spin Chern number to depth l according to $C_{s,\text{int}}(l) = \sum_{l'=1}^l \bar{C}_s(l')$, with $\bar{C}_s(l') = \frac{1}{2}[C_s(l') + C_s(l' + 1)]$ being the average of two neighboring layers [34]. The results are plotted in the lower panel in Fig. 3(c). Although the total spin Chern number of the slab vanishes, the spin Chern numbers on the bottom and top surfaces are half-quantized to $C_{s,\text{bot}} = -C_{s,\text{top}} = 1/2$, consistent with the surface partial quantum anomaly of a T -DAXI. Moreover, if we modify the slab by removing the topmost QSHI layer (a half unit cell) from the slab (resulting in $l \in [1, 2L - 1]$), the half-quantized plateau on the remaining surfaces persists while the sign of $C_{s,\text{top}}$ flips (i.e., $C_{s,\text{top}} = 1/2$). Consequently, the total spin Chern number of the modified slab becomes non-zero, $C_s = 1$.

C. Spin-magnetoelectric effect

For a magnetic AXI, the quantized axion angle $\theta = \pi$ implies a topological magnetoelectric effect: an applied magnetic field B induces a quantized charge polarization $\mathbf{P} = e^2 \mathbf{B} / 2h$ parallel to the magnetic field, so that electrons accumulate on one surface from the opposite surface [9,10] [see Fig. 4(a)]. In a T -DAXI, the partial axion angles $\theta^\pm = \pm\pi$ lead to a spin-magnetoelectric effect. Under a magnetic field, the net charge response vanishes because of time-reversal symmetry, but electrons carrying opposite spins will accumulate on two opposite surfaces, producing a nonlocal spin polarization parallel to the external magnetic field, as shown in Fig. 4(b).

To calculate the real-space nonlocal spin polarization in the gTCI model with parameters modified to s_y conservation, we consider an L -unit-cell slab under a static magnetic field $\mathbf{B} = (0, 0, B)$ applied along the z direction, which contributes the Peierls substitution $e^{(ie/\hbar) \int d\mathbf{l} \cdot \mathbf{A}}$ with $\mathbf{A} = (-yB, 0, 0)$. We obtain the s_y spin distribution via $q_s(z) = [\hbar/(2V)] \langle \hat{N}_s(z) \rangle$, where $\hat{N}_s(z)$ with $s = \uparrow_y$ and $\downarrow_y$ are the total-density operators at position z for spin up and spin down of s_y , respectively. V is the volume of the slab. In Fig. 4(c), we show the s_y spin distributions along the z

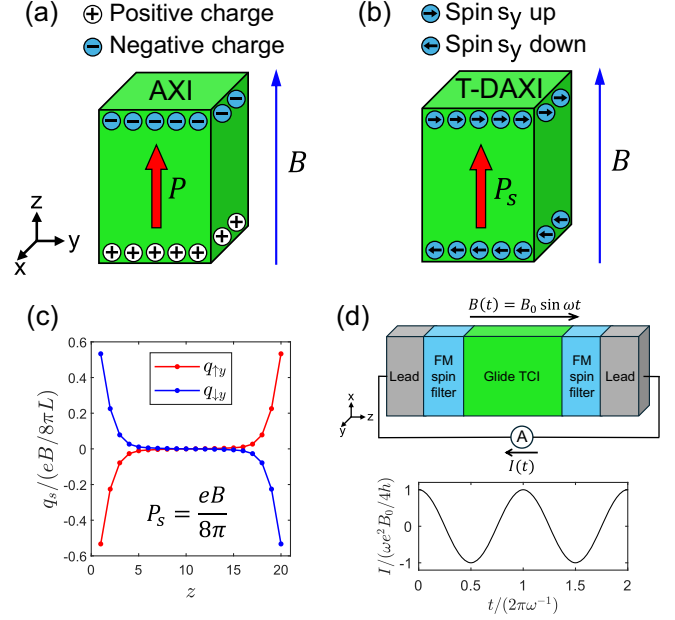


FIG. 4. (a) Topological charge polarization induced by an external magnetic field in a magnetic AXI. (b) Topological nonlocal spin polarization induced by an external magnetic field in a T -DAXI. (c) For s_y -conserved parameters by setting $v_x = A_y = t_3 = t_6 = 0$ and $t_1 = t_4 = 1.5$, the s_y spin distributions in each unit cell are shown along the z direction under a z -directed magnetic field. Red and blue dotted lines indicate s_y up and s_y down, respectively. The total nonlocal spin polarization reaches the quantized value $P_s = eB/8\pi$. (d) Alternating spin current in a gTCI tunneling junction induced by a time-periodic external magnetic field. Using y -directed polarized ferromagnetic (FM) spin filters, the spin-valve geometry can filter and convert the spin current into measurable charge current.

direction $q_s(z)$ for a 20-unit-cell slab, measured relative to an average $\bar{q}_s = \sum_z q_s(z)/L$. One clearly sees that s_y -up electrons transfer from the bottom surface to the top surface while s_y -down electrons transfer in the opposite direction, producing a real-space nonlocal spin polarization. We further quantify the nonlocal spin polarization by $P_s = \sum_z z[q_{\uparrow_y}(z) - q_{\downarrow_y}(z)]$, and it quantizes to $P_s = eB/8\pi$, determined by the partial axion angles. Moreover, if the applied magnetic field is time periodic with a frequency ω , $B(t) = B_0 \sin \omega t$, the nonlocal spin polarization should also be periodic and, thus, generate an alternating spin current with $I_s = dP_s(t)/dt = \omega e B_0 \cos(\omega t)/8\pi$ in a tunneling junction. Using y -directed polarized ferromagnetic (FM) spin filters, the spin-valve geometry can filter and convert the spin current into measurable charge current, as shown in Fig. 4(d). This provides a direct transport signature of the spin-magnetoelectric effect in a T -DAXI. When spin conservation is relaxed, although the T -DAXI phase is still well defined without closing the spin gap, the spin-magnetoelectric response should deviate from

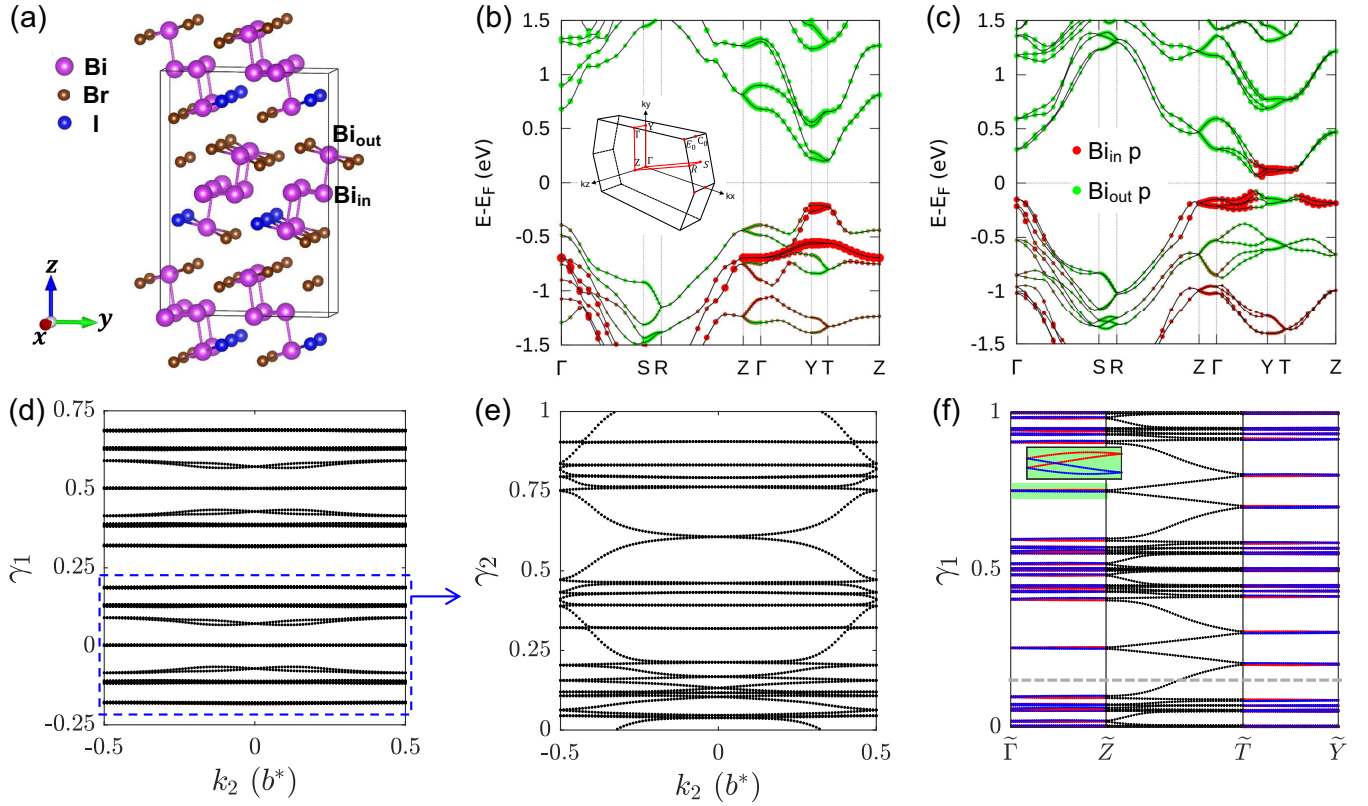


FIG. 5. (a) Crystal structure of $\text{Bi}_4\text{Br}_3\text{I}$. (b) Electronic band structure without SOC. Inset: Brillouin zone and high-symmetry paths. (c) Electronic band structure with SOC. The size of the red (green) circles indicate the p -orbital components of two kinds of Bi atoms, Bi_{in} and Bi_{out} labeled in (a). (d) WCCs of the k_z -directed Wilson loops of the occupied bands. (e) The nested Wilson loops for the k_z -directed Wilson bands around $\gamma_1 = 0$, depicted by a dashed blue frame in (d). It shows a zigzag pattern indicating the QSHI phase. (f) k_x -directed Wilson loops for the occupied bands, carrying the glide Z_4 value $\chi_y = 2$. Red and blue dots carry different glide eigenvalues $+ie^{-ik_z/2}$ (+ glide sector) and $-ie^{-ik_z/2}$ (− glide sector) on both $\tilde{\Gamma}\tilde{Z}$ and $\tilde{T}\tilde{Y}$ paths, respectively. The inset shows the enlargement highlighted in green. With a horizontal reference line (dashed gray line), the χ_y in Eq. (3) can be computed by simply counting the number of times of the Wilson bands crossing the line, i.e., $\chi_y = S^+ - S^- + 2S_{\tilde{Z}\tilde{T}}$. $S^\pm$ is defined as the number of positively sloped crossings minus the number of negatively sloped crossings in the $\pm$ glide sectors along both $\tilde{\Gamma}\tilde{Z}$ and $\tilde{T}\tilde{Y}$. $S_{\tilde{Z}\tilde{T}}$ is the number of crossings on $\tilde{Z}\tilde{T}$, with a factor of 2 due to the double degeneracy.

but lie close to the quantized value if the spin-nonconserving SOC is relatively weak (see details in Appendix C).

V. APPLICATION TO $\text{Bi}_4\text{Br}_x\text{I}_{4-x}$

The mixed bismuth monohalides $\text{Bi}_4\text{Br}_x\text{I}_{4-x}$ ($x = 1, 3$) have been synthesized experimentally [72], which crystallize in a base-centered structure belonging to the space group $Cmc2_1$ (#SG 36). We take $\text{Bi}_4\text{Br}_3\text{I}$ in Fig. 5(a) as an example in the main text. The chains extend along the a axis and assemble into layers within the ab plane. Two adjacent van der Waals layers form an AB stacking arrangement and are related by both glide g_y and screw s_2 symmetries, while an interlayer sliding breaks the inversion symmetry of the bulk crystal. The electronic band structure of $\text{Bi}_4\text{Br}_3\text{I}$ without and with SOC is plotted in Figs. 5(b) and 5(c), respectively, both showing

a global bulk gap. Upon including SOC, band inversion occurs along the Y - T path in the Brillouin zone. The orbital-projected band structures reveal that this band inversion involves bands with Bi p -orbital character at different positions [Bi_{in} and Bi_{out} in Fig. 5(a)]. Because of the time-reversal symmetry, $\text{Bi}_4\text{Br}_3\text{I}$ can be classified by four $\mathbb{Z}_2$ topological invariants. A Wilson loop calculation yields $(\nu_0; \nu_1\nu_2\nu_3) = (0; 000)$, indicating that the compound is neither a strong nor a weak 3D TI. Nevertheless, in Fig. 5(d), we show WCCs γ_1 of the k_z -directed Wilson loops of the occupied energy bands. Two sets of isolated WCCs are located around $\gamma_1 = 0$ and $\gamma_1 = 0.5$. Figure 5(e) further shows the k_1 -directed nested Wilson loop for the WCCs around $\gamma_1 = 0$ [inside the dashed blue frame in Fig. 5(d)]. A nontrivial zigzag pattern indicates a $\mathbb{Z}_2 = 1$ QSHI layer at $(001; 0)$ plane. Because of g_y and s_2 , another QSHI layer is located at $(001; c/2)$. By real-space layer construction, this reveals

a nonsymmorphic TCI protected by both g_y and s_2 , as illustrated in Figs. 1(a) and 1(c). In short, our calculations show that $\text{Bi}_4\text{Br}_3\text{I}$ is a nonsymmorphic TCI with $\delta_h = \delta_s = 1$ and $(\nu_0; \nu_1\nu_2\nu_3) = (0; 000)$. In addition, we calculate the glide-protected k_x -directed Wilson loop in Fig. 5(f) carrying the glide Z_4 value $\chi_y = 2$, which indicates a gTCI phase. Furthermore, we illustrate the s_y spin spectrum along high-symmetry path in Fig. 8(a) and calculate the global minimum spin gap in the whole Brillouin zone. The minimum spin gap is obtained to be $\Delta_{s_y} = 0.33$, which is larger than that ($\Delta_{s_x} = 0.26$) of $\alpha\text{-Bi}_4\text{Br}_4$ [60]. Therefore, in the s_y spin direction, $\text{Bi}_4\text{Br}_3\text{I}$ realizes a T -DAXI phase. To further verify the spin-resolved topology, we have performed the spin-resolved nested Wilson loop calculations (see Appendix B), whose results agree with the spin-resolved topological classification in nonsymmorphic TCIs discussed in Sec. II. Moreover, a new bulk phase of Bi_4Br_4 and Bi_4I_4 —denoted as the γ phase—is theoretically predicted to be dynamically stable [73] and also realizes T -DAXI in our calculations.

VI. CONCLUSION AND DISCUSSION

In summary, we have identified spin-resolved topological classifications and revealed T -DAXIs in nonsymmorphic TCIs. In certain spin-resolved directions, the T -DAXI is protected by nonsymmorphic symmetries. Explicitly, the g_y - s_2 - T -protected and T -DAXIs are indicated by the hourglass invariant $\delta_h = 1$ and the screw invariant $\delta_s = 1$, respectively, with trivial time-reversal $\mathbb{Z}_2$ indices $(\nu_0; \nu_1\nu_2\nu_3) = (0; 000)$. The nonsymmorphic T -DAXI is revealed to be characterized by several spin-resolved features: quantized partial axion angles, half-quantized surface spin Chern numbers, and topological nonlocal spin polarizations. Some novel experimentally accessible signatures of the T -DAXI can then be proposed. The glide- or screw-protected helical hinge states encircling the entire sample provide a spectroscopic signature accessible to angle-resolved photoemission spectroscopy or scanning tunneling microscopy. The surface quantum anomaly produces opposite, topologically contributed nonzero surface spin Hall conductivities, which are half-quantized to $-\sigma_{\text{top}}^{s,y} = \sigma_{\text{bot}}^{s,y} = e/4\pi$ on the top and bottom surfaces with spin conservation. This can be probed in a spin-transport experiment. Because of the spin-magnetoelectric effect, a time-periodic external magnetic field can generate an alternating spin current in a tunnel junction, providing a dynamical transport probe of the partial axion physics. These experiments can be performed in the mixed bismuth monohalides $\text{Bi}_4\text{Br}_x\text{I}_{4-x}$ and in other TCIs with nonsymmorphic symmetries. Furthermore, by changing the slab sample between even and odd layer counts, the total spin Chern number of a gTCI or sTCI can be controlled to vanish or quantize to 1, and the response of the system accordingly alternates between a T -DAXI and a QSHI.

This layer sensitivity suggests a route toward layer-manipulated “layertronics.” In addition, although this work focuses on T -invariant systems, the symmetry arguments should naturally generalize to magnetic gTCIs and sTCIs. In those magnetic nonsymmorphic TCIs, one can expect that chiral hinge states appear surrounding the whole samples and that the axion angles are quantized to π by the nonsymmorphic symmetries, with quantized magnetoelectric responses measurable without involving gapless boundary states. Finally, we anticipate that this work will motivate further experimental and theoretical studies on material realizations and device concepts that exploit partial axion physics.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: BUBBLE EQUIVALENCE AND SPIN-RESOLVED TOPOLOGICAL CLASSIFICATION

We employ the real-space topological classification method, bubble-equivalence analysis [74], to classify the spin-resolved layer constructions. In this approach, a bubbling process refers to a symmetry-preserving deformation in which topologically trivial layers are added to and/or removed from a layer construction and are then adiabatically deformed to generate another layer construction. Two layer constructions are regarded as topologically equivalent if they can be connected by such a bubbling process. Total inequivalent layer constructions yield the topological classification for the given symmetry class.

We first consider a T -invariant 3D insulator with glide symmetry g_y . In Fig. 6(a), for the S_y spin bands, a pair of QSHI layers with opposite spin Chern numbers can emerge at $r_z = r_z^0$ from trivial spin bands or perturbations. Because g_y persists in each sector of spin bands, another pair of QSHI layers should appear simultaneously at $r_z = r_z^0 + (c/2)$ [Fig. 6(b)]. Without breaking symmetries, the two pairs of QSHI layers can adiabatically evolve toward layer A and layer B . Consequently, a change of the total spin Chern number $\Delta C_{s,y}^A = -\Delta C_{s,y}^B = +2$ occurs, showing that the S_y spin bands are $\mathbb{Z}_2$ classified with $C_{s,y}^A = -C_{s,y}^B \bmod 2$ are topologically equivalent. Artificially, a $\mathbb{Z}_2$ invariant can

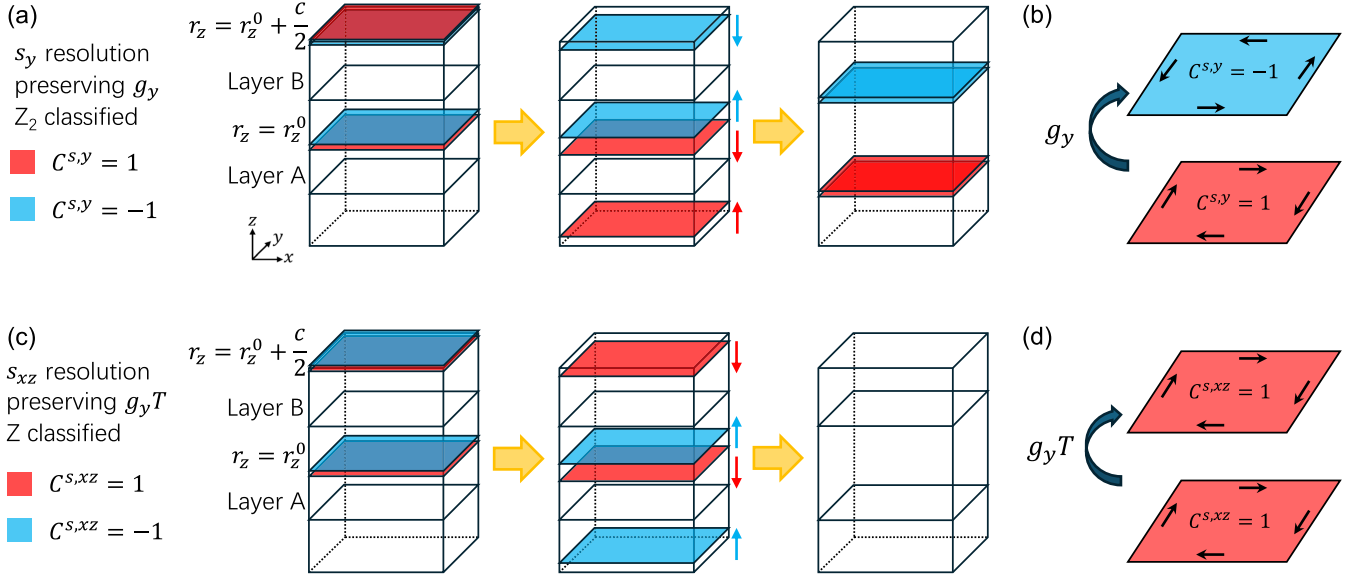


FIG. 6. In a T -invariant 3D insulator with glide g_y , bubble-equivalence processes for (a) the g_y -preserved s_y -projected spin subspaces and (c) the $g_y T$ -preserved s_{xz} -projected spin subspaces. (b),(d) Relations of the spin Chern number under symmetries g_y and $g_y T$.

be defined as $C_{s,y}^{AB} = (C_{s,y}^A - C_{s,y}^B)/2 \bmod 2$, and $C_{s,y}^{AB} = 1$ indicates a T -DAXI. Moreover, for a gTCI with g_y , $C_{s,y}^{AB} = 1$ inherits directly from the bulk $\mathbb{Z}_2$ -hourglass invariant $\delta_h = 1$ ($\delta_h = 1$ corresponds to stacking QSHIs at layer A and layer B).

For the s_{xz} spin resolution, the bubble equivalence shown in Figs. 6(c) and 6(d) demonstrates that adiabatic, symmetry-preserving perturbations do not alter the spin

Chern numbers at layer A or B due to $g_y T$. Consequently, a $\mathbb{Z}$ -classified 3D spin Chern number can be defined as $\gamma_{s,x/z} = C_{s,x/z}^A + C_{s,x/z}^B = 2C_{s,x/z}^A$, which corresponds to a 3D QSHI with a topological contribution to the bulk SHC $e\gamma_{s,x/z}/2\pi$. The bubble-equivalence analysis for screw symmetry s_2 is presented in Fig. 7, and we summarize the spin-resolved topological classifications discussed here in Table I in the main text.

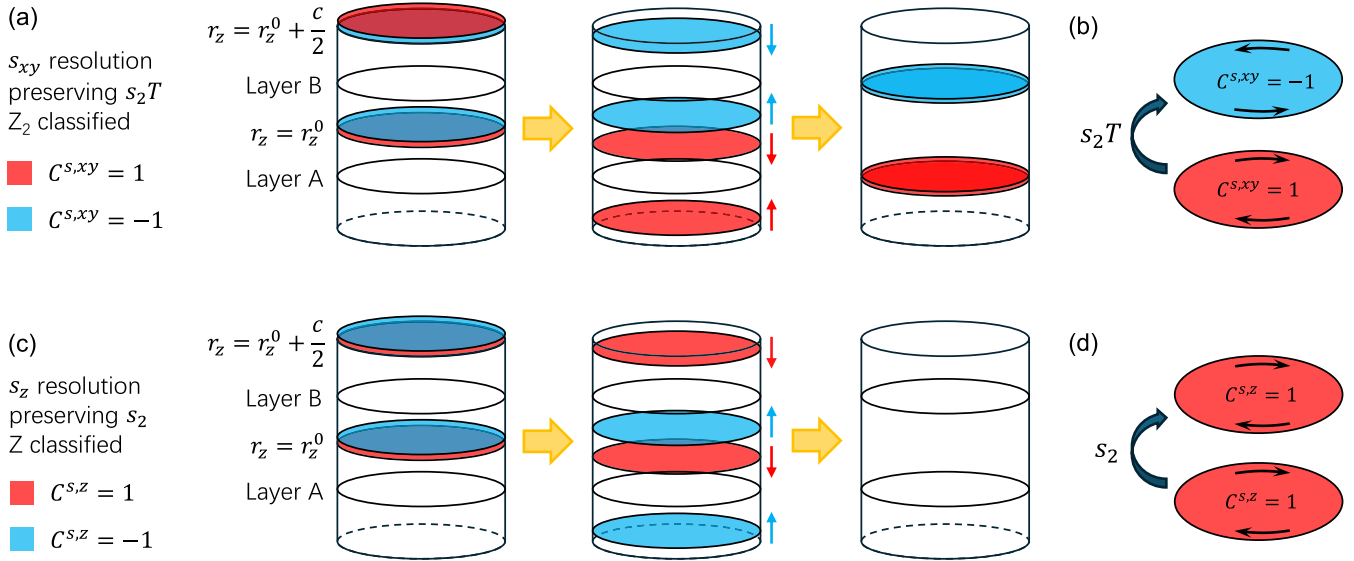


FIG. 7. In a T -invariant 3D insulator with screw s_2 , bubble-equivalence processes for (a) the $s_2 T$ -preserved s_{xy} -projected spin subspaces and (c) the s_2 -preserved s_z -projected spin subspaces. (b),(d) Relations of the spin Chern number under symmetries $s_2 T$ and s_2 .

APPENDIX B: SPIN-RESOLVED NESTED WILSON LOOP CHARACTERIZATION

In the spin-resolved topology, a T -DAXI can be considered as a stack of QSHI layers with alternating spin Chern numbers. This picture can be diagnosed by the spin-resolved nested Wilson loop method [60]. The s_y spin bands of $\text{Bi}_4\text{Br}_3\text{I}$ are shown in Fig. 8(a). One can clearly see that the occupied bands are separated into upper (positive eigenvalues) and lower (negative eigenvalues) spin bands. For the upper spin bands, we compute the k_z -directed Wilson loops, and their phases (Wilson bands) are plotted in Fig. 8(b). The Wilson bands form two separate groups. One group (colored red) is located near $z = 0$, and the other group (colored blue) is located near $z = \frac{1}{2}c$. We then compute the k_1 -directed nested Wilson loops for each group of these Wilson bands, and the obtained nested Wilson-loop phases are shown in Fig. 8(c). The opposite windings indicate that the red-colored states near $z = 0$ have partial Chern number $C^+ = +1$, while the blue-colored states near $z = \frac{1}{2}c$ have $C^+ = -1$. Therefore, the corresponding opposite spin Chern numbers on adjacent layers signal a T -DAXI in the presence of g_y/s_2T and time-reversal symmetry. This numerical result exactly matches the spin-resolved layer construction in Figs. 1(b) and 1(d). In Figs. 8(d)–8(f), we show another work flow of the spin-resolved nested Wilson loop for the s_z resolution. This work flow shows that the upper spin sectors of both

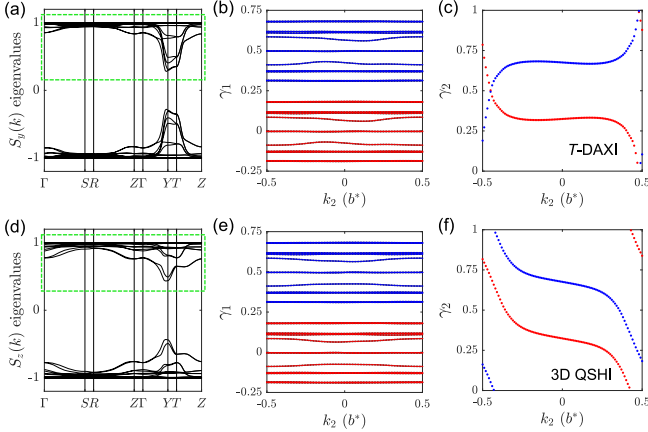


FIG. 8. (a)–(c) Work flow of the spin-resolved nested Wilson loops in the s_y resolution. (a) Spin bands formed by eigenvalues of $S_y(k)$, where a spin-band gap is clearly observed. (b) Partial WCCs γ_1 of the k_z -directed spin-resolved Wilson loops for the upper spin bands λ^+ [inside the dashed green frame in (a)]. (c) The red (blue) dotted phases γ_2 of the k_1 -directed spin-resolved nested Wilson loops calculated using the red (blue) dotted Wilson bands in (b). (d)–(f) Work flow for the spin-resolved 3D QSHI phase in the s_z resolution with a 3D spin Chern number $C_s = 2$.

layers located near $z = 0$ and $z = \frac{1}{2}c$ have the same partial Chern number $C^+ = 1$, indicating a 3D QSHI phase with a total 3D spin Chern number $C_s = 2$. These results agree with the spin-resolved topological classification in nonsymmorphic TCIs discussed in Sec. II.

APPENDIX C: SPIN-MAGNETOELECTRIC EFFECT IN SPIN NONCONSERVING NONSYMMORPHIC T -DAXIS

To demonstrate the spin-magnetoelectric effect in spin non-conserving nonsymmorphic T -DAXIs, we calculate the real-space nonlocal spin polarization using the gTCI model Eq. (2), with parameters breaking the s_y symmetry. Specifically, we tune the s_y -breaking terms $-t_3 = t_6$ from 0 to 1. The evolutions of the resulting minimum spin gap of the s_y spin spectrum Δ_{s_y} and the nonlocal spin polarization P_s are shown in Fig. 9(a), demonstrated by the blue and red dotted lines, respectively. One can see that, when the spin conservation is relaxed, the nonlocal spin polarization perturbatively deviates from its quantized value but lies close to that value if the spin-nonconserving terms are relatively weak. We further decrease the minimum spin gap to $\Delta_{s_y} = 0.36$, which is on the order of that in $\text{Bi}_4\text{Br}_3\text{I}$, and specifically calculate the s_y -spin distributions shown in Fig. 9(b). Opposite spins still clearly accumulate on opposite surfaces, resulting in a nonzero nonlocal spin polarization $P_s = 0.24eB/8\pi$. Hence, we suggest that the nonsymmorphic real-material T -DAXI $\text{Bi}_4\text{Br}_3\text{I}$ provides a promising platform for experimental detection of the spin-magnetoelectric effect.

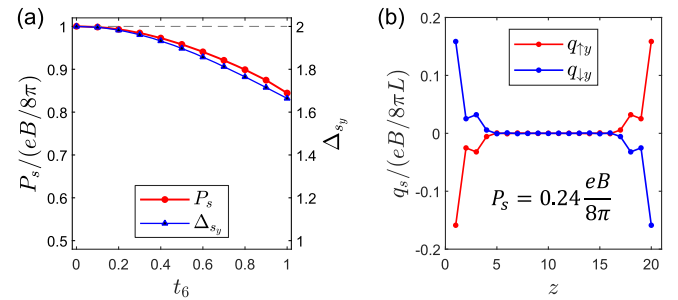


FIG. 9. (a) The evolutions of the nonlocal spin polarization P_s and the s_y -minimum spin gap Δ_{s_y} against the increasing of s_y -symmetry-breaking strength. Modified parameters are $v_x = A_y = 0$, $t_1 = t_4 = 1.5$, and $-t_3 = t_6$, with t_6 tuned from 0 to 1. (b) The s_y spin distributions in each unit cell of a 20-unit-cell slab under a z -directed magnetic field. Red and blue dotted lines indicate s_y up and s_y down, respectively. The total nonlocal spin polarization is $P_s = 0.24eB/8\pi$. Modified parameters are $t_1 = t_4 = 0.4$ and $v_x = A_y = -t_3 = t_6 = 2$, which give rise to a minimum s_y -spin gap $\Delta_{s_y} = 0.36$.

APPENDIX D: CALCULATION AND METHODOLOGY

We carried out first-principles calculations based on density functional theory with the projector augmented wave method [75,76], as implemented in the Vienna *ab initio* simulation package (VASP) [77,78]. The generalized gradient approximation in the form of the Perdew-Burke-Ernzerhof functional [79] was employed for the exchange-correlation potential. The kinetic energy cutoff for the plane-wave expansion was set to 450 eV. The Brillouin zone was sampled by the Monkhorst-Pack method in the self-consistent process, with a $16 \times 16 \times 4$ $\mathbf{k}$ mesh for the primitive cell. The maximally localized Wannier functions and the Wannier-based tight-binding Hamiltonian for the Bi p , Br p , and I p orbitals of $\text{Bi}_4\text{Br}_3\text{I}$ were constructed using the WANNIER90 package [80,81]. The (spin-resolved) nested Wilson loop of $\text{Bi}_4\text{Br}_3\text{I}$ was calculated using the Wannier-based Hamiltonian. The atomic coordinates and lattice constants of $\text{Bi}_4\text{Br}_3\text{I}$ ($a = 4.35585$ Å, $b = 13.4532$ Å, and $c = 19.3272$ Å) are adopted from Ref. [72]. In our calculations of the mixed bismuth monohalide phase, the Br atoms occupy three of the four $4a$ Wyckoff positions, while the I atoms occupy the remaining one $4a$ Wyckoff position.

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