

Reconstructing the Wave Function of Magnetic Topological Insulators MnBi_2Te_4 and MnBi_4Te_7 Using Spin-Resolved Photoemission

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Despite their importance for exotic quantum effects, the surface electronic structure of magnetic topological insulators MnBi_2Te_4 and MnBi_4Te_7 remains poorly understood. Using high-efficiency spin- and angle-resolved photoemission spectroscopy, we directly image the spin-polarization and orbital character of the surface states in both compounds and map our observations onto a model wave function to describe the complex spin-orbital texture, which solidifies our understanding of the surface band structure by establishing the single-band nature of the most prominent states. Most importantly, our analysis reveals a new mechanism for reducing the magnetic gap of the topological surface states based on the orbital composition of the wave function.

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I. INTRODUCTION

$\text{MnBi}_{2n}\text{Te}_{3n+1}$ (MBT) compounds have been intensively studied in recent years as they constitute the first intrinsic bulk magnetic topological insulator family that has been synthesized [1–4]. When time-reversal symmetry (TRS) is spontaneously broken, MBT has been shown to host exotic quantum phenomena such as the quantum anomalous Hall effect [5] and second- and third-order nonlinear Hall effects [6–8], which result from nontrivial quantum geometry. Despite these consequences of broken TRS, angle-resolved photoemission spectroscopy (ARPES) studies predominantly show a gapless Dirac cone insensitive to the magnetic phase transition [9–16], in contradiction to theory calculations [17–22].

In conventional topological insulators (TIs) such as Bi_2Se_3 and Bi_2Te_3 , the measured band structure consists of well-defined bulk and surface states, and therefore the

interpretation of even the earliest ARPES data was decisive [23,24]. In contrast, ARPES data on MBT exhibits a multitude of bands of uncertain bulk or surface character without clear correspondences in electronic structure calculations, thus precluding a straightforward assignment of the observed bands [11,12]. Considering the important controversy surrounding its magnetic behavior, it is critical to first establish a foundational understanding of the electronic structure. To provide information beyond the dispersions measured by high-resolution ARPES, we shall demonstrate that probing the structure of the wave function itself, including the entangled spin and orbital textures, can be used to help understand the Dirac cone's insensitivity to the magnetic phase transition in MBT.

In this work, we perform spin-resolved ARPES measurements on MnBi_2Te_4 and MnBi_4Te_7 to systematically track the spin-polarization and orbital character as a function of momentum k . By mapping these experimental observations onto a model for the wave function and its governing Hamiltonian, we show that the most prominent bands are well described by a single-band picture dominated by p orbitals and free from hybridization with neighboring bands, reconciling disparate interpretations and solidifying band assignments in the MBT family [15,16,25–27]. Our methodology demonstrates that spin- and orbital-resolved ARPES describes the electronic states

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microscopically and predicts meaningful experimental observables. Most importantly, we quantitatively show in MnBi_2Te_4 that a non-negligible contribution of in-plane p orbitals has an antagonistic effect on the surface state gap, thus providing critical insight into the issue of the gapless Dirac cone in the MBT family.

II. SPIN-ORBITAL TEXTURE OF TOPOLOGICAL SURFACE STATES

A. Experiment

The measurement geometry of our spin-resolved ARPES setup is shown in Fig. 1(a). We measure along k_x by rotating the sample about the θ axis, and our high-efficiency spin detector resolves the tangential in-plane spin polarization S_y and out-of-plane spin polarization S_z , as described in Appendix A and elsewhere [28,29]. Photoemission is performed using 6-eV photons with either s or p linear polarization, which we denote as s -pol or p -pol, respectively.

To establish the baseline electronic structure free from magnetism, the measurements in this work are performed at 80 K, which is above the Néel temperatures of MnBi_2Te_4 ($T_N = 24$ K) and MnBi_4Te_7 ($T_N = 13.5$ K) (see Appendix B for synthesis methods). When TRS is preserved, MBT shares the same C_{3v} rotational symmetry as the Bi_2Se_3 family [10,30]. MnBi_2Te_4 consists of stacked septuple layers (SLs), while MnBi_4Te_7 consists of alternative stacking of SLs and Bi_2Te_3 quintuple layers (QLs) and therefore exhibits two different surface terminations [12,16,19,20,31,32].

Figure 1(b) illustrates the established dispersion and spin texture of a topological surface state (TSS) obeying C_{3v} symmetry. Near Γ , the energy contour is circular and exhibits helical in-plane spin texture. At higher momenta the energy contour becomes hexagonally warped and develops finite out-of-plane spin polarization along Γ - K , as has been experimentally observed in Bi_2Te_3 [33–35]. The effective Hamiltonian is given by the third-order $k \cdot p$ theory [36]:

$$H(k) = \alpha(k_x\sigma_y - k_y\sigma_x) + \gamma(k_+^3 + k_-^3)\sigma_z, \quad (1)$$

where σ_x , σ_y , and σ_z are spin Pauli matrices, and $k_{\pm} = k_x \pm ik_y$. α defines the in-plane spin-momentum locking, while γ introduces the warping and out-of-plane spin.

Next, we show the in-plane (S_y) and out-of-plane (S_z) spin-resolved band structures of MnBi_2Te_4 and QL-terminated MnBi_4Te_7 in Fig. 1. The TSS of both materials exhibits the expected spin-momentum locking, with helical in-plane texture down to the Dirac point as reported previously [1,4,15,16,37,38]. In addition, for both surfaces we also observe out-of-plane spin developing at higher k , which is well described by the γ term in the

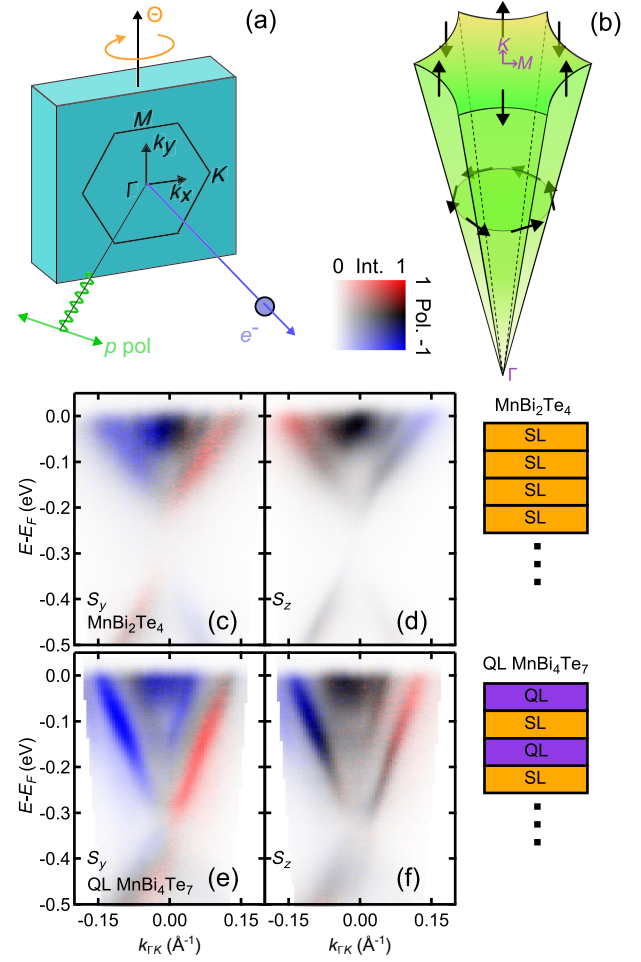


FIG. 1. (a) A schematic of the experimental geometry for spin-resolved ARPES measurements. Momentum space is mapped along k_x (Γ - K) by rotating the sample about the θ axis. Data in this figure are taken with p -polarized light. (b) A simplified illustration of the surface state spin texture in materials with C_{3v} symmetry. Near Γ the surface state hosts in-plane helical spin texture, which becomes out of plane approaching lower binding energy. In the following, spin-resolved ARPES data are plotted with the 2D color scale shown, where red-blue denotes the spin polarization and white-black denotes the photoemission intensity. (c) In-plane S_y and (d) out-of-plane S_z measurement for MnBi_2Te_4 , which consists of septuple layers (SL) stackings. (e), (f) Same for quintuple layer (QL) terminated MnBi_4Te_7 , which consists of alternative stacking of QL and SL.

effective Hamiltonian [Eq. (1)]. We note that the S_z polarization direction depends on the sample orientation (see Fig. 6 of Appendix F). Additional measurements of the in-plane spin along Γ - M confirm the helical spin texture of the TSS, which are shown in Fig. 7 of Appendix G.

While Fig. 1 suggests that the illustration in Fig. 1(b) provides a complete description of the TSS, we next show that a richer picture emerges when the orbital degrees of freedom are considered. Based on optical selection rules

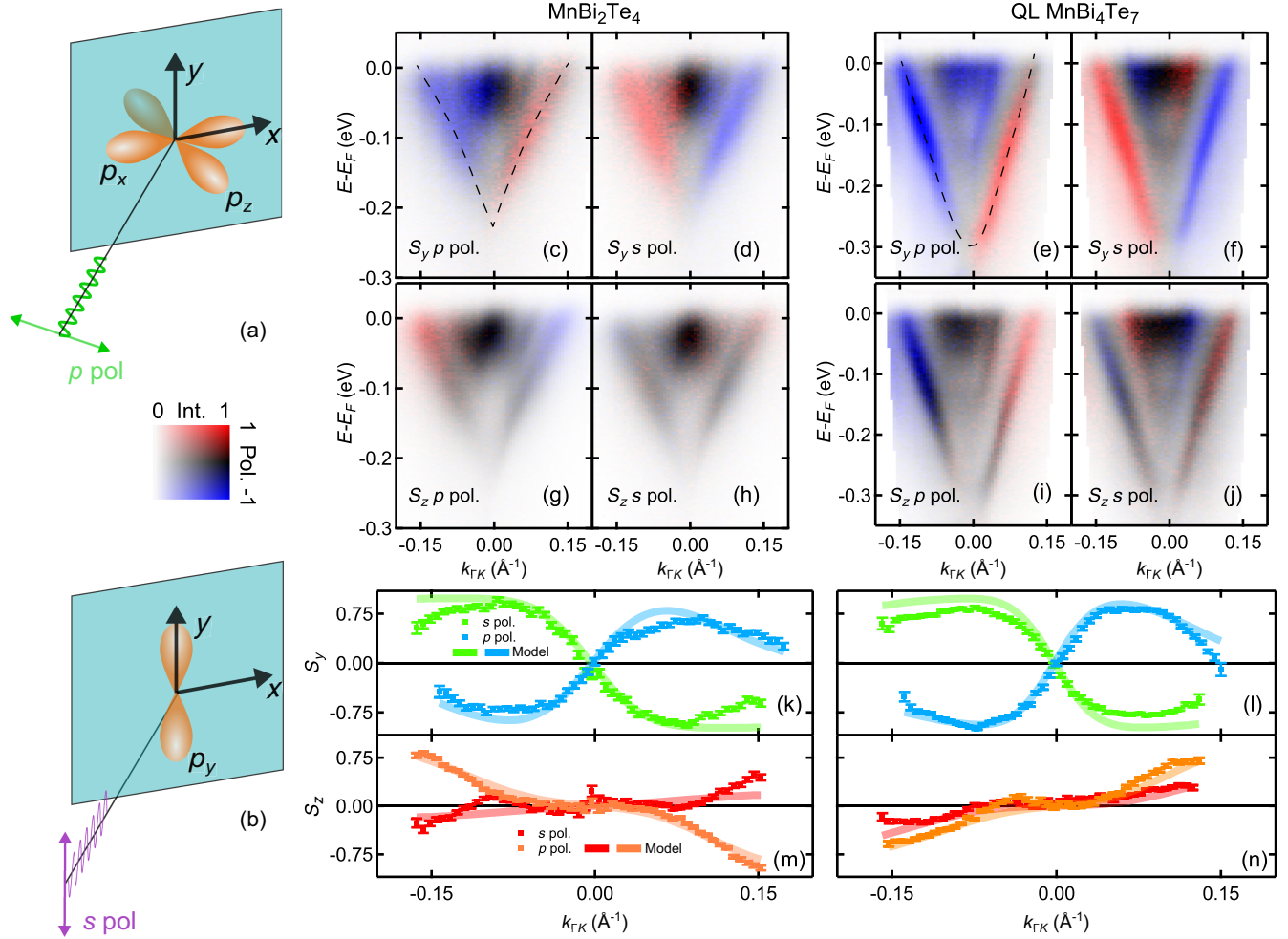


FIG. 2. (a) Measurement schematic with p -polarized light, which mainly couples to p_x and p_z orbitals. (b) Similarly, s -polarized light mainly couples to p_y orbitals. (c), (d) S_y of MnBi_2Te_4 measured with p - and s -pol, respectively. (e), (f) Same but for QL MnBi_4Te_7 . (g), (h) S_z of MnBi_2Te_4 measured with p - and s -pol, respectively. (i), (j) Same but for QL MnBi_4Te_7 . (k) S_y extracted from the MnBi_2Te_4 surface state measured with both light polarizations (markers) overlapped with the model (lines). (l) Same but for QL MnBi_4Te_7 . (m) S_z extracted from the MnBi_2Te_4 surface state measured with both light polarizations, overlapped with the model. (n) Same but for QL MnBi_4Te_7 . We note that asymmetries in the p -pol data with respect to $k = 0$ are attributed to the measurement geometry, which is included in the modeling (see Appendix C).

governing photoemission matrix elements [39,40], measurements using p - and s -polarized light directly project different orbital components of the wave function. Specifically for p orbitals, p -pol couples to p_x and p_z orbitals [Fig. 2(a)], and s -pol selectively photoemits p_y orbitals [Fig. 2(b)].

Whereas Fig. 1 was measured using only p -pol, the corresponding measurements using both p - and s -pol are shown in Figs. 2(c)–2(j). To facilitate a quantitative discussion, we also extract the spin polarizations integrated within a 43-meV energy window traced along the band dispersions [dashed lines in Figs. 2(c) and 2(e)], which are plotted using markers in Figs. 2(k)–2(n). We highlight several observations. (1) S_y behaves qualitatively the same in both compounds, with an overall reversal between p - and s -pol [Figs. 2(k) and 2(l)]. (2) Depending on the

material, S_z may or may not reverse with light polarization [Figs. 2(m) and 2(n)]. (3) The absolute values of $|S_z|$ measured with p - and s -pol can be quite different; most strikingly, $|S_z|$ nearly vanishes for s -pol measurements on MnBi_2Te_4 , as shown in Figs. 2(h) and 2(m). Such a comparison of S_z measured by p - and s -pol has never been reported in previous spin-resolved ARPES measurements of conventional TIs [35,39,41,42]. Similarly, previous spin-resolved ARPES measurements on the MBT family have established spin-momentum locking, but did not reveal this complex orbital-dependent behavior [1,4,15,16,37,38]. Such phenomena pose a challenge to our understanding of the wave function; therefore, it is necessary to develop a more comprehensive model to describe our observations quantitatively.

B. Wave function model

We use the effective Hamiltonian shown in Eq. (1). To capture the orbital degrees-of-freedom coupling to spin, we construct the wave function basis following the methodology of Ref. [43], which preserves total angular momentum $J_z = \pm 1/2$, and is expanded with respect to momentum up to first order. The basis wave function based on Ref. [43] is written as $|\psi_{J_z=\pm 1/2}\rangle = |\psi_{\pm(1/2)}^{(0)}\rangle + |\psi_{\pm(1/2)}^{(1)}\rangle$, including the zeroth-order contribution,

$$|\psi_{\pm 1/2}^{(0)}\rangle = u_0|p_z, \uparrow(\downarrow)\rangle + v_0|p_{\pm}, \downarrow(\uparrow)\rangle, \quad (2)$$

and the first-order contribution,

$$|\psi_{\pm 1/2}^{(1)}\rangle = \pm k_{\pm}(iu_1|p_{\mp}, \uparrow(\downarrow)\rangle + iv_1|p_z, \downarrow(\uparrow)\rangle) \mp ik_{\mp}w_1|p_{\pm}, \uparrow(\downarrow)\rangle, \quad (3)$$

where u_0, v_0, u_1, v_1, w_1 are material-dependent parameters taken to be real numbers, which control the relative ratio of different wave function components. The arrows denote spin angular momentum, and (p_x, p_y) represent the two in-plane p orbitals, with $p_{\pm} = \mp (1/\sqrt{2})(p_x \pm ip_y)$ contributing ± 1 unit of angular momentum along the z axis. Each term in the wave function separately combines orbital and spin angular momenta to give a total angular momentum $J_z = \pm 1/2$. The first-order contribution [Eq. (3)] enables the orbital character to evolve with momentum. After diagonalizing the two band Hamiltonian [Eq. (1)] and expanding under this basis wave function, we obtain the 2 eigenfunctions $|\Phi_{1,2}\rangle$ as a linear combination of $|\psi_{\pm 1/2}\rangle$. We can then derive the spin texture coupled to different p orbitals to calculate the quantitative momentum evolution of spin and orbital textures. The key distinction of our methodology from the formalism of Ref. [43] is the addition of the γ term to the Hamiltonian in Eq. (1) which is necessary to describe the observed out-of-plane spin polarization. Moreover, Ref. [43] used first principles calculations to obtain the material-specific parameters for Bi_2Se_3 ; such an approach is not feasible here since the electronic structure of MBT is not well described by density-functional theory (DFT) [17,18,21,22].

To overcome this challenge, we use our exhaustive dataset—comprising the k -dependent orbital-resolved spin polarizations as well as the band dispersions—to experimentally constrain the material-dependent parameters. Our formalism, detailed in Appendix C, is based on s -type final states for electrons photoemitted from the TSS with 6-eV photons. The nature of the final states has been well established for Bi-based topological insulators in the literature [35,40], including an extensive theoretical and experimental study employing spin-resolved ARPES, circular dichroism (CD) ARPES, and one-step-model photoemission calculations [44]. From our analysis, we obtain

TABLE I. Parameters used for the model describing different surfaces. The units for the Hamiltonian parameters are α (eV Å), γ (eV Å³). The wave function parameters u_0 and v_0 are unitless, with $u_0 \equiv 1$ to facilitate comparison of other parameter values. The higher-order wave function parameters (u_1, v_1, w_1) have units (Å). Note that γ has the opposite sign for MnBi_2Te_4 due to its different sample orientation (see Appendix F).

Surface	α	γ	u_0	v_0	u_1	v_1	w_1
MnBi_2Te_4	-1.7	-39	1	1.12	-4.8	-1.8	-8
QL MnBi_4Te_7	-1.9	71	1	0.74	4.6	0.56	-16
Bi_2Te_3	-1.9	69	1	0.06	4.6	-2.4	-20

Hamiltonian parameters α and γ and the wave function parameters [see Eqs. (2) and (3)]. We show a comparison with the data in Figs. 2(k)–2(n), where the results from the model are shown in solid lines. Table I reports the parameters we obtain for all compounds. Next, we explain how the diverse observed behaviors are successfully reproduced by this single unified model.

Focusing on our first observation, we note that the light polarization-dependent in-plane spin S_y [Figs. 2(k) and 2(l)] is consistent with previous studies on Bi_2Se_3 [39,41,42], and has been well understood from the zeroth-order wave function basis alone [Eq. (2)] [40,43,45–47]. The observation of similar S_y reversal behavior in MBT further showcases the applicability of the p -orbital basis set. Now we turn our attention to the second observation, which was that S_z reverses direction between p - and s -pol in MnBi_2Te_4 [Fig. 2(m)], while in QL MnBi_4Te_7 [Fig. 2(n)] it does not. Such distinct S_z behaviors can be quantitatively described by the basis set: The ratio of different wave function components [specifically, ku_1/v_0 ; see Eqs. (2) and (3)] controls the sign of out-of-plane spin that develops at larger k for in-plane orbitals. We also perform this analysis for Bi_2Te_3 (see Appendix E), which has the same termination as QL MnBi_4Te_7 . The similar absence of S_z reversal shows that this behavior manifests the distinct wave function properties of each surface termination. Furthermore, as mentioned in our third observation, the reduced $|S_z|$ when measured with s -pol, which is particularly pronounced for MnBi_2Te_4 [Fig. 2(m)] can also be captured by the basis wave function parameters [specifically, the ratio w_1/u_1 in Eq. (3)] which tune the magnitude of S_z coupled to in-plane orbitals at higher k .

To further confirm the validity of our model, we have also benchmarked our analysis with CD ARPES (see Appendix D), which has been extensively used to study conventional TIs [48–50] as well as MBT [15,25,27].

III. SPIN-ORBITAL TEXTURE OF HYBRIDIZED SURFACE BANDS

Next, we turn to SL-terminated MnBi_4Te_7 , which exhibits a more complex band structure whose assignments

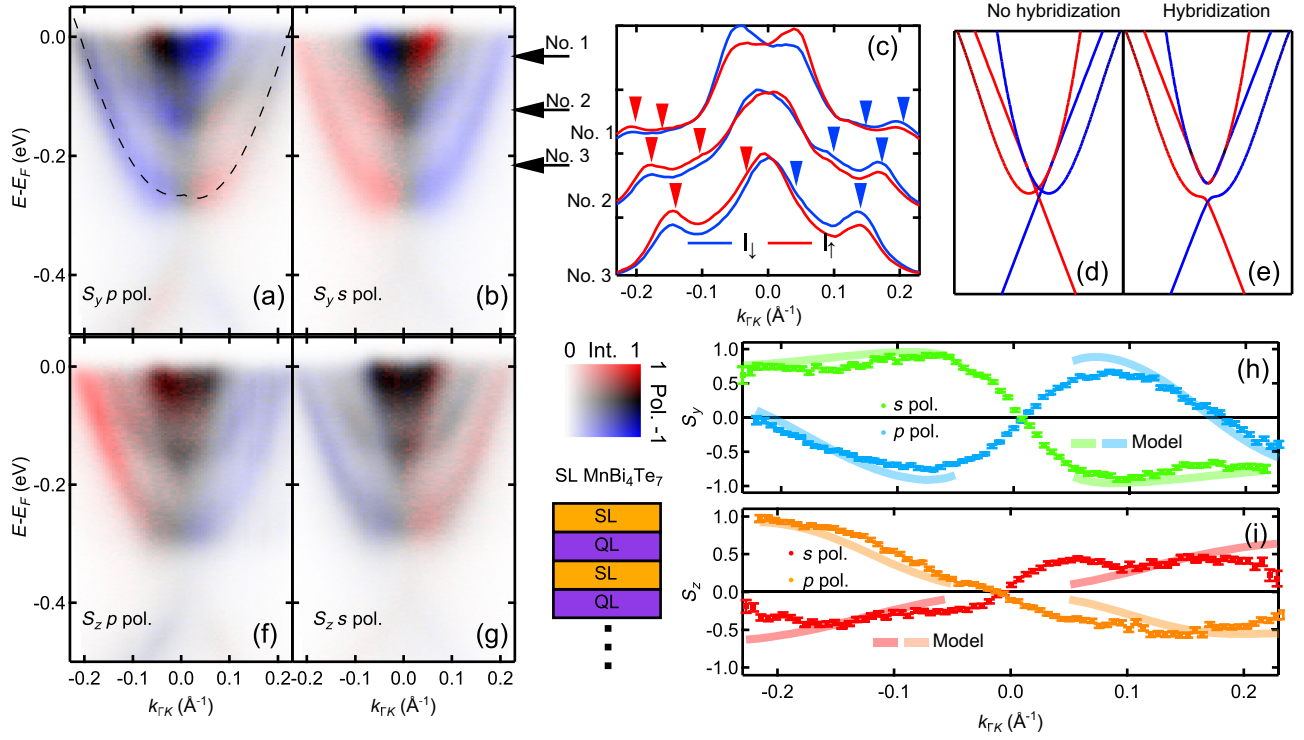


FIG. 3. Spin-resolved ARPES measurements of SL MnBi₄Te₇. (a), (b) S_y data with p - and s -pol light. (c) The corresponding momentum distribution curves (MDCs) of spin-up $I_\uparrow$ (+ y direction) and spin-down $I_\downarrow$ ($-y$ direction) intensities. Each MDC is integrated within an energy window of 33 meV. Each MDC pair is normalized by the maximum intensity for that pair to facilitate a comparison between MDCs at different energies. The markers denote peak positions of both bands, with blue-red coloring indicating the overall polarization of each peak. (d) Cartoon model of a pair of Rashba-split states and Dirac TSS without band hybridization, where color denotes S_y . (e) The same, with hybridization. (f), (g) S_z images with p - and s -pol. (h) S_y extracted along the black dashed line in (a), with 43-meV integration window for both light polarizations (markers) overlapped with the model (lines). The data within $k = \pm 0.05 \text{ \AA}^{-1}$ are excluded from the comparison due to the number of overlapping bands in this region. (i) Same but for S_z .

are even less well understood compared to the other terminations. High-resolution ARPES shows multiple bands intersecting near Γ [12,27], and the most prominent band, which has a parabolic dispersion, is absent in DFT [16]. Our spin-resolved ARPES measurements of S_y and S_z measured with both p - and s -pol are shown in Fig. 3. Unlike the other studied terminations, we cannot resolve a distinct TSS due to the highly overlapping nature of the bands and our limited k resolution. Nevertheless, we show that our spin-resolved data allow us to offer insights into the observed band structure.

A leading interpretation in literature is that the outermost band belongs to a pair of spin-split bands induced by the Rashba effect, which we will refer to as “Rashba-split” states. To study this more systematically, we plot momentum distribution curves (MDCs) of spin-up and spin-down intensities at three different binding energies in Fig. 3(c), with color denoting the spin channel. The triangle markers denote the position of not only the outermost band, but also a weaker inner band. The MDCs reveal that these two bands have parallel spin polarizations, indicating that they are not a Rashba-split pair, but states of different origins. We note that this differs from previous CD studies,

where their opposite relative CD signals suggest an antiparallel alignment [15,27]. Nevertheless, our observation is conceptually consistent with previous interpretations which attributed the bands to hybridization between Rashba-split and Dirac states [27]. This idea is illustrated in the illustrations in Fig. 3, which show the Dirac and Rashba-split states in Fig. 3(d) hybridizing into the states shown in Fig. 3(e).

Finally, we investigate the spin-orbital texture of the outer band of the Rashba-split pair [28,51,52]. We follow Ref. [53] and write out the Rashba Hamiltonian H_R obeying C_{3v} symmetry as

$$\begin{aligned}
 H_R(k) = & E_0(k_x^2 + k_y^2) + \alpha(k_x\sigma_y - k_y\sigma_x) \\
 & + \beta[(k_x^3 + k_xk_y^2)\sigma_y - (k_x^2k_y + k_y^3)\sigma_x] \\
 & + \gamma(k_+^3 + k_-^3)\sigma_z.
 \end{aligned} \quad (4)$$

This is similar to the TSS Hamiltonian [Eq. (1)], but with an additional term with coefficient β that has been shown to be important in systems that show prominent Rashba effects [28,53]. In addition, the E_0 term is spin independent and gives a quadratic dispersion which ensures trivial

TABLE II. Parameters used for the model describing SL MnBi₄Te₇. The units for the Hamiltonian parameters are E_0 (eV Å²), α (eV Å), β and γ (eV Å³). The wave function parameters u_0 and v_0 are unitless, with $u_0 \equiv 1$ to facilitate comparison of other parameter values. The higher-order wave function parameters (u_1, v_1, w_1) have units (Å).

Surface	E_0	α	β	γ	u_0	v_0	u_1	v_1	w_1
SL MnBi ₄ Te ₇	16	1.1	-8	33	1	-0.56	1.2	-1.2	1.9

topology. The data and model comparisons are shown in Figs. 3(h) and 3(i). Note that we exclude the range within $k = \pm 0.05$ Å⁻¹, since multiple bands overlap in this region and cannot be separated within our resolution. Remarkably, under the single-band picture and same basis wave function set that we previously used to describe the TSSs, we can also capture the quantitative spin texture for the Rashba-split states. The parameters we use for the Rashba-split pair are separately shown in Table II.

IV. DISCUSSION AND CONCLUSIONS

We now discuss the implications of our results for understanding the surface band structures of the MBT family. We have shown that the complex spin-orbital texture of the TSS in both MnBi₂Te₄ and QL MnBi₄Te₇ is well described by a single-band model composed of p orbitals with $J_z = \pm 1/2$. In other words, the wave function properties of the TSS are qualitatively similar to those of conventional TIs such as Bi₂Se₃. We emphasize the important role of spin information for arriving at this conclusion, since the curvature of the band dispersion and reversal behavior in CD naturally lead to more complex interpretations based on interband hybridizations [25,26]. SL-terminated MnBi₄Te₇, in contrast, does exhibit interband hybridizations, with the band assignments and wave function characters clearly demonstrated by our analysis. However, despite the qualitative similarity to conventional TIs, Table I shows a strong material dependence to the orbital compositions, thus pointing out the importance of systematic studies of the TSS wave functions. In addition, the ability to extract Hamiltonian and wave function parameters allows us to experimentally quantify quantum geometry related properties including Berry curvature and quantum metric [54,55], which give rise to exotic topological transport behavior such as higher-order quantum Hall effects [56,57]. A specific case calculation is shown in Appendix H.

Beyond the interpretation of dispersions and quantum geometry, the most important question is how the wave function information provides insight on the issue of the gapless Dirac cone in MBT [10–16]. There have so far been many studies exploring the issue in literature, and the possible explanations mainly include magnetic reconstruction [10,18,58–60] and defect-induced TSS

relocalization [61–63]. Both pictures involve factors extrinsic to the nominal magnetic and structural configuration of MBT, and they are challenging to be experimentally verified in ARPES studies.

Our wave function analysis suggests an intrinsic mechanism that reduces the TSS gap size compared to that predicted by DFT. When TRS is broken, the gap Δ is proportional to the strength of the Zeeman interaction between the effective magnetic field B_{eff} generated by the Mn layer and the magnetic moment μ of the TSS [64]:

$$\Delta \propto \mu \cdot B_{\text{eff}} \propto \langle \psi | \mathbf{L} + 2\mathbf{S} | \psi \rangle \cdot B_{\text{eff}}, \quad (5)$$

where the magnetic moment includes both orbital $\mathbf{L}$ and spin $\mathbf{S}$ angular momenta. Since we are interested in the behavior near the Γ point, we take the $k \rightarrow 0$ limit of Eq. (2):

$$\Delta \propto \frac{|u_0|^2}{|u_0|^2 + |v_0|^2} = \frac{r}{1+r}, \quad (6)$$

where $r = u_0^2/v_0^2$ is the relative weight of out-of-plane and in-plane p orbitals.

Equation (6) reveals an antagonistic effect of in-plane p orbitals: A larger proportion of in-plane orbitals results in a smaller TSS gap. Based on this mechanism, we perform a direct comparison between our model and DFT calculations, focusing on MnBi₂Te₄ since in both terminations of MnBi₄Te₇ the Dirac point is hybridized with bulk bands, so the gapping behavior and orbital characters are less clearly defined.

For MnBi₂Te₄ we obtained $r = 0.8$ (Table I), showing a dominance of in-plane p orbitals. In contrast, DFT calculations produce a value $r = 2.7$ (see Appendix I for the DFT electronic structure), which shows a dominance of out-of-plane p orbitals instead. Based on Eq. (6), this discrepancy corresponds to a 40% reduction in TSS gap size compared to DFT prediction. In other words, DFT underestimates the in-plane orbital contribution and therefore overestimates the magnitude of the TSS gap. We emphasize that this behavior is intrinsic to the wave function, and it must necessarily coexist with extrinsic mechanisms (such as defects) which may additionally contribute to the gap reduction.

Finally, we briefly comment on ferromagnetic TIs, which are proposed to be more robust against disorder compared to antiferromagnetic TIs [62]. Indeed, magnetic gaps have been experimentally observed in ferromagnetic bulk MnBi₈Te₁₃ [65] and monolayer MnBi₂Te₄/Bi₂Te₃ [66], yet their magnitudes remain a factor of 2 smaller than theoretical predictions [67]. This suggests that the intrinsic gap-reducing mechanism revealed in this work may be operative in ferromagnetic TIs as well, which will be the subject of future investigations.

In conclusion, our work provides a systematic study of the MnBi_2Te_4 and MnBi_4Te_7 surface state wave functions. The data showcase the nontrivial orbital-coupled spin texture, and our analysis establishes the quantitative applicability of the $k \cdot p$ model for unraveling the surface electronic structure. Most importantly, we propose a distinct intrinsic mechanism in which the contribution of in-plane p orbitals reduces the TSS gap. This provides crucial insights into the contradiction between theory and experiment and guides future efforts to discover and optimize magnetic topological insulators.

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APPENDIX A: PHOTOEMISSION METHODS

Our spin-resolved ARPES setup is based on a spectrometer with high efficiency attributed to its combination of exchange scattering for spin discrimination and time-of-flight analysis for resolving energy. We map out the momentum space along k_x by rotating the sample with respect to axis θ [see Fig. 1(a)], with Γ - K and Γ - M trajectories selected by azimuthal rotation of the sample about its normal. Spin discrimination is achieved via low-energy exchange scattering from a ferromagnetic thin film [10 ML Co/W(110)], with the scattered electrons detected by a multichannel plate detector. Spin contrast is obtained by reversing the magnetization direction of the film using Helmholtz coils. The spin detector can measure the horizontal and vertical spin components (in the lab frame) by rotation of the magnetic scattering crystal, corresponding to S_y and S_z , respectively. A more detailed description of the system can be found in Ref. [29], with additional technical information in Refs. [68,69].

The laser source for spin-resolved photoemission is a commercial ytterbium fiber laser amplifier (Coherent

Monaco) providing up to 80 μJ and 60 W at 1035-nm wavelength with < 300 fs pulse duration. The fifth harmonic of the fiber laser system generates the 6-eV photons for photoemission [70].

CD ARPES measurements are performed with a Scienta R4000 electron analyzer and a Ti:sapphire oscillator with photon energy quadrupling through two stages of second harmonic generation, outputting 6-eV photons for photoemission.

APPENDIX B: SAMPLE SYNTHESIS AND PREPARATION

The $\text{MnBi}_{2n}\text{Te}_{3n+1}$ ($n = 1$ and 2) single crystals in this study were grown from Mn (99.95%), Bi (99.999%), and Te (99.999%) blocks by using the self-flux method. The mixture with a specific molar ratio of 1:8:13 was put into an alumina crucible, which was then sealed into a quartz tube in vacuum. The assembly was heated in a furnace up to 700 $^\circ\text{C}$ within 10 h and kept at that temperature for 10 h, then cooled down to 610 $^\circ\text{C}$ in 10 h and slowly further cooled down to 600 $^\circ\text{C}$ and 590 $^\circ\text{C}$ for $n = 1$ and 2 , respectively. Finally, the assemblies were taken from the furnace and immediately put into a centrifuge to separate black crystals with shining surfaces from the flux.

APPENDIX C: LIGHT POLARIZATION COUPLED SPIN TEXTURE FORMALISM

Since we focus on only one of the two bands of the model, we denote the eigenfunction as $|\Phi\rangle$. We project the eigenfunction $|\Phi\rangle$ onto the desired basis to obtain the p -orbital coupled spin texture. We define the projections as

$$c_{p_i, \uparrow(\downarrow)_j} = \langle p_i, \uparrow(\downarrow)_j | \Phi \rangle. \quad (\text{C1})$$

Here $i, j = x, y, z$ represent the p -orbital and spin direction. For example, $c_{p_x, \uparrow_x}$ denotes the $|p_x, \uparrow_x\rangle$ component. The weight of the orbital p_i can be then defined as

$$w_{p_i} = |c_{p_i, \uparrow}|^2 + |c_{p_i, \downarrow}|^2. \quad (\text{C2})$$

To connect the output of this model to our measurements, we must account for the experimental geometry. With s -type final states (see main text), the measured spin polarization $\langle S_j \rangle$ along quantization axis j can be derived as [71]

$$\langle S_j \rangle_{p\text{-pol}} = \frac{\cos^2(\eta)(|c_{p_x, \uparrow_j}|^2 - |c_{p_x, \downarrow_j}|^2) + \sin^2(\eta)(|c_{p_z, \uparrow_j}|^2 - |c_{p_z, \downarrow_j}|^2) + 2 \cos(\eta) \sin(\eta) (\text{Re}[c_{p_z, \uparrow_j}^* c_{p_z, \uparrow_j}] - \text{Re}[c_{p_z, \downarrow_j}^* c_{p_z, \downarrow_j}])}{\cos^2(\eta)w_{p_x} + \sin^2(\eta)w_{p_z} + 2 \cos(\eta) \sin(\eta) (\text{Re}[c_{p_z, \uparrow_j}^* c_{p_z, \uparrow_j}] + \text{Re}[c_{p_z, \downarrow_j}^* c_{p_z, \downarrow_j}])}, \quad (\text{C3})$$

$$\langle S_j \rangle_{s\text{-pol}} = \frac{|c_{p_y, \uparrow j}|^2 - |c_{p_y, \downarrow j}|^2}{w_{p_y}}, \quad (\text{C4})$$

where $\eta = 45^\circ - \theta$ is the angle between the incoming laser and the sample surface normal. The spin polarization we experimentally measure has contributions from different p orbitals depending on the light polarization and sample orientation. As can be seen from Eq. (C3), the relative weight of p orbitals probed by p -pol depends on the sample rotation η . When $\eta = 0^\circ$, spin polarization probed by p -polarized light is solely due to the p_x orbital contributions. When $\eta = 90^\circ$, only p_z orbitals contribute to the signal. On the other hand, according to Eq. (C4), s -polarized light solely probes p_y orbital contributions, and is independent of the angle between sample normal and incident light. After computing the momentum-dependent spin polarization from this model, the final result is convolved with a Gaussian function to take into account the finite momentum resolution in the experiment.

To highlight the need for these corrections related to experimental geometry, we note that Eq. (C3) shows that the spin polarization measured with p -pol is asymmetric with respect to $k = 0 \text{ \AA}^{-1}$ due to the way contributions from p_x and p_z orbitals are mixed as the sample is rotated. In contrast, s -pol data should be symmetric in magnitude with respect to $k = 0 \text{ \AA}^{-1}$. These behaviors are indeed observed in the experimental data and well described by our model (Figs. 2 and 3).

APPENDIX D: CONNECTION TO CIRCULAR DICHROISM ARPES

To show that the spin-orbital texture of the TSS wave function is correctly described by the model in the main text, we here benchmark the model by using it to compute a separate experimental observable: circular dichroism. We perform CD ARPES on QL MnBi_4Te_7 using the measurement geometry shown in Fig. 4, where there is a 50° angle between the incident circularly polarized light and sample normal (see Appendix A). We repeat the measurement after rotating the sample azimuthally by 180° to test the consequences of the C_{3v} symmetry. Figures 4(c) and 4(d) present the CD signal along the TSS, which depends on sample orientation.

To calculate CD, we assume circularly polarized light projects the wave function onto the orbital angular momentum basis $|p_\pm\rangle$, which refers to $m_l = \pm 1$ along the axis defined by the light propagation direction [72]. Based on the geometry shown in Fig. 4, this basis can be written as

$$|p_{\pm, \uparrow(\downarrow)}\rangle = \mp \frac{1}{\sqrt{2}} [|p_{x, \uparrow(\downarrow)}\rangle \pm i(\cos(\kappa)|p_{y, \uparrow(\downarrow)}\rangle + \sin(\kappa)|p_{z, \uparrow(\downarrow)}\rangle)], \quad (\text{D1})$$

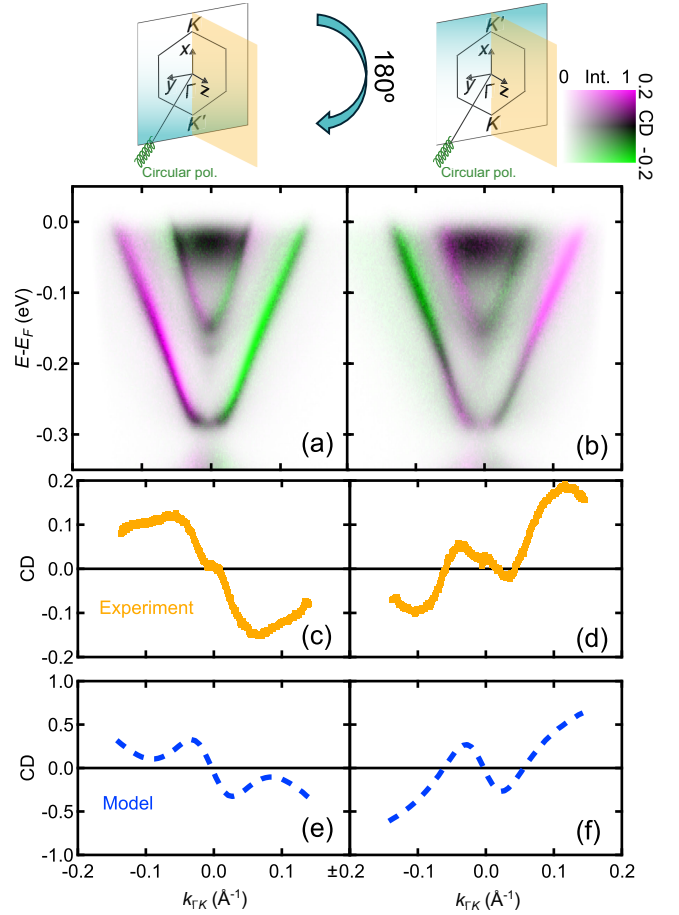


FIG. 4. Measurement geometry for circular dichroism (CD) ARPES of QL MnBi_4Te_7 . Circularly polarized light is incident at 50° with respect to the surface normal. Γ - K is along the x axis. The yellow plane indicates the plane from which the electrons are collected. Panels (a) and (b) show the CD ARPES data before and after 180° rotation of the sample, plotted in the 2D color scale as shown. (c), (d) CD of the surface state before and after sample rotation. (e), (f) CD yielded from our model with wave function parameters derived from the spin-resolved measurements.

where $\kappa = 50^\circ$ is the angle between the light propagation and the sample normal. As a result, the total projection on the orbitals for plus and minus circularly polarized light can be written as

$$\text{CD}_\pm = |\langle p_{\pm, \uparrow} | \Phi \rangle|^2 + |\langle p_{\pm, \downarrow} | \Phi \rangle|^2, \quad (\text{D2})$$

Hence, the normalized circular dichroism is given as

$$\text{CD} = \frac{\text{CD}_+ - \text{CD}_-}{\text{CD}_+ + \text{CD}_-}. \quad (\text{D3})$$

The calculation results, plotted in Figs. 4(e) and 4(f), qualitatively reproduce the CD observed experimentally, including the azimuthal angle dependence.

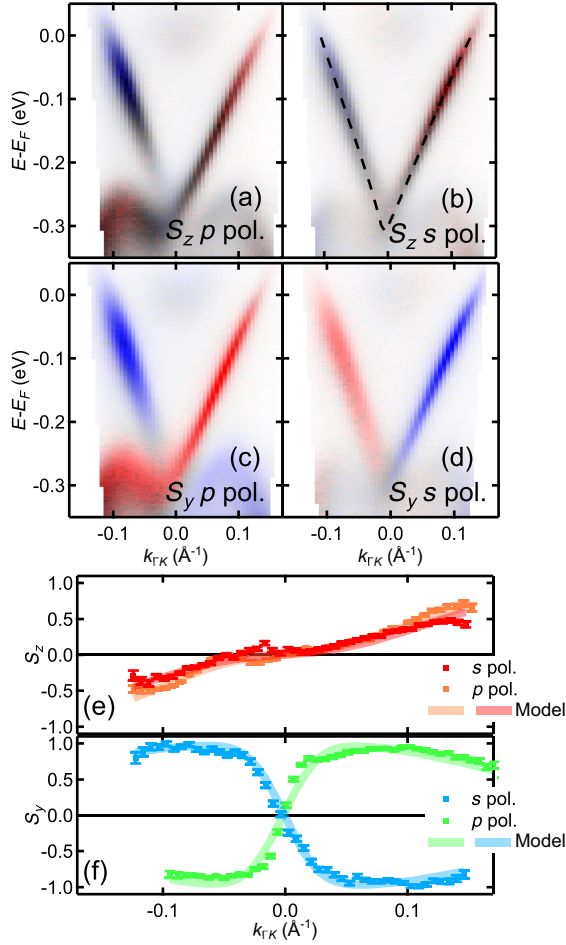


FIG. 5. Data for Bi_2Te_3 taken at room temperature along Γ - K . Specific measurements are S_z with (a) p -pol and (b) s -pol, and S_y with (c) p -pol and (d) s -pol. (e) S_z with both p and s -pol from spin image (dots), overlapped with result yielded from model (lines). (f) Same but for S_y .

Intuitively, CD measures the orbital angular momentum (OAM) projected onto the axis of light propagation, which in this geometry is a linear combination of y and z directions. The behavior at higher k is associated with the OAM derived from the γ term of the Hamiltonian, which obeys threefold rotational symmetry and therefore reverses sign upon 180° rotation [48,73]. The composite effects of in-plane and out-of-plane OAM lead to a complex CD texture that depends sensitively on the light-sample geometry. The fact that this is captured by our wave function evidences the intricate coupling of orbital and spin angular momenta, and further corroborates the validity of our model.

APPENDIX E: COMPARISON TO Bi_2Te_3

We perform similar wave function analysis for Bi_2Te_3 , the results of which are shown in Fig. 5. The model again captures the measured spin texture. It can be seen that S_y flips [Fig. 5(f)], while S_z does not flip between p -pol and s -pol [Fig. 5(e)]. Such behavior is the same as QL-terminated MnBi_4Te_7 as discussed in the main text [Figs. 2(i) and 2(j)], which further showcases the distinct wave function properties of each surface termination. See Table I for the model parameters for Bi_2Te_3 .

APPENDIX F: OUT-OF-PLANE SPIN TEXTURE ALONG Γ - K

Figure 6 shows different sets of S_z data of MnBi_2Te_4 along Γ - K taken on different cleaves at different times and temperatures. Each time it was prepared and remounted so the orientation could be integer multiples of 60° off from each other, due to the hexagonal symmetry of the Fermi surface. It can be seen that S_z for Figs. 6(a) and 6(b) is opposite to Figs. 6(c) and 6(d). The difference in S_z depends on the orientation of the sample.

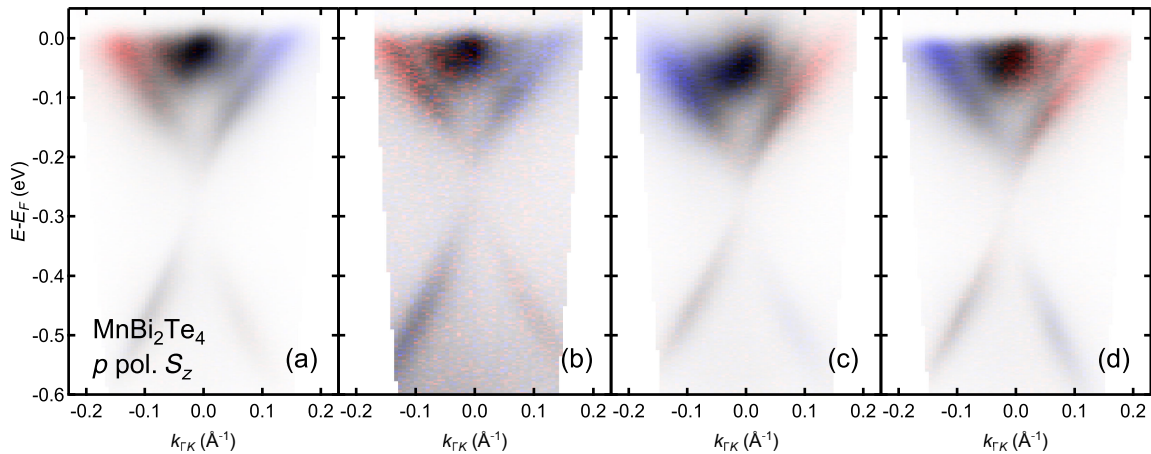


FIG. 6. Four different measurements of MnBi_2Te_4 . Out-of-plane spin polarization S_z taken with p -polarized light at temperature (a) 80 K, (b) 80 K, (c) room temperature, and (d) 18 K. Note that S_z in (a) and (b) is opposite to that in (c) and (d) because of a 180° difference in the azimuthal sample orientation, which produces a reversal of the out-of-plane spin components [see Fig. 1(b)].

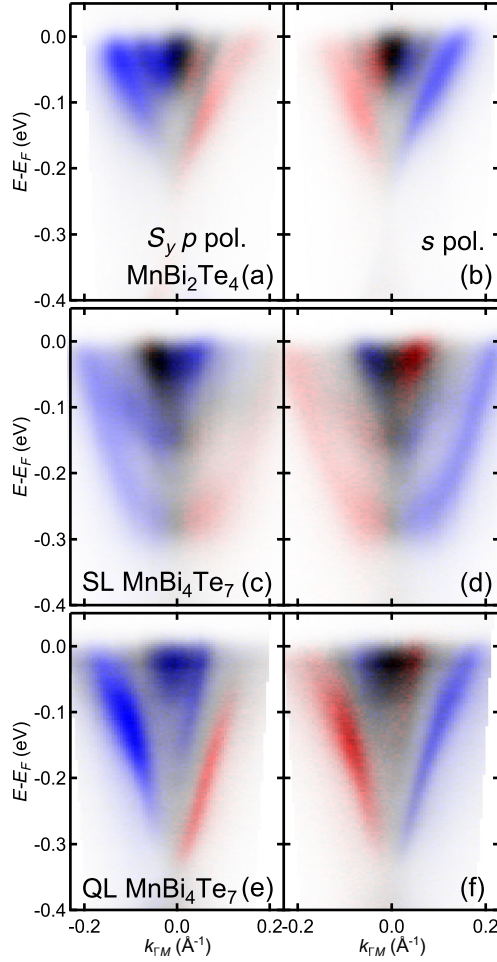


FIG. 7. (a), (b) S_y along Γ M for MnBi_2Te_4 , taken with p - and s -polarized light. (c), (d) Same but for SL MnBi_4Te_7 and (e), (f) QL MnBi_4Te_7 . Color scale same as figures in main text.

APPENDIX G: IN-PLANE SPIN TEXTURE ALONG Γ -M

We show in Fig. 7 the tangential in-plane spin measurements S_y of MnBi_2Te_4 and MnBi_4Te_7 along Γ -M. We rotate the sample azimuthally so that Γ -M is along k_x as shown in Fig. 1(a). Under the constraint of time-reversal symmetry and mirror symmetry along Γ -M, there is no S_z allowed in the paramagnetic phase; therefore, here we focus only on S_y . The measured S_y along Γ -M (Fig. 7) agrees with that measured along Γ -K qualitatively, revealing the helical spin texture of the surface states.

APPENDIX H: EXTRACTING THE QUANTUM GEOMETRY: BERRY CURVATURE AND BERRY CURVATURE MULTIPLES

The extracted wave function parameters can be used to quantify quantum geometry, which is the basis for the quantum anomalous and nonlinear Hall effects. Here we provide a simple example by calculating the Berry

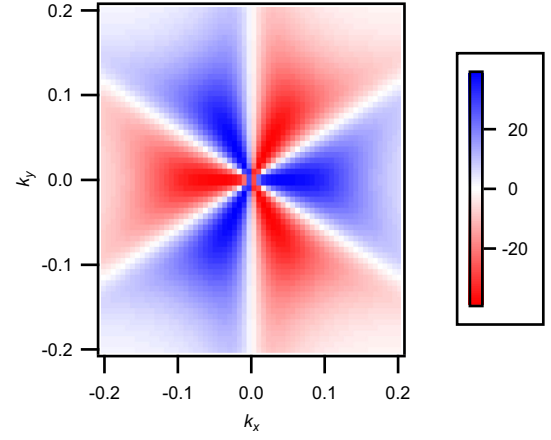


FIG. 8. Simulated Berry curvature of QL MnBi_4Te_7 .

curvature. Based on the Hamiltonian Eq. (1) and Ref. [74], the Berry curvature Ω can be calculated as

$$\Omega(k_x, k_y) = \frac{\alpha^2 [k_x(-3k_y^2 + k_x^2)\gamma]}{[\alpha^2(k_x^2 + k_y^2) + k_x(k_x^2 - 3k_y^2)\gamma]^{1.5}} \quad (\text{H1})$$

where α and γ are the Hamiltonian parameters extracted from our analysis.

Figure 8 shows the calculated Ω for QL MnBi_4Te_7 . In addition, Berry curvature multipoles (dipole, quadrupole, hexapole, etc.) [57] and quantum metric (the real part of quantum geometry) can also be derived from a similar manner [56].

While local Berry curvature in Fig. 8 is finite, the integral across momentum space is zero due to time-reversal symmetry. However, the integral of higher-order multipoles can still be nonzero, and hence can lead to nonlinear Hall conductivities [75]. Therefore, our methodology provides a quantitative pathway to extract nontrivial phenomena related to quantum geometry.

APPENDIX I: DFT CALCULATION

DFT calculation on the surface states of MnBi_2Te_4 is performed using slab models. The MnBi_2Te_4 slab comprises five septuple layers. To prevent interactions between periodic images, a vacuum thickness of at least 12 Å was included in all slab models. We considered intralayer ferromagnetic and interlayer antiferromagnetic configurations, with local magnetic moments collinearly aligned along the out-of-plane direction. All calculations were performed using DFT as implemented in the Vienna *ab initio* simulation package (VASP) [76]. The Perdew-Burke-Ernzerhof generalized gradient approximation [77] was employed for the exchange-correlation functional. A plane-wave energy cutoff of 350 eV was used, and the two-dimensional Brillouin zone was sampled with a k -point grid denser than 6×6 . A Hubbard U (5 eV) correction was applied to the Mn 3d orbitals. Spin-orbit coupling

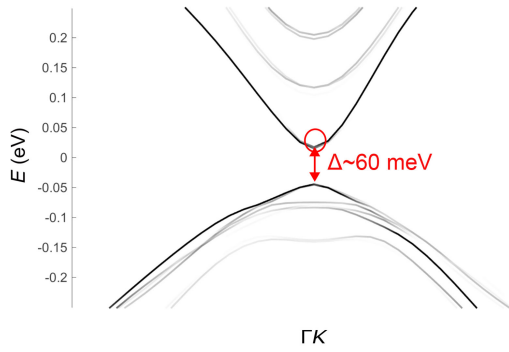


FIG. 9. DFT slab calculations of the band structure of MnBi_2Te_4 . The red circle denotes the Γ point from which the p -orbital weights are extracted. The red arrow represents the TSS gap, with the gap size Δ also labeled.

was included in all electronic structure calculations to ensure accurate description of the surface state properties.

Figure 9 shows the electronic structure of MnBi_2Te_4 near Γ along Γ -K. The intensity represents the weight projected to the surface. We directly extract the p -orbital weights of the TSS at Γ , at the energy-momentum location indicated by the red circle.

- [1] E. D. L. Rienks *et al.*, *Large magnetic gap at the Dirac point in $\text{Bi}_2\text{Te}_3/\text{MnBi}_2\text{Te}_4$ s heterostructures*, *Nature (London)* **576**, 423 (2019).
- [2] M. M. Otrokov *et al.*, *Prediction and observation of an antiferromagnetic topological insulator*, *Nature (London)* **576**, 416 (2019).
- [3] Z. S. Aliev, I. R. Amiraslanov, D. I. Nasonova, A. V. Shevelkov, N. A. Abdullayev, Z. A. Jahangirli, E. N. Orujlu, M. M. Otrokov, N. T. Mamedov, M. B. Babanly, and E. V. Chulkov, *Novel ternary layered manganese bismuth tellurides of the $\text{MnTe-Bi}_2\text{Te}_3$ system: Synthesis and crystal structure*, *J. Alloys Compd.* **789**, 443 (2019).
- [4] I. I. Klimovskikh *et al.*, *Tunable 3D/2D magnetism in the $(\text{MnBi}_2\text{Te}_4)(\text{Bi}_2\text{Te}_3)_m$ topological insulators family*, *npj Quantum Mater.* **5**, 54 (2020).
- [5] Y. Deng, Y. Yu, M. Z. Shi, Z. Guo, Z. Xu, J. Wang, X. H. Chen, and Y. Zhang, *Quantum anomalous Hall effect in intrinsic magnetic topological insulator MnBi_2Te_4* , *Science* **367**, 895 (2020).
- [6] N. Wang, D. Kaplan, Z. Zhang, T. Holder, N. Cao, A. Wang, X. Zhou, F. Zhou, Z. Jiang, C. Zhang, S. Ru, H. Cai, K. Watanabe, T. Taniguchi, B. Yan, and W. Gao, *Quantum-metric-induced nonlinear transport in a topological antiferromagnet*, *Nature (London)* **621**, 487 (2023).
- [7] A. Gao *et al.*, *Quantum metric nonlinear Hall effect in a topological antiferromagnetic heterostructure*, *Science* **381**, 181 (2023).
- [8] H. Li, C. Zhang, C. Zhou, C. Ma, X. Lei, Z. Jin, H. He, B. Li, K. T. Law, and J. Wang, *Quantum geometry quadrupole-induced third-order nonlinear transport in antiferromagnetic topological insulator MnBi_2Te_4* , *Nat. Commun.* **15**, 7779 (2024).
- [9] H. Li *et al.*, *Dirac surface states in intrinsic magnetic topological insulators EuSn_2As_2 and $\text{MnBi}_{2n}\text{Te}_{3n+1}$* , *Phys. Rev. X* **9**, 041039 (2019).
- [10] Y.-J. Hao *et al.*, *Gapless surface Dirac cone in antiferromagnetic topological insulator MnBi_2Te_4* , *Phys. Rev. X* **9**, 041038 (2019).
- [11] Y. J. Chen *et al.*, *Topological electronic structure and its temperature evolution in antiferromagnetic topological insulator MnBi_2Te_4* , *Phys. Rev. X* **9**, 041040 (2019).
- [12] Y. Hu, L. Xu, M. Shi, A. Luo, S. Peng, Z. Y. Wang, J. J. Ying, T. Wu, Z. K. Liu, C. F. Zhang, Y. L. Chen, G. Xu, X. H. Chen, and J. F. He, *Universal gapless Dirac cone and tunable topological states in $(\text{MnBi}_2\text{Te}_4)_m(\text{Bi}_2\text{Te}_3)_n$ heterostructures*, *Phys. Rev. B* **101**, 161113(R) (2020).
- [13] D. Nevola, H. X. Li, J.-Q. Yan, R. G. Moore, H.-N. Lee, H. Miao, and P. D. Johnson, *Coexistence of surface ferromagnetism and a gapless topological state in MnBi_2Te_4* , *Phys. Rev. Lett.* **125**, 117205 (2020).
- [14] P. Swatek, Y. Wu, L.-L. Wang, K. Lee, B. Schunk, J. Yan, and A. Kaminski, *Gapless Dirac surface states in the antiferromagnetic topological insulator MnBi_2Te_4* , *Phys. Rev. B* **101**, 161109(R) (2020).
- [15] R. C. Vidal, H. Bentmann, J. I. Facio, T. Heider, P. Kagerer, C. I. Fornari, T. R. F. Peixoto, T. Figgemeier, S. Jung, C. Cacho, B. Büchner, J. van den Brink, C. M. Schneider, L. Plucinski, E. F. Schwier, K. Shimada, M. Richter, A. Isaeva, and F. Reinert, *Orbital complexity in intrinsic magnetic topological insulators MnBi_4Te_7 and $\text{MnBi}_6\text{Te}_{10}$* , *Phys. Rev. Lett.* **126**, 176403 (2021).
- [16] X. Wu *et al.*, *Distinct topological surface states on the two terminations of MnBi_4Te_7* , *Phys. Rev. X* **10**, 031013 (2020).
- [17] J. Li, Y. Li, S. Du, Z. Wang, B.-L. Gu, S.-C. Zhang, K. He, W. Duan, and Y. Xu, *Intrinsic magnetic topological insulators in van der Waals layered MnBi_2Te_4 -family materials*, *Sci. Adv.* **5**, eaaw5685 (2019).
- [18] J. Li, C. Wang, Z. Zhang, B.-L. Gu, W. Duan, and Y. Xu, *Magnetically controllable topological quantum phase transitions in the antiferromagnetic topological insulator MnBi_2Te_4* , *Phys. Rev. B* **100**, 121103(R) (2019).
- [19] R. C. Vidal *et al.*, *Topological electronic structure and intrinsic magnetization in MnBi_4Te_7* , *Phys. Rev. X* **9**, 041065 (2019).
- [20] J. Wu, F. Liu, M. Sasase, K. Ienaga, Y. Obata, R. Yukawa, K. Horiba, H. Kumigashira, S. Okuma, T. Inoshita, and H. Hosono, *Natural van der Waals heterostructural single crystals with both magnetic and topological properties*, *Sci. Adv.* **5**, eaax9989 (2019).
- [21] D. Zhang, M. Shi, T. Zhu, D. Xing, H. Zhang, and J. Wang, *Topological axion states in the magnetic insulator MnBi_2Te_4 with the quantized magnetoelectric effect*, *Phys. Rev. Lett.* **122**, 206401 (2019).
- [22] A. M. Shikin, N. L. Zaitsev, A. V. Tarasov, T. P. Makarova, D. A. Glazkova, D. A. Estyunin, and I. I. Klimovskikh, *Electronic and spin structure of topological surface states in MnBi_4Te_7 and $\text{MnBi}_6\text{Te}_{10}$ and their modification by an applied electric field*, *JETP Lett.* **116**, 556 (2022).
- [23] Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, *Observation of a large-gap topological-insulator class with a single Dirac cone on the surface*, *Nat. Phys.* **5**, 398 (2009).

- [24] Y. L. Chen, J. G. Analytis, J.-H. Chu, Z. K. Liu, S.-K. Mo, X. L. Qi, H. J. Zhang, D. H. Lu, X. Dai, Z. Fang, S. C. Zhang, I. R. Fisher, Z. Hussain, and Z.-X. Shen, *Experimental realization of a three-dimensional topological insulator*, *Bi₂Te₃*, *Science* **325**, 178 (2009).
- [25] C. Yan, S. Fernandez-Mulligan, R. Mei, S. H. Lee, N. Protic, R. Fukumori, B. Yan, C. Liu, Z. Mao, and S. Yang, *Origins of electronic bands in the antiferromagnetic topological insulator MnBi₂Te₄*, *Phys. Rev. B* **104**, L041102 (2021).
- [26] A. Liang, C. Chen, H. Zheng, W. Xia, K. Huang, L. Wei, H. Yang, Y. Chen, X. Zhang, X. Xu, M. Wang, Y. Guo, L. Yang, Z. Liu, and Y. Chen, *Approaching a minimal topological electronic structure in antiferromagnetic topological insulator MnBi₂Te₄ via surface modification*, *Nano Lett.* **22**, 4307 (2022).
- [27] W. Lee, S. Fernandez-Mulligan, H. Tan, C. Yan, Y. Guan, S. H. Lee, R. Mei, C. Liu, B. Yan, Z. Mao, and S. Yang, *Layer-by-layer disentanglement of Bloch states*, *Nat. Phys.* **19**, 950 (2023).
- [28] J. Qu, X. Han, S. Sakamoto, C. J. Jia, J. Liu, H. Li, D. Guan, Y. J. Zeng, M. Schüler, P. S. Kirchmann, B. Moritz, Z. Hussain, T. P. Devereaux, Z. X. Shen, and J. A. Sobota, *Reversal of spin-polarization near the Fermi level of the Rashba semiconductor BiTeCl*, *npj Quantum Mater.* **8**, 13 (2023).
- [29] X. Han, J. Qu, S. Sakamoto, D. Liu, D. Guan, J. Liu, H. Li, C. R. Rotundu, N. Andresen, C. Jozwiak, Z. Hussain, Z.-X. Shen, and J. A. Sobota, *Development of deflector mode for spin-resolved time-of-flight photoemission spectroscopy*, *Rev. Sci. Instrum.* **94**, 103906 (2023).
- [30] G. Naselli, A. G. Moghaddam, S. Di Napoli, V. Vildosola, I. C. Fulga, J. van den Brink, and J. I. Facio, *Magnetic warping in topological insulators*, *Phys. Rev. Res.* **4**, 033198 (2022).
- [31] L. Xu *et al.*, *Persistent surface states with diminishing gap in MnBi₂Te₄/Bi₂Te₃ superlattice antiferromagnetic topological insulator*, *Sci. Bull.* **65**, 2086 (2020).
- [32] C. Hu, K. N. Gordon, P. Liu, J. Liu, X. Zhou, P. Hao, D. Narayan, E. Emmanouilidou, H. Sun, Y. Liu, H. Brawer, A. P. Ramirez, L. Ding, H. Cao, Q. Liu, D. Dessau, and N. Ni, *A van der Waals antiferromagnetic topological insulator with weak interlayer magnetic coupling*, *Nat. Commun.* **11**, 97 (2020).
- [33] S. Souma, K. Kosaka, T. Sato, M. Komatsu, A. Takayama, T. Takahashi, M. Kriener, K. Segawa, and Y. Ando, *Direct measurement of the out-of-plane spin texture in the Dirac-cone surface state of a topological insulator*, *Phys. Rev. Lett.* **106**, 216803 (2011).
- [34] M. Nomura, S. Souma, A. Takayama, T. Sato, T. Takahashi, K. Eto, K. Segawa, and Y. Ando, *Relationship between Fermi surface warping and out-of-plane spin polarization in topological insulators: A view from spin- and angle-resolved photoemission*, *Phys. Rev. B* **89**, 045134 (2014).
- [35] H. Bentmann, H. Maaß, J. Braun, C. Seibel, K. A. Kokh, O. E. Tereshchenko, S. Schreyeck, K. Brunner, L. W. Molenkamp, K. Miyamoto, M. Arita, K. Shimada, T. Okuda, J. Kirschner, C. Tusche, H. Ebert, J. Minár, and F. Reinert, *Profiling spin and orbital texture of a topological insulator in full momentum space*, *Phys. Rev. B* **103**, L161107 (2021).
- [36] L. Fu, *Hexagonal warping effects in the surface states of the topological insulator Bi₂Te₃*, *Phys. Rev. Lett.* **103**, 266801 (2009).
- [37] R. C. Vidal *et al.*, *Surface states and Rashba-type spin polarization in antiferromagnetic MnBi₂Te₄ (0001)*, *Phys. Rev. B* **100**, 121104(R) (2019).
- [38] A. M. Shikin *et al.*, *Nature of the Dirac gap modulation and surface magnetic interaction in axion antiferromagnetic topological insulator MnBi₂Te₄*, *Sci. Rep.* **10**, 13226 (2020).
- [39] Z. H. Zhu, C. N. Veenstra, S. Zhdanovich, M. P. Schneider, T. Okuda, K. Miyamoto, S. Y. Zhu, H. Namatame, M. Taniguchi, M. W. Haverkort, I. S. Elfimov, and A. Damascelli, *Photoelectron spin-polarization control in the topological insulator Bi₂Se₃*, *Phys. Rev. Lett.* **112**, 076802 (2014).
- [40] J. H. Ryoo and C. H. Park, *Spin-conserving and reversing photoemission from the surface states of Bi₂Se₃ and Au (111)*, *Phys. Rev. B* **93**, 085419 (2016).
- [41] C. Jozwiak, C. H. Park, K. Gottlieb, C. Hwang, D. H. Lee, S. G. Louie, J. D. Denlinger, C. R. Rotundu, R. J. Birgeneau, Z. Hussain, and A. Lanzara, *Photoelectron spin-flipping and texture manipulation in a topological insulator*, *Nat. Phys.* **9**, 293 (2013).
- [42] Z. Xie *et al.*, *Orbital-selective spin texture and its manipulation in a topological insulator*, *Nat. Commun.* **5**, 3382 (2014).
- [43] H. Zhang, C.-X. Liu, and S.-C. Zhang, *Spin-orbital texture in topological insulators*, *Phys. Rev. Lett.* **111**, 066801 (2013).
- [44] J. Sánchez-Barriga, A. Varykhalov, J. Braun, S. Y. Xu, N. Alidoust, O. Kornilov, J. Minár, K. Hummer, G. Springholz, G. Bauer, R. Schumann, L. V. Yashina, H. Ebert, M. Z. Hasan, and O. Rader, *Photoemission of Bi₂Se₃ with circularly polarized light: Probe of spin polarization or means for spin manipulation?*, *Phys. Rev. X* **4**, 011046 (2014).
- [45] C. X. Liu, X. L. Qi, H. J. Zhang, X. Dai, Z. Fang, and S. C. Zhang, *Model Hamiltonian for topological insulators*, *Phys. Rev. B* **82**, 045122 (2010).
- [46] Z. H. Zhu, C. N. Veenstra, G. Levy, A. Ubal dini, P. Syers, N. P. Butch, J. Paglione, M. W. Haverkort, I. S. Elfimov, and A. Damascelli, *Layer-by-layer entangled spin-orbital texture of the topological surface state in Bi₂Se₃*, *Phys. Rev. Lett.* **110**, 216401 (2013).
- [47] A. Pertsova and C. M. Canali, *Probing the wavefunction of the surface states in Bi₂Se₃ topological insulator: A realistic tight-binding approach*, *New J. Phys.* **16**, 063022 (2014).
- [48] Y. H. Wang, D. Hsieh, D. Pilon, L. Fu, D. R. Gardner, Y. S. Lee, and N. Gedik, *Observation of a warped helical spin texture in Bi₂Se₃ from circular dichroism angle-resolved photoemission spectroscopy*, *Phys. Rev. Lett.* **107**, 207602 (2011).
- [49] M. R. Scholz, J. Sánchez-Barriga, J. Braun, D. Marchenko, A. Varykhalov, M. Lindroos, Y. J. Wang, H. Lin, A. Bansil, J. Minár, H. Ebert, A. Volykhov, L. V. Yashina, and O. Rader, *Reversal of the circular dichroism in angle-resolved*

- photoemission from Bi_2Te_3 , *Phys. Rev. Lett.* **110**, 216801 (2013).
- [50] S. Cho, J. H. Park, S. Huh, J. Hong, W. Kyung, B. G. Park, J. D. Denlinger, J. H. Shim, C. Kim, and S. R. Park, *Studying local Berry curvature in 2H-WSe₂ by circular dichroism photoemission utilizing crystal mirror plane*, *Sci. Rep.* **11**, 1684 (2021).
- [51] Q. Liu, X. Zhang, J. A. Waugh, D. S. Dessau, and A. Zunger, *Orbital mapping of energy bands and the truncated spin polarization in three-dimensional Rashba semiconductors*, *Phys. Rev. B* **94**, 125207 (2016).
- [52] J. A. Waugh, T. Nummy, S. Parham, Q. Liu, X. Zhang, A. Zunger, and D. S. Dessau, *Minimal ingredients for orbital-texture switches at Dirac points in strong spin-orbit coupled materials*, *npj Quantum Mater.* **1**, 16025 (2016).
- [53] S. Vajna, E. Simon, A. Szilva, K. Palotas, B. Ujfalussy, and L. Szunyogh, *Higher-order contributions to the Rashba-Bychkov effect with application to the Bi/Ag(111) surface alloy*, *Phys. Rev. B* **85**, 075404 (2012).
- [54] D. Xiao, M.-C. Chang, and Q. Niu, *Berry phase effects on electronic properties*, *Rev. Mod. Phys.* **82**, 1959 (2010).
- [55] Y. Gao, S. A. Yang, and Q. Niu, *Field induced positional shift of Bloch electrons and its dynamical implications*, *Phys. Rev. Lett.* **112**, 166601 (2014).
- [56] K. Das, S. Lahiri, R. B. Atencia, D. Culcer, and A. Agarwal, *Intrinsic nonlinear conductivities induced by the quantum metric*, *Phys. Rev. B* **108**, L201405 (2023).
- [57] C. P. Zhang, X. J. Gao, Y. M. Xie, H. C. Po, and K. T. Law, *Higher-order nonlinear anomalous Hall effects induced by Berry curvature multipoles*, *Phys. Rev. B* **107**, 115142 (2023).
- [58] R.-X. Zhang, F. Wu, and S. Das Sarma, *Möbius insulator and higher-order topology in $\text{MnBi}_{2n}\text{Te}_{3n+1}$* , *Phys. Rev. Lett.* **124**, 136407 (2020).
- [59] K. F. Garrity, S. Chowdhury, and F. M. Tavazza, *Topological surface states of MnBi_2Te_4 at finite temperatures and at domain walls*, *Phys. Rev. Mater.* **5**, 024207 (2021).
- [60] Z. Yang and H. Zhang, *Evolution of surface states of antiferromagnetic topological insulator MnBi_2Te_4 with tuning the surface magnetization*, *New J. Phys.* **24**, 073034 (2022).
- [61] A. M. Shikin, D. A. Estyunin, N. L. Zaitsev, D. Glazkova, I. I. Klimovskikh, S. O. Filnov, A. G. Rybkin, E. F. Schwier, S. Kumar, A. Kimura, N. Mamedov, Z. Aliev, M. B. Babanly, K. Kokh, O. E. Tereshchenko, M. M. Otrokov, E. V. Chulkov, K. A. Zvezdin, and A. K. Zvezdin, *Sample-dependent Dirac-point gap in and its response to applied surface charge: A combined photoemission and ab initio study*, *Phys. Rev. B* **104**, 115168 (2021).
- [62] H. Tan and B. Yan, *Distinct magnetic gaps between antiferromagnetic and ferromagnetic orders driven by surface defects in the topological magnet MnBi_2Te_4* , *Phys. Rev. Lett.* **130**, 126702 (2023).
- [63] M. Liu, C. Lei, H. Kim, Y. Li, L. Frammolino, J. Yan, A. H. Macdonald, and C.-K. Shih, *Visualizing the interplay of Dirac mass gap and magnetism at nanoscale in intrinsic magnetic topological insulators*, *Proc. Natl. Acad. Sci. U.S.A.* **119**, e2207681119 (2022).
- [64] S. Xiao, X. Xiao, F. Zhan, J. Fan, X. Wu, and R. Wang, *Spin-polarized topological phases in a ferromagnetic $\text{Bi}_2\text{Te}_3/\text{MnBi}_2\text{Te}_4$ bilayer tuned by electric and magnetic fields*, *Phys. Rev. B* **105**, 125126 (2022).
- [65] R. Lu *et al.*, *Half-magnetic topological insulator with magnetization-induced Dirac gap at a selected surface*, *Phys. Rev. X* **11**, 011039 (2021).
- [66] P. Kagerer *et al.*, *Two-dimensional ferromagnetic extension of a topological insulator*, *Phys. Rev. Res.* **5**, L022019 (2023).
- [67] M. M. Otrokov, T. V. Menshchikova, M. G. Vergniory, I. P. Rusinov, A. Yu Vyazovskaya, Y. M. Koroteev, G. Bihlmayer, A. Ernst, P. M. Echenique, A. Arnau, and E. V. Chulkov, *Highly-ordered wide bandgap materials for quantized anomalous Hall and magnetoelectric effects*, *2D Mater.* **4**, 025082 (2017).
- [68] C. Jozwiak, J. Graf, G. Lebedev, N. Andresen, A. K. Schmid, A. V. Fedorov, F. El Gabaly, W. Wan, A. Lanzara, and Z. Hussain, *A high-efficiency spin-resolved photoemission spectrometer combining time-of-flight spectroscopy with exchange-scattering polarimetry*, *Rev. Sci. Instrum.* **81**, 053904 (2010).
- [69] K. Gotlieb, Z. Hussain, A. Bostwick, A. Lanzara, and C. Jozwiak, *Rapid high-resolution spin- and angle-resolved photoemission spectroscopy with pulsed laser source and time-of-flight spectrometer*, *Rev. Sci. Instrum.* **84**, 093904 (2013).
- [70] Y. Ishida, T. Otsu, A. Ozawa, K. Yaji, S. Tani, S. Shin, and Y. Kobayashi, *High repetition pump-and-probe photoemission spectroscopy based on a compact fiber laser system*, *Rev. Sci. Instrum.* **87**, 123902 (2016).
- [71] S. Moser, *A toy model for dichroism in angle resolved photoemission*, *J. Electron Spectrosc. Relat. Phenom.* **262**, 147278 (2023).
- [72] J.-H. Park, C. H. Kim, J.-W. Rhim, and J. H. Han, *Orbital Rashba effect and its detection by circular dichroism angle-resolved photoemission spectroscopy*, *Phys. Rev. B* **85**, 195401 (2012).
- [73] A. S. Ketterl, S. Otto, M. Bastian, B. Andres, C. Gahl, J. Minár, H. Ebert, J. Braun, O. E. Tereshchenko, K. A. Kokh, T. Fauster, and M. Weinelt, *Origin of spin-polarized photocurrents in the topological surface states of Bi_2Se_3* , *Phys. Rev. B* **98**, 155406 (2018).
- [74] Z. Li and J. P. Carbotte, *Hexagonal warping on spin texture, Hall conductivity, and circular dichroism of topological insulators*, *Phys. Rev. B* **89**, 165420 (2014).
- [75] I. Sodemann and L. Fu, *Quantum nonlinear Hall effect induced by Berry curvature dipole in time-reversal invariant materials*, *Phys. Rev. Lett.* **115**, 216806 (2015).
- [76] G. Kresse and J. Furthmüller, *Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set*, *Comput. Mater. Sci.* **6**, 15 (1996).
- [77] J. P. Perdew, K. Burke, and M. Ernzerhof, *Generalized gradient approximation made simple*, *Phys. Rev. Lett.* **77**, 3865 (1996).