

Supplementary Information: Rashba Spin-Splitting Driven Inverse Spin Hall Effect in MnBi₂Te₄

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SUPPLEMENTARY NOTE 1: SPIN HALL CONDUCTIVITY

Base on the Kubo formula, spin Hall conductivity (SHC) can be written as^[1, 2]

$$\sigma_{\beta\gamma}^{\alpha} = -\frac{e^2}{\hbar} \frac{1}{VN_k^3} \sum_{\mathbf{k}} \Omega_{\beta\gamma}^{\alpha}(\mathbf{k}), \quad (\text{Supplementary equation 1})$$

where V is the volume of crystal structure, and N_k^3 is the number of k points in the Brillouin zone, and the k -resolved term can be represented as

$$\Omega_{\beta\gamma}^{\alpha}(\mathbf{k}) = \sum_n f_{n\mathbf{k}} \Omega_{n,\beta\gamma}^{\alpha}(\mathbf{k}), \quad (\text{Supplementary equation 2})$$

where $f_{n\mathbf{k}}$ is the Fermi distribution function, and the band-projected Berry curvature term is

$$\Omega_{n,\beta\gamma}^{\alpha}(\mathbf{k}) = \hbar^2 \sum_{m \neq n} \frac{-2 \text{Im} [\langle n\mathbf{k} | \frac{1}{2} \{ \hat{\sigma}_{\alpha}, \hat{v}_{\beta} \} | m\mathbf{k} \rangle \langle m\mathbf{k} | \hat{v}_{\gamma} | n\mathbf{k} \rangle]}{(\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}})^2}, \quad (\text{Supplementary equation 3})$$

where m and n are the band indexes, ϵ_i ($i = m, n$) are the eigenvalues. For SHC, the spin-current operator is given by

$$\hat{j}_x = \frac{1}{2} \{ \hat{s}_z, \hat{v}_x \}.$$

Assuming the spin is oriented in the z -direction, we have

$$\hat{j}_{\text{spin},z} = \frac{1}{2} (\hat{s}_z \hat{v}_x + \hat{v}_x \hat{s}_z).$$

It is clear that the intrinsic SHC mainly depends on the spin operator $\hat{s}_z$ and the velocity operators $\hat{v}_x$ and $\hat{v}_y$. Thus we can qualitatively state that the sign reversal of SHC is mainly a result of the transition in the type of band splitting and changes in the spin distribution, leading to the opposite signs of the Berry curvature.

SUPPLEMENTARY NOTE 2: THE ORIGIN OF RASHBA SOC

In the following, we present a succinct explanation of the origin of the Rashba spin-orbit coupling (SOC). When an electron carrying momentum $\mathbf{p}$ moves within a magnetic field of strength $\mathbf{B}$, it experiences a Lorentz force $\mathbf{F} = -e\mathbf{p} \times \mathbf{B}/m$, perpendicular to its motion direction. This motion results in the generation of Zeeman energy $\mu_B \boldsymbol{\sigma} \cdot \mathbf{B}$, where the Bohr magneton $\mu_B = 9.27 \times 10^{-24} \text{ JT}^{-1}$, $\boldsymbol{\sigma}$ represents the Pauli spin matrix-vector, and m and e denote the electron's mass and charge, respectively. Let's now consider an electron moving through an electric field $\mathbf{E}$. Utilizing the electron as a rest frame while the electric field is in motion, the electron encounters an effective magnetic field $\mathbf{B}_{\text{eff}} \sim \mathbf{E} \times \mathbf{p}/mc^2$, arising from the moving electric field (with c being the speed of light). This effective magnetic field triggers the SOC, expressed as $\hat{H}_{\text{SO}} \sim \mu_B (\mathbf{E} \times \mathbf{p}) \cdot \boldsymbol{\sigma}/mc^2$, where $\mathbf{E}$ originates from the gradient of the crystal potential within the crystal, denoted as $\mathbf{E} = -\nabla V$. This results in the emergence of the spin-orbit

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field $\mathbf{so}(\mathbf{p}) = -\mu_B(\nabla V \times \mathbf{p})/mc^2$, which is momentum-dependent. It is essential to note that the SOC preserves time-reversal symmetry (TRS), as reflected in $(\mathbf{so}(\mathbf{p}) \cdot \boldsymbol{\sigma} = -\mathbf{so}(-\mathbf{p}) \cdot \boldsymbol{\sigma})$, indicating that $\mathbf{so}(-\mathbf{p}) = -\mathbf{so}(\mathbf{p})$. This peculiar property implies that the spin-orbit field must exhibit singularity in electron momentum $\mathbf{p}$, typically found in systems with broken space inversion symmetry $\mathcal{I}$. Hence, in systems adhering to TRS, $\mathcal{I}$ must be disrupted to facilitate induced energy band spin splitting, denoted by $\mathbf{B}_{\text{eff}}(\mathbf{p}) \neq 0$. This spin splitting effect correlates with a spin-momentum locking phenomenon. Vas'ko[3] and Bychkov/Rashba[4] proposed the Rashba SOC characteristic, described by Eq. [Supplementary equation 4](#), when considering an interface electric field $\mathbf{E} = E_z \mathbf{z}$ linearly dependent on $\mathbf{z}$ in the $\mathbf{z}$ direction.

$$\hat{H}_R = (\alpha_R/\hbar) (\mathbf{z} \times \mathbf{p}) \cdot \boldsymbol{\sigma} \quad (\text{Supplementary equation 4})$$

where α_R is the Rashba parameter.

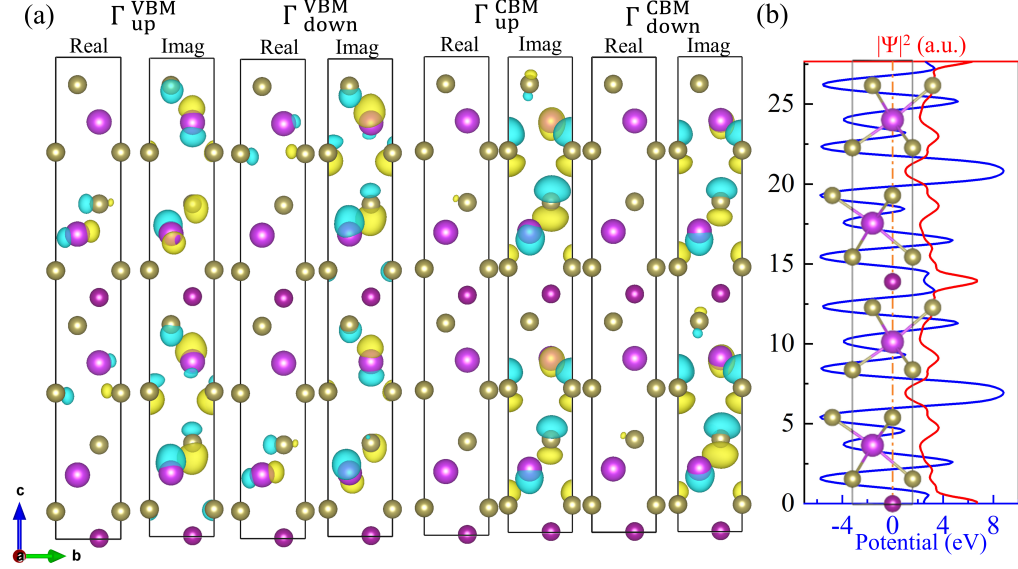


FIG. S1. Wavefunction distributions and charge density. (a) CBM and VBM at the Γ point distinguish between the wavefunction distributions of the upper and lower spins. (b) Dependence on the electrostatic potential and the surface charge density (mode squared of the wavefunction) in the z direction.

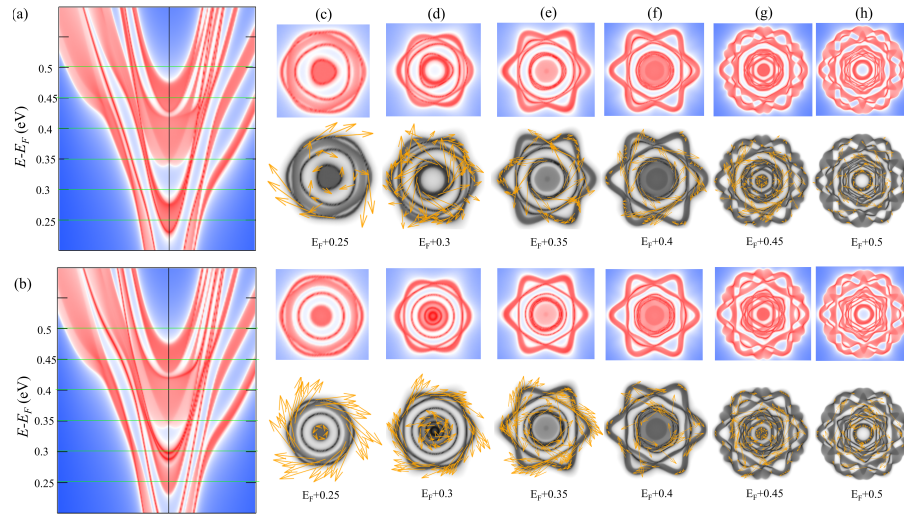


FIG. S2. Fermi arcs of different energy cross-sections. Surface states on (001) plane of (a) left and (b) right termination. (c)-(h) Spin textures for different energy sections.

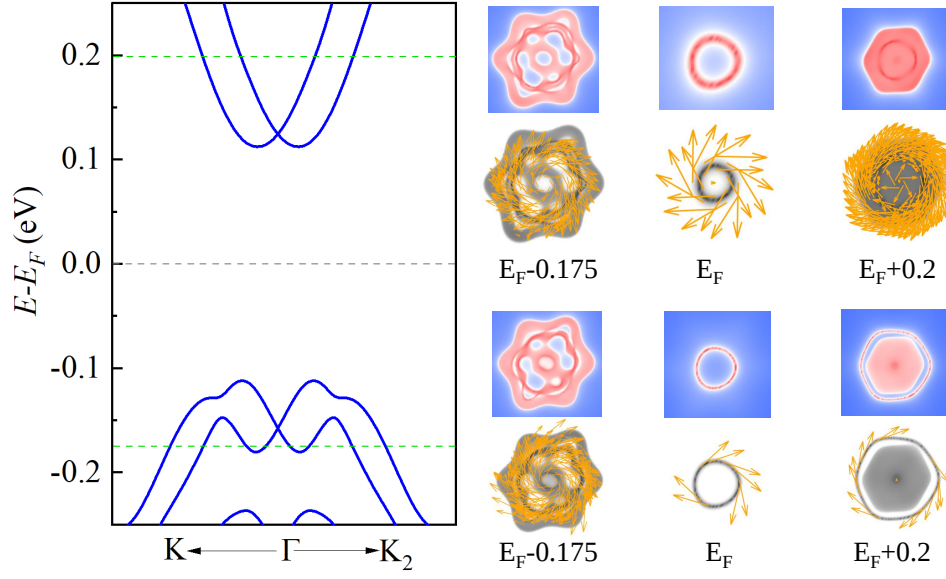


FIG. S3. Fermi arcs of different energy cross-sections in Lifshitz splitting system. Lifshitz-type splitting with Fermi surfaces and spin textures across different energy cross-sections.

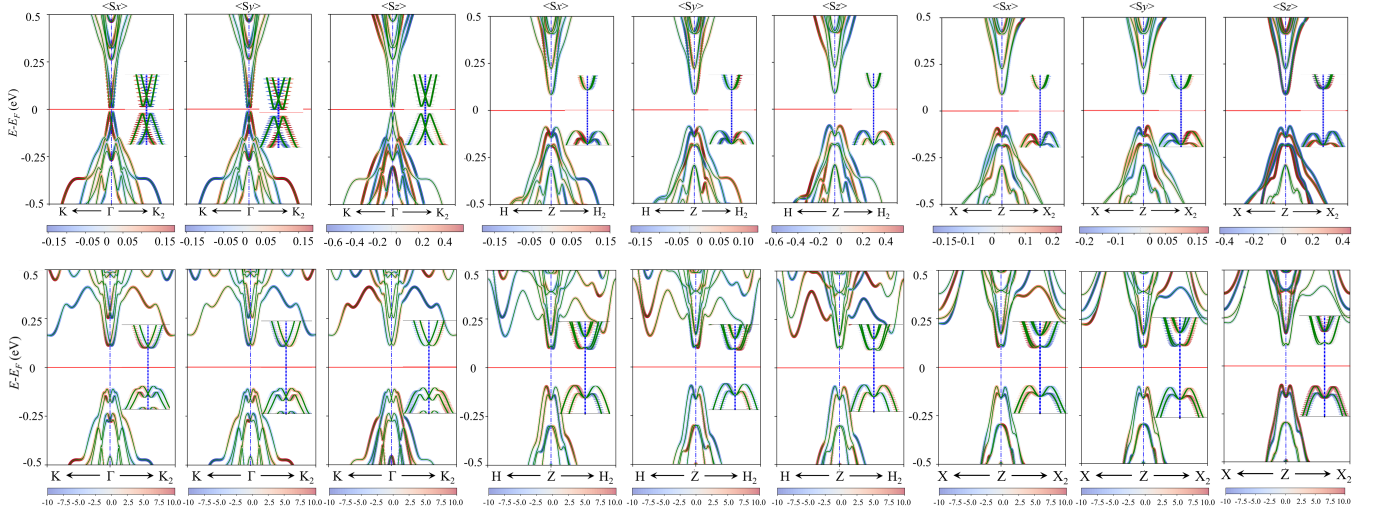


FIG. S4. Spin distribution of two splitting types. The Rashba split (upper column) and Lifshitz split (lower column) distinguish energy bands in the spin direction on the iso z -plane $K - \Gamma - K_2$ path, and the trans z -plane $H - Z - H_2$ and $X - Z - X_2$ paths. The high symmetric paths are shown in Fig. 1(d). Red represents spin up and blue spin down.

SUPPLEMENTARY NOTE 3: ELECTRIC POLARIZATION

R-MBT classifies it as a polarized material within the $3m1'$ magnetic point group. With polarization along the z -axis, both AFM order structures (AFM- x and AFM- z) exhibit a significant electric polarization of $0.51 \text{ C per } m^2$, while linear ferromagnetic order structures (FM- x and FM- z) show a polarization of $0.37 \text{ C per } m^2$. This substantial spontaneous polarization is comparable to well-known materials such as BaTiO_3 ($0.26 \text{ C per } m^2$) [5], and HfO_2 in the $Pca2_1$ ($0.52 \text{ C per } m^2$) and $Pmn2_1$ ($0.56 \text{ C per } m^2$) phases [6]. Although reversing ferroelectric polarization in this bulk structure is challenging, layered materials offer potential for induced ferroelectric polarization through intentional interlayer shifts or stacking variations. Alternatively, non-switchable electric polarization may exhibit pyroelectric properties similar to those found in compounds like $\text{CaBaCo}_4\text{O}_7$ with an orthorhombic $Pbn2_1$ space group [7–9]. This suggests potential for screening band spin splitting types through polarization modulation by magnetic configurations.

SUPPLEMENTARY NOTE 4: RASHBA SPLITTING

Detecting Rashba splitting in 3D bulk materials is rare and significant. To explore the physical implications of Rashba splitting due to $\mathcal{I}$ breaking, we calculated wave functions at the conduction band minimum (CBM) and valence band maximum (VBM) near the high symmetry point Γ , as shown in Fig. S1(a). The analysis reveals that Rashba splitting primarily originates from imaginary components, with substantial contributions from Bi- p_z and Te- p_z orbitals. Additionally, Fig. S1(b) in the SM displays the electrostatic potential distribution and the average surface charge density along the z -direction. The electrostatic potential difference between Bi and Te atoms creates an intrinsic electric field that induces polarization and drives the Rashba effect.

In the energy range $(-0.15, 0.15)$ eV, pronounced Rashba spin splitting is evident in both the conduction and valence bands near the Fermi level. The Rashba splitting magnitude is described by $\alpha_R = \frac{2E_R}{k_0}$, with $E_R = \frac{\hbar^2 k_0^2}{2m^*}$ and $k_0 = \frac{\alpha_R m^*}{\hbar^2}$. We can calculate $\alpha_R^{VBM} = 4.631$ eVÅ, $\alpha_R^{CBM} = 4$ eVÅ, which is much larger than that of BiTeI ($\alpha_R = 3.85$ eVÅ)[10], and the valence-band splitting is also larger than the largest bulk Rashba state at the M point in the PtBi₂ system $\alpha_R = 4.36 \pm 0.14$ eVÅ. And it has a similar degree of Rashba splitting to systems such as KSnSb_xBi_{1-x} ($\alpha_R = 4.83$ eVÅ)[11], BiTeI ($\alpha_R = 4.548$ eVÅ), GeTe ($\alpha_R = 4.352$ eVÅ), BiTeCl ($\alpha_R = 3.564$ eVÅ), Sb₂TeSe₂ ($\alpha_R = 3.885$ eVÅ)[12], and the recently reported RbSnBi ($\alpha_R = 3.33$ eVÅ), CsSnBi ($\alpha_R = 2.68$ eVÅ)[13]. Although giant Rashba splitting zones RbSnBi ($\alpha_R = 4.26$ eVÅ), CsSnBi ($\alpha_R = 6.4$ eVÅ)[13] have also been reported at the top of the valence zone, this seems to look more like the Lifshitz-type splitting zone.

SUPPLEMENTARY NOTE 5: SPIN DISTRIBUTION

To investigate the anisotropic spin splitting induced by the Rashba effect, we analyzed spin component weights for two spin splitting configurations of R-MBT along various paths, as shown in Fig. S4. Along the K - Γ - K_2 path in the $k_z=0$ plane, we observed significant band spin splittings, including Rashba and Lifshitz types, in the valence band. Lifshitz-type splits result from the deformation of the second-highest valence band, causing spin redistribution. For Rashba-type splitting along the K - Γ - K_2 path, all three spin components exhibit opposite spin chirality distributions between the symmetric momentum path centered at the Γ point and the two splitting subbands. Conversely, Lifshitz-type splitting in the valence band on the K - Γ - K_2 path shows opposing spin orientations between the two subbands, maintaining an antisymmetric spin distribution around the Γ point in momentum space. This shift in valence band spin splitting type along the $k_z=0$ plane path significantly impacts spin distribution and transport behavior. Transitioning to Lifshitz-type spin splitting is observed when selecting high symmetry line paths across distinct k_z planes. Except for the out-of-plane spin component $\langle S_z \rangle$ along the X - Z - X_2 path, other spin component distributions across the k_z planes remain consistent with the transition to valence band splitting type along the in-plane path. The X - Z - X_2 and H - Z - H_2 paths, both high symmetry lines spanning the k_z plane, exhibit similar chiral laws for the in-plane spin components $\langle S_x \rangle$ and $\langle S_y \rangle$. Additionally, the $\langle S_z \rangle$ spin components of the H - Z - H_2 paths share the same cross-spin chirality as the K - Z - K_2 paths due to their positions at similar corners of the Brillouin zone.

SUPPLEMENTARY NOTE 6: TB MODEL

The magnetic space group of the MnBi₂Te₄ system whose phase changes to the C_{3v} point group after structural inversion symmetry breaking is the grey group 158. Based on the inputs of the magnetic group, the lattice parameters, the atomic Wyckoff occupation sites, and the consideration of the p_z orbitals of the SOC as a basis function, the TB model has been constructed and the Hamiltonian quantities as shown have been obtained by using the MagneticTB software, with the computational procedure taking into account the next-nearest-neighbour atoms.

The TB model Hamiltonian constructed to coincide with the DFT computation on the K - Γ - K_2 path is shown in Fig. S6, where $\mathcal{R}_l$ ($l=1,2,3,4$) is shown in Eq. Supplementary equation 5-Supplementary equation 8. Then the φ_k , $\mathcal{H}_i$, c_l and $E_j^{(x,y)}$ involved in $\mathcal{R}_l$ (integers $i=1-6$, $j=1-8$, $k=1-2$, $l=1-4$, and the upper index in $E_j^{(x,y)}$ is denoted $\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} t_2 \\ t_3 \end{pmatrix} = \begin{pmatrix} r_2 \\ r_3 \end{pmatrix}$ as in Eqs. Supplementary equation 9-Supplementary equation 11.

The diagonal element of the $\mathcal{R}_i$ matrix consists of the product of the c_l constant coefficients, the φ_k trinomials, and the atomic positional information $\mathcal{H}_i$, which can no longer be referred to the common factor due to the more complex interactions in the non-diagonal element, and is denoted by the $E_j^{(x,y)}$ in a complex relationship.

As shown in Fig. 1(b), the Bi and Te atoms of an septuple (SL) single cell are distinguished as Bi₁, Bi₂ and Te₁, Te₂, Te₃, and Te₄, respectively, and the positions of the corresponding atoms of the other equivalent SL of the AFM

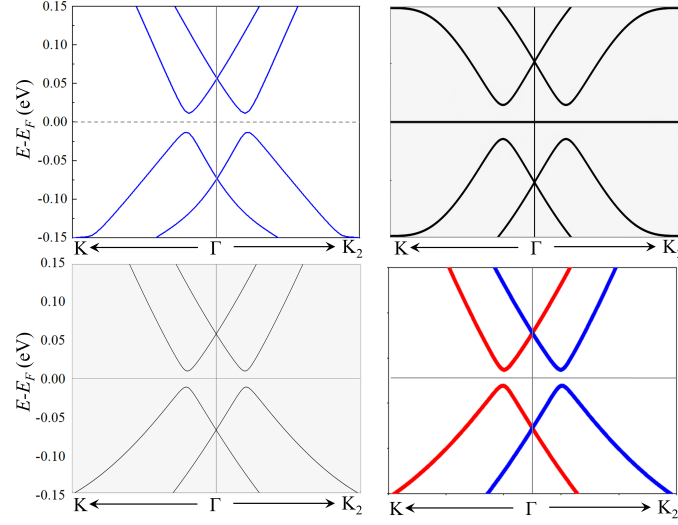


FIG. S5. Band structures of DFT, TB model and $k \cdot p$ model. (a) DFT calculations and (b) tightly bound model (c) energy band structure obtained by $k \cdot p$ model fitting. (d) $k \cdot p$ model results distinguishing between upper and lower spins.

	1	2	3	4	5	6	7	8	9	10	11	12
	Bi ₂ ↑	Bi ₂ ↓	Bi ₂ '↑	Bi ₂ '↓	Te ₁ ↑	Te ₁ ↓	Te ₁ '↑	Te ₁ '↓	Te ₄ ↑	Te ₄ ↓	Te ₄ '↑	Te ₄ '↓
1	Bi ₂ ↑	e3	0	0	0	$\mathcal{R}_1$			$\mathcal{R}_4$			
2	Bi ₂ ↓	0	e3	0	0							
3	Bi ₂ '↑	0	0	e3	0							
4	Bi ₂ '↓	0	0	0	e3							
5	Te ₁ ↑	$\mathcal{R}_2$			e2	0	0	0	0	0	0	0
6	Te ₁ ↓				0	e2	0	0	0	0	0	0
7	Te ₁ '↑				0	0	e2	0	0	0	0	0
8	Te ₁ '↓				0	0	0	e2	0	0	0	0
9	Te ₄ ↑	$\mathcal{R}_3$			0	0	0	0	e1	0	0	0
10	Te ₄ ↓				0	0	0	0	0	e1	0	0
11	Te ₄ '↑				0	0	0	0	0	0	e1	0
12	Te ₄ '↓				0	0	0	0	0	0	0	e1

FIG. S6. Schematic diagram of the Hamiltonian of the TB model consistent with the results of the DFT calculations.

$$\mathcal{R}1 = \begin{pmatrix} c_2 \varphi_2 \mathcal{H}_1 & \frac{1}{3} E_8^{(t_2, t_3)} \mathcal{H}_6 & 0 & 0 \\ \frac{1}{3} E_7^{(t_2, t_3)} \mathcal{H}_6 & c_1 \varphi_2 \mathcal{H}_1 & 0 & 0 \\ 0 & 0 & c_1 \varphi_2 \mathcal{H}_1 & \frac{1}{3} E_6^{(t_2, t_3)} \mathcal{H}_6 \\ 0 & 0 & \frac{1}{3} E_5^{(t_2, t_3)} \mathcal{H}_6 & c_2 \varphi_2 \mathcal{H}_1 \end{pmatrix} \quad (\text{Supplementary equation 5})$$

$$\mathcal{R}2 = \begin{pmatrix} c_1 \varphi_1 \mathcal{H}_2 & \frac{1}{3} E_4^{(t_2, t_3)} \mathcal{H}_5 & 0 & 0 \\ \frac{1}{3} E_3^{(t_2, t_3)} \mathcal{H}_5 & c_2 \varphi_1 \mathcal{H}_2 & 0 & 0 \\ 0 & 0 & c_2 \varphi_1 \mathcal{H}_2 & \frac{1}{3} E_2^{(t_2, t_3)} \mathcal{H}_5 \\ 0 & 0 & \frac{1}{3} E_1^{(t_2, t_3)} \mathcal{H}_5 & c_1 \varphi_1 \mathcal{H}_2 \end{pmatrix} \quad (\text{Supplementary equation 6})$$

$$\mathcal{R}3 = \begin{pmatrix} c_4 \varphi_2 \mathcal{H}_3 & \frac{1}{3} E_2^{(r_2, r_3)} \mathcal{H}_3 & 0 & 0 \\ \frac{1}{3} E_1^{(r_2, r_3)} \mathcal{H}_3 & c_3 \varphi_2 \mathcal{H}_3 & 0 & 0 \\ 0 & 0 & c_3 \varphi_2 \mathcal{H}_3 & \frac{1}{3} E_4^{(r_2, r_3)} \mathcal{H}_3 \\ 0 & 0 & \frac{1}{3} E_3^{(r_2, r_3)} \mathcal{H}_3 & c_4 \varphi_2 \mathcal{H}_3 \end{pmatrix} \quad (\text{Supplementary equation 7})$$

$$\mathcal{R}_4 = \begin{pmatrix} c_3\varphi_1\mathcal{H}_4 & \frac{1}{3}E_6^{(r_2,r_3)}\mathcal{H}_4 & 0 & 0 \\ \frac{1}{3}E_5^{(r_2,r_3)}\mathcal{H}_4 & c_4\varphi_1\mathcal{H}_4 & 0 & 0 \\ 0 & 0 & c_4\varphi_1\mathcal{H}_4 & \frac{1}{3}E_8^{(r_2,r_3)}\mathcal{H}_4 \\ 0 & 0 & \frac{1}{3}E_7^{(r_2,r_3)}\mathcal{H}_4 & c_3\varphi_1\mathcal{H}_4 \end{pmatrix} \quad (\text{Supplementary equation 8})$$

configuration are based on this with an apostrophe in the upper right corner to show the distinction. The Hamiltonian quantity construction of the above TB model selects the orbitals ($|P1_z^+, \uparrow\rangle, |P2_z^-, \uparrow\rangle, |P1_z^+, \downarrow\rangle, |P2_z^-, \downarrow\rangle$) as the base. The $P1_z^+$ and $P2_z^-$ represent the p_z orbitals of Bi or Te atoms (Bi_2 , Te_1 and Te_4 and their Equivalent Wyckoff site) with positive (+1) and negative (-1) metrics, and the $\uparrow / \downarrow$ denotes the electron spin. The Hamiltonian quantities shown in Figs. S6 consider a total of 12 orbitals for the basis group. The $\mathcal{R}_1$ and $\mathcal{R}_2$ matrices are contributed by the nearest-neighbor atomic pairs $\text{Bi}_{2/2'}$ and $\text{Te}_{1/1'}$ (nearest-neighbor hopping parameters t_l ($l=1-4$)), while the $\mathcal{R}_3$ and $\mathcal{R}_4$ matrices are contributed by the next-nearest-neighbor atomic pairs $\text{Bi}_{2/2'}$ and $\text{Te}_{4/4'}$ (next-nearest-neighbor hopping parameters r_l ($l=1-4$)). The diagonal elements of the R_l matrices are primarily represented by parameters r_x and t_x ($x=1, 4$), indicating hopping between aligned spin states of the two types of atoms, while the off-diagonal elements are represented by r_y and t_y ($y=2, 3$), indicating hopping between anti-aligned spin states of the two types of atoms.

To fit the energy band structure of the DFT under the $K\text{-}\Gamma\text{-}K_2$ path, where the nonzero parameters are set to $r_1 \rightarrow 0.0065, r_3 \rightarrow 0.04, t_1 \rightarrow -0.01, t_2 \rightarrow -0.058, t_3 \rightarrow 0.035, t_4 \rightarrow 0.01$, and a comparison of the fitted results obtained is shown in Figure S5.

Figures S5(a)-(c) present the energy band structures from DFT calculations, TB model fitting, and $k \cdot p$ model fitting, respectively. The spin splitting within the $k \cdot p$ model bands, shown in Figure S5(d), closely matches the DFT results shown in Figure S4.

$$\begin{aligned} \varphi_1 &= (1 + e^{ik_x} + e^{i(k_x+k_y)}); \varphi_2 = (1 + e^{ik_y} + e^{i(k_x+k_y)}); \\ \mathcal{H}_1 &= e^{-\frac{1}{3}i(2k_x+k_y) + \frac{63ik_z}{1000}}; \mathcal{H}_2 = e^{-\frac{1}{3}i(k_x+2k_y) - \frac{63ik_z}{1000}}; \\ \mathcal{H}_3 &= e^{-\frac{1}{3}i(k_x+2k_y) + \frac{19ik_z}{250}}; \mathcal{H}_4 = e^{-\frac{1}{3}i(2k_x+k_y) - \frac{19ik_z}{250}}; \\ \mathcal{H}_5 &= e^{-\frac{1}{3}i(2k_x+k_y) - \frac{63ik_z}{1000}}; \mathcal{H}_6 = e^{-\frac{1}{3}i(k_x+2k_y) + \frac{63ik_z}{1000}}. \end{aligned} \quad (\text{Supplementary equation 9})$$

$$\begin{aligned} c_1 &= it_1 + t_4; c_2 = -it_1 + t_4; \\ c_3 &= ir_1 + r_4; c_4 = -ir_1 + r_4. \end{aligned} \quad (\text{Supplementary equation 10})$$

$$\begin{aligned} E_j^{(x,y)} &= \begin{pmatrix} E_1^{(x,y)} \\ E_2^{(x,y)} \\ E_3^{(x,y)} \\ E_4^{(x,y)} \end{pmatrix} = Q_1 \begin{pmatrix} x \\ y \end{pmatrix} + Q_2 \begin{pmatrix} x \\ y \end{pmatrix} e^{ik_x} + Q_3 \begin{pmatrix} x \\ y \end{pmatrix} e^{i(k_x+k_y)}; \\ E_j^{(x,y)} &= \begin{pmatrix} E_5^{(x,y)} \\ E_6^{(x,y)} \\ E_7^{(x,y)} \\ E_8^{(x,y)} \end{pmatrix} = -Q_3 \begin{pmatrix} x \\ y \end{pmatrix} - Q_2 \begin{pmatrix} x \\ y \end{pmatrix} e^{ik_y} - Q_1 \begin{pmatrix} x \\ y \end{pmatrix} e^{i(k_x+k_y)}. \end{aligned} \quad (\text{Supplementary equation 11})$$

The parameter matrices P_m and Q_m ($m=1, 2, 3$) in $E_j^{(x,y)}$ are given below:

$$\begin{aligned} P_1 &= \begin{pmatrix} -(d-d^*) & d^* \\ -(d-d^*) & -d \\ -d^* & d-d^* \end{pmatrix}; P = \begin{pmatrix} d & d-d^* \\ -d^* & d-d^* \\ -(d-d^*) & -d \end{pmatrix}; P_3 = \begin{pmatrix} -d^* & -d \\ d & d^* \\ d & d^* \end{pmatrix}; \\ Q_1 &= \begin{pmatrix} d & d-d^* \\ -d^* & d-d^* \\ d & d^* \end{pmatrix}; Q = \begin{pmatrix} -d^* & -d \\ d & d^* \\ -d^* & d-d^* \end{pmatrix}; Q_3 = \begin{pmatrix} -(d-d^*) & d^* \\ -(d-d^*) & -d \\ -(d-d^*) & -d \end{pmatrix}. \end{aligned}$$

where $d = 3 + \sqrt{3}i$, and d^* is the complex conjugate of d .

SUPPLEMENTARY NOTE 7: $\mathbf{k} \cdot \mathbf{p}$ MODEL

Based on the magnetic group symmetry of the system and atomic information we constructed the kp model using MagneticKP. The Hamiltonian is shown in Eq. [Supplementary equation 12](#), where the matrix elements are labeled below them.

$$\mathcal{H}(k) = \begin{pmatrix} \mathcal{H}_{00} & \mathcal{H}_{01} & \mathcal{H}_{02} & \mathcal{H}_{03} \\ \mathcal{H}_{10} & \mathcal{H}_{11} & \mathcal{H}_{12} & \mathcal{H}_{13} \\ \mathcal{H}_{20} & \mathcal{H}_{21} & \mathcal{H}_{22} & \mathcal{H}_{23} \\ \mathcal{H}_{30} & \mathcal{H}_{31} & \mathcal{H}_{32} & \mathcal{H}_{33} \end{pmatrix} \quad (\text{Supplementary equation 12})$$

$$\begin{aligned} \mathcal{H}_{01} &= (C_{1,2} + C_{1,4})k_y; \mathcal{H}_{10} = (C_{1,2} + C_{1,4})k_y; \\ \mathcal{H}_{23} &= (-C_{1,2} + C_{1,4})k_y; \mathcal{H}_{32} = (-C_{1,2} + C_{1,4})k_y; \\ \mathcal{H}_{12} &= -2ik_xk_yC_{2,6} - ik_yk_zC_{2,4} + k_yC_{1,3}; \mathcal{H}_{21} = 2ik_xk_yC_{2,6} + ik_yk_zC_{2,4} + k_yC_{1,3}; \\ \mathcal{H}_{03} &= -2ik_xk_yC_{2,6} - ik_yk_zC_{2,4} + k_yC_{1,3}; \mathcal{H}_{30} = 2ik_xk_yC_{2,6} + ik_yk_zC_{2,4} + k_yC_{1,3}; \\ \mathcal{H}_{00} &= (C_{2,5} + C_{2,8})(k_x^2 + k_y^2) + (C_{1,2} + C_{1,4})k_x + (C_{2,1} + C_{2,3})k_z^2 + C_{0,1} + C_{0,3}; \\ \mathcal{H}_{11} &= (C_{2,5} + C_{2,8})(k_x^2 + k_y^2) - (C_{1,2} + C_{1,4})k_x + (C_{2,1} + C_{2,3})k_z^2 + C_{0,1} + C_{0,3}; \\ \mathcal{H}_{22} &= (-C_{2,5} + C_{2,8})(k_x^2 + k_y^2) + (-C_{1,2} + C_{1,4})k_x + (-C_{2,1} + C_{2,3})k_z^2 - C_{0,1} + C_{0,3}; \\ \mathcal{H}_{33} &= (-C_{2,5} + C_{2,8})(k_x^2 + k_y^2) + (C_{1,2} - C_{1,4})k_x + ((-C_{2,1} + C_{2,3}) + k_z^2 - C_{0,1} + C_{0,3}); \\ \mathcal{H}_{02} &= C_{2,6}(ik_x^2 - ik_y^2) + C_{2,7}(k_x^2 + k_y^2) - ik_xk_zC_{2,4} + k_xC_{1,3} + k_z^2C_{2,2} - ik_zC_{1,1} + C_{0,2}; \\ \mathcal{H}_{20} &= C_{2,6}(ik_y^2 - ik_x^2) + C_{2,7}(k_x^2 + k_y^2) + ik_xk_zC_{2,4} + k_xC_{1,3} + k_z^2C_{2,2} + ik_zC_{1,1} + C_{0,2}; \\ \mathcal{H}_{13} &= C_{2,6}(ik_y^2 - ik_x^2) + C_{2,7}(k_x^2 + k_y^2) + ik_xk_zC_{2,4} - k_xC_{1,3} + k_z^2C_{2,2} - ik_zC_{1,1} + C_{0,2}; \\ \mathcal{H}_{31} &= C_{2,6}(ik_x^2 - ik_y^2) + C_{2,7}(k_x^2 + k_y^2) - ik_xk_zC_{2,4} - k_xC_{1,3} + k_z^2C_{2,2} + ik_zC_{1,1} + C_{0,2}. \end{aligned}$$

The Hamiltonian of the R-MBT system along specific paths depends on constant terms $C_{0,i}$ ($i=1-4$), first-order terms $C_{1,j}$ ($j=2,3,4$), and second-order terms $C_{2,k}$ ($k=6,7,8$). The imaginary coefficient $C_{2,6}$ contributes to the Rashba splitting; adjusting it and $C_{0,2}$ to zero, while making $C_{1,2}$ negative and appropriately tuning related parameters, will transition to Lifshitz-type splitting.

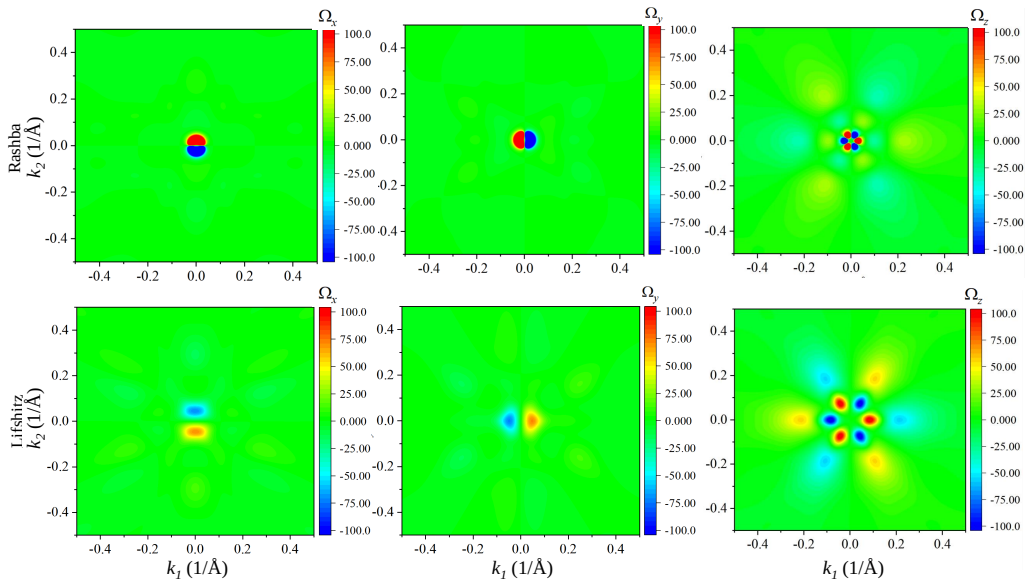


FIG. S7. Rashba and Lifshitz splitting involve the summation of Berry curvature from occupied bands in different planes.

SUPPLEMENTARY METHODS

Based on the Maximum Local Wannier Functions (MLWFs) we construct the tight-binding (TB) model. Then based on the surface Green's function method [14–17], the surface state, Berry curvature, spin Hall conductivity and Fermi surface calculations of the semi-infinite surface was realized by the WannierTools package [18]. The TB model and $\mathbf{k} \cdot \mathbf{p}$ model were constructed via MagneticTB[19] and MagneticKP[20], respectively.

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