

Tunable spin texture in ferroelectric Bi₆O₉

Li-Qi Huang,^{1,2} Ming Li^{3,*}, Hang Zhou,^{1,4} Zi-An Wang,^{1,2} Yue-Wen Fang⁵, Yu-Ping Sun^{1,6,7}
Wen-Jian Lu^{1,†} and Ding-Fu Shao^{1,‡}

¹Key Laboratory of Materials Physics, *Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China*

²University of Science and Technology of China, Hefei 230026, China

³School of Physics, *University of Electronic Science and Technology of China, Chengdu 611731, China*

⁴Institute of Physical Science and Information Technology, *Anhui University, Hefei 230601, China*

⁵*Centro de Física de Materiales (CSIC-UPV/EHU), Manuel de Lardizabal Pasealekua 5, 20018 Donostia/San Sebastián, Spain*

⁶Anhui Province Key Laboratory of Low-Energy Quantum Materials and Devices, *High Magnetic Field Laboratory, HFIPS, Chinese Academy of Sciences, Hefei, Anhui 230031, China*

⁷Collaborative Innovation Center of Microstructures, *Nanjing University, Nanjing 210093, China*



(Received 20 January 2025; revised 13 October 2025; accepted 16 October 2025; published 10 November 2025)

Momentum-dependent spin polarization exists in ferroelectric materials with strong spin-orbit coupling (SOC), which can be controlled by ferroelectric switching, promising for nonvolatile applications in spintronics. In the present work, we investigate the SOC-induced spin texture in orthorhombic Bi₆O₉, a recently discovered ferroelectric material with robust polarization down to the atomic limit. Utilizing first-principles calculations, we reveal the SOC-induced giant band splitting around the Γ point and notable spin texture, which can be well described by a $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian with sizable Rashba parameters of $\lambda_R = 0.65$ eV Å and Dresselhaus parameters $\lambda_D = -0.23$ eV Å at the conduction-band minimum. We also find that the SOC parameters can be effectively modulated by strain, resulting from band splitting and band anticrossing collectively, supported by substrate and strain-dependent calculations. The highly tunable spin texture indicates the opportunities for using Bi₆O₉ for the nonvolatile charge-spin conversion useful in spintronics.

DOI: [10.1103/12t3-n7r1](https://doi.org/10.1103/12t3-n7r1)

I. INTRODUCTION

Materials with spontaneous multistable states that can be switchable by external stimuli are crucial for nonvolatile electronic devices. A typical example is ferroelectric materials, where the spontaneous electric polarizations serve as the state variable for information processing and storage. However, conventional ferroelectric devices usually utilize only the charge degree of freedom, leaving the spin degree of freedom unexploited. Different approaches have been proposed to address this shortage. For example, in multiferroic systems with strong magnetoelectric coupling, the electric-field-driven ferroelectric switching is used to control the magnetic order parameters, promising for the high-speed and low-power write-in for spintronics. Nevertheless, the applicable room-temperature bulk multiferroics are uncommon. In multiferroic heterostructures, the interfacial magnetoelectric coupling can be strong, and hence the interface magnetization can be controlled by ferroelectric switching [1]. However, this approach requires precise engineering of interfacial configurations [2–5], which may be complicated for the design of realistic devices.

The recent exploration of spin-textured ferroelectrics with strong spin-orbit coupling (SOC) opens a new route to tailor

the ferroelectricity and the spin-dependent transport properties [6,7]. The SOC-driven spin texture in momentum space originates from the inversion symmetry breaking of a nonzero gradient of electrostatic potential intrinsic in ferroelectrics, which turns on the Rashba [8] and Dresselhaus [9] effects described with a Hamiltonian,

$$H_{\text{SOC}} = \mathbf{\Omega}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (1)$$

where $\mathbf{\Omega}(\mathbf{k})$ is an effective field and linear in the wave vector $\mathbf{k}$, and $\boldsymbol{\sigma}$ is the spin Pauli matrix. Such a Hamiltonian does not break the time-reversal symmetry and hence does not result in a spontaneous spin polarization. However, a nonequilibrium spin polarization can be introduced by an external electric field via an Edelstein effect [10,11], which can be used to switch the magnetization in a spin-torque device [12–15] or to control spin-dependent transport properties in a spin transistor [16,17]. In particular, the ferroelectric switching can reverse the spin textures and hence the nonequilibrium spin polarization, making the associated functionalities controllable by an external electric field [18–22]. Recently, various spin-textured ferroelectrics have been identified, including complex oxides and nitrides [19,23–29], organic perovskites [30–32], semiconductors [33,34], and two-dimensional (2D) materials [35,36]. Moreover, various new spin-textured ferroelectrics have been predicted recently based on the inverse design [37].

Generally, the performance of a ferroelectric material in a spintronic device utilizing the Edelstein effect is associated with two aspects. First, the ferroelectric material should have sufficient SOC to generate a sizable spin splitting in

*Contact author: ming.li7@uestc.edu.cn

†Contact author: wjl@issp.ac.cn

‡Contact author: dfshao@issp.ac.cn

band edges, supportive of a strong Edelstein effect. Second, the ferroelectric material should have a robust ferroelectricity even with a small thickness, allowing the implementation in a nanoscale device. In this sense, the recently discovered ferroelectric material Bi_6O_9 [38] is a promising candidate for the above-mentioned functionalities. It hosts the heavy element Bi, guaranteeing a strong SOC. It is compatible with a couple of substrates, offering miscellaneous choices for industrial manufacturing. It is found that a large remanent polarization is robust even with the size reduced down to 1 nanometer, and the high endurance of the switching behavior is confirmed in a ferroelectric tunnel junction [39].

In this work, we predict the SOC-driven giant spin splitting and tunable spin texture in Bi_6O_9 . Based on first-principles density functional theory (DFT) calculations, we derive the notable Rashba and Dresselhaus parameters in Bi_6O_9 . Notably, we find that these SOC parameters can be effectively modulated by strain, resulting collectively from the band splitting and band anticrossing between the Rashba split bands. Our results suggest that Bi_6O_9 is a promising spin-textured ferroelectric with great potential for spintronic applications.

II. METHODS

We employ DFT calculations using the projector-augmented-wave (PAW [40,41]) method as implemented in the Vienna Ab Initio Simulation Package (vasp [42]), applying the generalized gradient approximation (GGA [43]) and the Perdew-Burke-Ernzerhof for solids (PBEsol [44]) exchange-correlation functional. Both the lattice and parameters of the freestanding ferroelectric Bi_6O_9 are relaxed without SOC until the Hellmann-Feynman forces are less than 10^{-4} eV/Å on each atom. Epitaxial strain is introduced to simulate the properties of Bi_6O_9 films by varying the in-plane lattice parameters from a compressive to tensile regime or constraining them to match the epitaxial growth on substrates such as SrTiO_3 (STO) and LaAlO_3 (LAO), and in this regard, only the z -axis parameters are optimized. The optimized lattice parameters are listed in Table S4 of the Supplemental Material [45]. An energy cutoff of 550 eV and a $27 \times 12 \times 11$ k -point mesh are set for self-consistent computations. Postprocessing of electronic structures, e.g., density of states (DOS) and band structures are treated using vaspkit [46]. To calculate the spin textures, k points are evenly distributed in the Brillouin zone around the Γ point on the valence-band maximum (VBM) and conduction-band minimum (CBM) in the $k_z = 0$ plane.

III. RESULTS AND DISCUSSIONS

The orthorhombic ferroelectric Bi_6O_9 of space group $Pmm2$ is presented in Figs. 1(a)–1(c). It hosts two mirror planes M_x and M_y perpendicular to the x and y axes, respectively, and a twofold rotation C_{2z} around the z axis, enforcing a spontaneous polarization pointing along the $[001]$ direction. The stability of ferroelectric properties of Bi_6O_9 is evaluated by calculating the total energies of a series of structures denoted by a normalized dimensionless order parameter μ , whose atomic displacements are interpolated between the two equivalent oppositely spontaneously polarized states, corresponding to $\mu = \pm 1$, respectively. The resulting energy

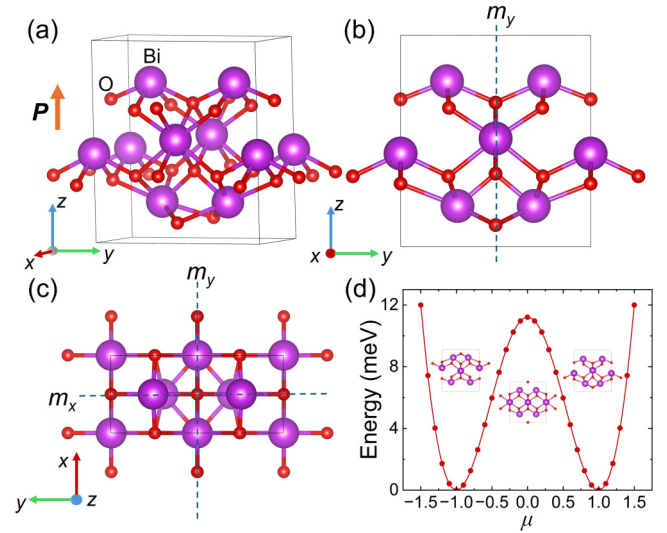


FIG. 1. (a) Crystal structure of bulk Bi_6O_9 in the ferroelectric phase. The polarization P is indicated by the orange arrow, which is along the $[001]$ direction. (b),(c) Mapping the crystalline arrangement onto the (b) (100) plane and (c) (001) plane. The blue dashed lines indicate the symmetry of bulk Bi_6O_9 in the $Pmm2$ space group, emphasizing the mirror reflection about the xz (m_y) and yz (m_x) planes in the ferroelectric Bi_6O_9 . (d) The total energy of Bi_6O_9 varying with the ferroelectric order μ of Bi_6O_9 . Insets: From left to right, the polarization of the crystal structure is along the $[00\bar{1}]$ direction, there is no polarization (paraelectric phase), and the polarization is along the $[001]$ direction.

profile displays the conventional double-well characteristic, featuring a sizable energy barrier of 11.21 meV per atom, indicating the stability of the ferroelectric phase.

The band structure of the ferroelectric Bi_6O_9 is first calculated in the absence of SOC, as shown in Fig. 2(a), exhibiting a direct band gap of 0.819 eV with CBM and VBM both located at the Γ point. When the SOC is taken into account, a notable splitting, up to 28.5 meV around the CBM at the Γ point, arises in conduction and valence bands [Fig. 2(b)]. Meanwhile, the splitting lowers the band gap to 0.75 eV. Overall, the spin splitting of CBM is stronger than that of VBM. This is because the CBM is majorly contributed by the Bi- p_z orbital and slightly contributed by the O- p_z orbital, while the VBM is majorly contributed by the O- p_y/p_z and slightly contributed by the Bi- s orbitals. The stronger SOC of Bi thus leads to a stronger spin splitting of CBM. A special instance is noted that the degeneracy still holds along Γ - Z , reflecting the symmetry-preserved polar direction and zero k_x (k_y). The side panels in Fig. 2 display the orbital-resolved DOS without and with SOC, accordingly. In either case, the conduction band is dominated by Bi-6 p orbitals and the valence band by O-2 p , which reveals the role of the heavy atom Bi in SOC and explains the more prominent splitting at CBM. The DOS with a wider range and more details is included in Fig. S1 in the Supplemental Material [45].

Zooming in on the band splitting around the Γ point, we then project the spin components, s_x and s_y , onto the band structure, as demonstrated in Fig. 3(a). It is a pure s_x (s_y) contribution to the energy bands along the path connecting

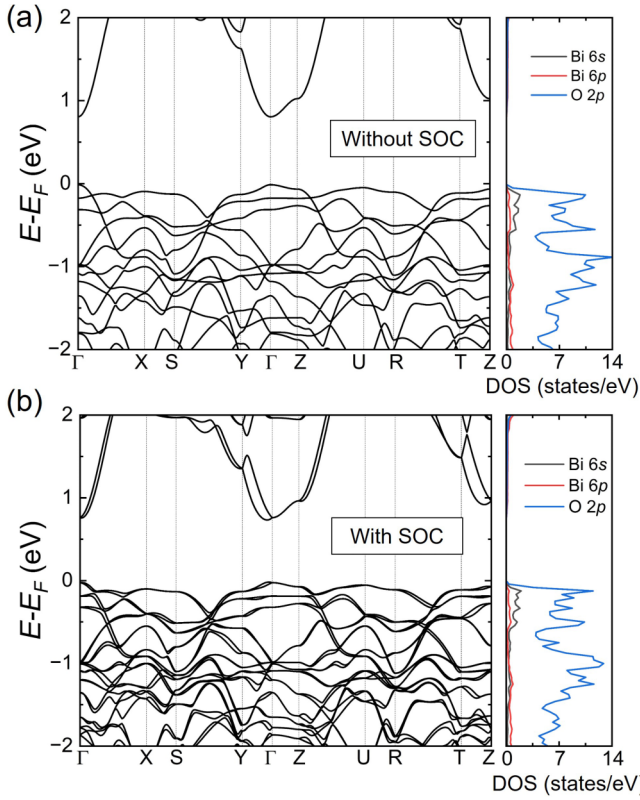


FIG. 2. (a) The band structure of ferroelectric Bi_6O_9 without considering the SOC along the path of $\Gamma(0, 0, 0)$ - $X(0.5, 0, 0)$ - $S(0.5, 0.5, 0)$ - $Y(0, 0.5, 0)$ - $\Gamma(0, 0, 0)$ - $Z(0, 0, 0.5)$ - $U(0.5, 0, 0.5)$ - $R(0.5, 0.5, 0.5)$ - $T(0, 0.5, 0.5)$ - $Z(0, 0, 0.5)$ which are all high-symmetry points in the first Brillouin zone, and projection of the density of states (DOS) onto the Bi-6s, Bi-6p, and O-2p orbitals. (b) The band structure of ferroelectric Bi_6O_9 considering the SOC along the same path, and projection of the DOS onto the Bi-6s, Bi-6p, and O-2p orbitals. The Fermi levels were both positioned at the maximum of the valence band.

selected high-symmetry points Γ - $Y(X)$, regardless of energy levels. This is due to the symmetry transformations,

$$M_x(k_x, k_y, k_z, s_x, s_y, s_z) = (-k_x, k_y, k_z, s_x, -s_y, -s_z),$$

$$M_y(k_x, k_y, k_z, s_x, s_y, s_z) = (k_x, -k_y, k_z, -s_x, s_y, -s_z), \quad (2)$$

forbidding s_x and s_z (s_y and s_z) when $k_y = 0$ ($k_x = 0$). Moreover, for the Γ - Z direction where $k_x = k_y = 0$, all the spin components are forbidden by combining M_x and M_y , leading to the spin-degenerate band structure in this direction.

Here we denote the outer (inner) conduction/valence bands surrounding the Γ point as CBM1(2)/VBM1(2) and illustrate the spin textures on them in the $k_z = 0$ plane [Figs. 3(b) and 3(c)], individually. We find that the spin textures show a clockwise or anticlockwise chirality, indicating that the Rashba-type SOC is dominant for all considered bands. The out-of-plane component s_z is vanishing for these spin textures due to symmetry transformations combining the time-reversal symmetry T and C_{2z} :

$$T(k_x, k_y, k_z, s_x, s_y, s_z) = (-k_x, -k_y, -k_z, -s_x, -s_y, -s_z),$$

$$C_{2z}(k_x, k_y, k_z, s_x, s_y, s_z) = (-k_x, -k_y, k_z, -s_x, -s_y, s_z). \quad (3)$$

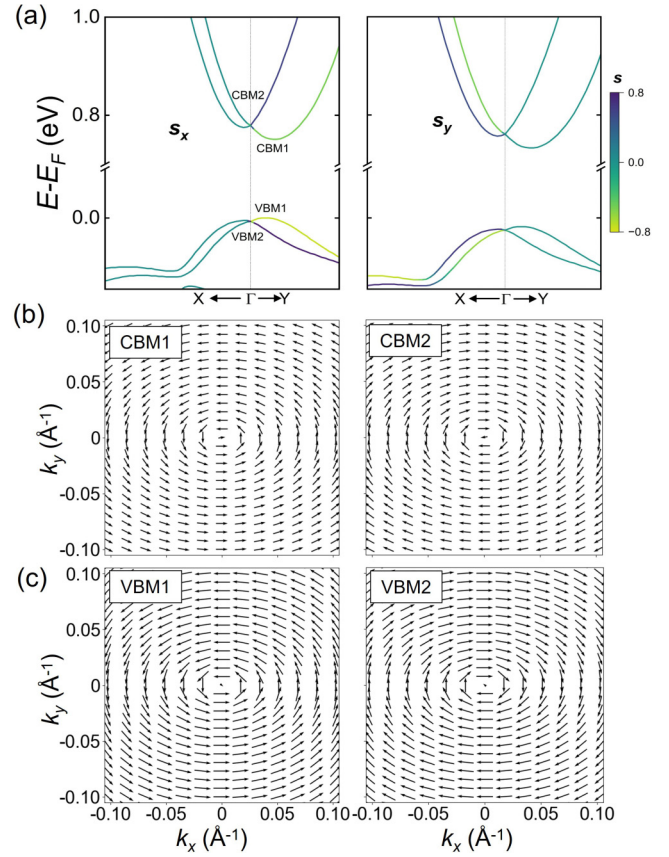


FIG. 3. (a) Spin-projected band structures of ferroelectric Bi_6O_9 along the $X(\frac{1}{2}, 0, 0) - \Gamma(0, 0, 0) - Y(0, \frac{1}{2}, 0)$ path, which were projected onto the s_x and s_y when polarization is along the $[001]$ direction. (b) Spin textures of the band CBM1 and CBM2. (c) Spin textures of the band VBM1 and VBM2. Both are around the Γ point and in the $k_z = 0$ plane.

We also find that the chirality can be reversed by the switching of ferroelectric polarization in the crystal [21].

Starting from the DFT calculated spin-polarized band structures and taking the symmetry transformations of the C_{2v} point group listed in Table S3 in the Supplemental Material [45] into account, we can describe the spin textures around the Γ point utilizing the Hamiltonian that was derived based on symmetry, which contains the free-electron and SOC terms given by Eq. (1),

$$H = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + \mathbf{\Omega}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \quad (4)$$

When $k_z = 0$, the effective SOC field can be simplified as $\mathbf{\Omega}(\mathbf{k}) = (\beta k_y, \alpha k_x, 0)$, where the parameters $\alpha = \lambda_D + \lambda_R$ and $\beta = \lambda_D - \lambda_R$, and λ_R and λ_D are Rashba and Dresselhaus parameters, respectively. This brings the deduced Hamiltonian [20],

$$H = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + \alpha k_x \sigma_y + \beta k_y \sigma_x, \quad (5)$$

which leads to band energies,

$$E_k = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} \pm \sqrt{\alpha^2 k_x^2 + \beta^2 k_y^2}. \quad (6)$$

TABLE I. λ_R and λ_D on the CBM and VBM of bulk ferroelectric Bi_6O_9 and Bi_6O_9 epitaxially grown on SrTiO_3 and LaAlO_3 substrates.

	CBM		VBM	
	λ_R (eV Å)	λ_D (eV Å)	λ_R (eV Å)	λ_D (eV Å)
Bi_6O_9	0.65	-0.23	0.22	-0.08
$\text{Bi}_6\text{O}_9_{\text{-SrTiO}_3}$	0.56	-0.13	0.34	-0.21
$\text{Bi}_6\text{O}_9_{\text{-LaAlO}_3}$	0.36	0	0	0

Fitting the polynomials in Eq. (4) with the calculated bands along Γ -X and Γ -Y in Fig. 3(a), we extract λ_R and λ_D at the CBM and VBM, as listed in the first row of Table I. The magnitude of λ_R is, overall, triple the value of λ_D , reaching ~ 0.65 eV Å at the CBM, confirming the dominance of the Rashba SOC reflected by the chiral spin textures shown in Figs. 3(b) and 3(c). Furthermore, we find that the spin textures can be fully switched upon polarization reversal, as shown in Fig. S4 in the Supplemental Material [45]. This indicates the nonvolatile switching of the spin texture in the ferroelectric Bi_6O_9 by an external field above ε_c , which is estimated to be about 0.26 MeV/cm according to $\varepsilon_c = (\frac{4}{3})^{\frac{2}{3}} \frac{E_1}{P_1}$ [47], where E_1 is the energy of the fully polarized states with respect to the paraelectric state, and P_1 is the spontaneous polarization ($\sim 38.96 \mu\text{C}/\text{cm}^2$) calculated using the Berry phase method in vasp. The sizable SOC parameters indicate the strong Edelstein effect that is promising for spintronics.

When implementing a material in a nanoscale device, an epitaxial growth of its film on a substrate is required. We thus investigate the electronic properties of Bi_6O_9 with epitaxial strains from the usual substrates such as STO and LAO by relaxing the structure with the in-plane crystal parameters of STO and LAO. As seen from Figs. 4(a) and 4(b), the anisotropy of bands along high-symmetry lines Γ -Y and Γ -X is reduced for Bi_6O_9 when the epitaxial strains are included, due to diminishment of inequality in in-plane lattice parameters. This suppresses the band splitting in CBM, leading to the smaller SOC parameters (Table I). However, we find the λ_R of CBM is still sizable, indicating the spintronic functionalities will be sustained in realistic epitaxial devices. Moreover, we find the band splitting at the VBM is negligible when the epitaxial strain from LAO substrate is included. This is because the in-plane strains can effectively modulate the hybridizations associated with O- p_y , O- p_z , and Bi- s orbitals, and thus strongly influence the dispersion of bands near the VBM. This modulation is revealed straightforwardly by the differential charge density calculations (Fig. S6 in the Supplemental Material [45]). We expect that a tensile (compressive) in-plane strain is associated with the decrease (increase) of the out-of-plane lattice constant, which enhances (reduces) the hybridization of O- p_y and Bi- s orbitals at VBM, and makes the associated bands more (less) dispersive. Therefore, the epitaxial growth of Bi_6O_9 on the LAO substrate introduces the remarkable compressive strain, reducing the hybridization between the Bi and O atoms, as shown in Fig. S6 in the Supplemental Material [45], making the SOC parameters for VBM negligible. On the other hand, we find it is no-

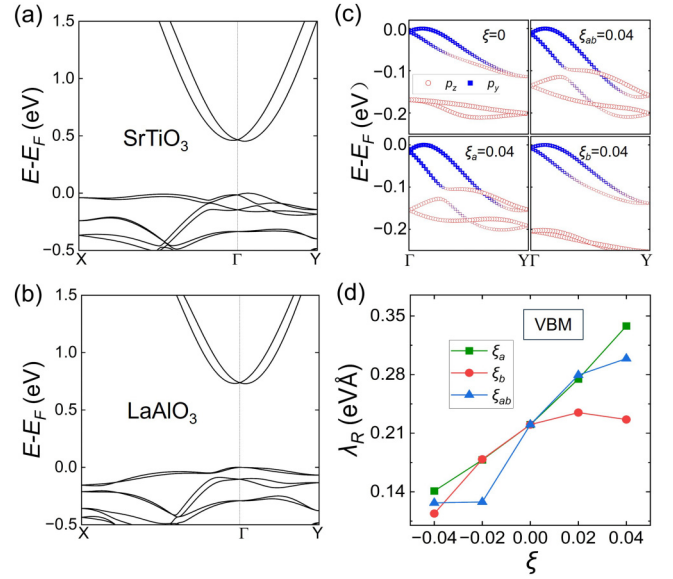


FIG. 4. (a) Band structure of ferroelectric Bi_6O_9 grown on an SrTiO_3 substrate along the $X(\frac{1}{2}, 0, 0) - \Gamma(0, 0, 0) - Y(0, \frac{1}{2}, 0)$ path. (b) Band structure of ferroelectric Bi_6O_9 grown on an LaAlO_3 substrate along the $X(\frac{1}{2}, 0, 0) - \Gamma(0, 0, 0) - Y(0, \frac{1}{2}, 0)$ path. (c) Orbital-projected band structures of bulk Bi_6O_9 when no strain exists, where (a) increases by 0.04, (b) increases by 0.04, and (a) and (b) increase by 0.04 simultaneously, contributed by the p_y , p_z orbital. (d) λ_R of the CBM varying with the strain -0.04 , -0.02 , 0 , 0.02 , 0.04 applied on (a) (ξ_a), (b) (ξ_b), and both (a) and (b) (ξ_{ab}) of Bi_6O_9 .

tably enhanced by the epitaxial strain from the STO substrate (Fig. S6 in the Supplemental Material [45]). This indicates a more complicated mechanism beyond the intuitively monotonic relation between the energy band splitting and the SOC parameters, and it requires extensive examination of the strain dependence of λ_R and λ_D since it points out possible substrate effects when there is no charge transfer or any other interfacial interactions, as for our calculations.

Hence, we calculate the electronic structures and SOC parameters for a series of structures with uniaxial strains ξ_a along the a axis and ξ_b along the b axis or a biaxial strain ξ_{ab} simultaneously, influencing the lattice constants of the a and b axes, as shown in Figs. 4(c) and 4(d), and Figs. S2 and S3 in the Supplemental Material [45]. We find that the anticrossing behavior occurs between the second and third bands below the VBM with a tensile strain ξ_a or ξ_{ab} , in contrast with those for bulk Bi_6O_9 or with the strain ξ_b , as displayed in Fig. 4(c). This “anticrossing” behavior between the Rashba split bands has been proposed as a design principle for classifying compounds with the large Rashba coefficients, along with the requirements of noncentrosymmetric space group and the emergence of SOC [48]. The importance of this behavior can be understood by considering the ratio $2E_R/k_R$ between band splitting E_R and momentum offset k_R [49,50], which qualitatively determines the magnitude of λ_R . The emergence of the band anticrossing can dramatically suppress k_R , and consequently drastically promote λ_R , leading to the nonmonotonic dependence of λ_R on splitting E_R . Thus, the distinct trend in the ξ_b dependence of λ_R at the VBM in Fig. 4(d)

is comprehensible, compared with the other two curves of which the band structures manifest anticrossing. Similarly, in the case for the STO substrate, the band anticrossing also occurs at the VBM (Fig. S3 in the Supplemental Material [45]), resulting in the enhancement of the SOC parameters at the VBM compared to that for pristine Bi_6O_9 where the band anticrossing is absent.

We note that the semiconducting behavior of Bi_6O_9 is robust against strain [45]. On the other hand, the band gap varies with the strains, indicating tunable electrostatic potentials within Bi_6O_9 and possible changes in transport properties that are commonly expected in ferroelectric materials. In the Bi_6O_9 films with substantial thickness, distortions at interfaces are not expected to generate a non-negligible influence on the bulk properties of Bi_6O_9 . However, the interfacial distortion may significantly influence the performance of an ultrathin Bi_6O_9 film, which is worthy of investigation in the future.

IV. CONCLUSION

To conclude, we explore the electronic structures and spin textures of the orthorhombic ferroelectric Bi_6O_9 , revealing a direct band gap at the Γ point and Rashba-type SOC around both the CBM and the VBM, whose chirality is associated with the ferroelectric polarization. We predict the SOC parameters using a derived Hamiltonian and achieve large Rashba and Dresselhaus parameters (λ_R and λ_D) as high as $0.65 \text{ eV \AA}$. How the substrate would affect the SOC

parameters is also evaluated, presenting generally increased magnitude of λ_R and λ_D when band splitting is larger, along with an interestingly opposite tendency at the VBM on STO, which can be perfectly explained by the anticrossing found in the band structure near the Γ point. Strain dependence of SOC parameters further confirms the collaborative effects of band splitting and band anticrossing on λ_R and λ_D . These results suggest the great potential of the spin-textured ferroelectric Bi_6O_9 to be a promising element in nanoscale spintronic devices for high-performance and low-power applications.

ACKNOWLEDGMENTS

This work was supported by the National Key Research and Development Program of China (Grant No. 2024YFB3614101), the National Science Foundation of China (NSFC Grants No. 12274411, No. 12241405, No. 52250418, and No. G0512504098), the Basic Research Program of the Chinese Academy of Sciences Based on Major Scientific Infrastructures (Grant No. JZHKYPT-2021-08), and the CAS Project for Young Scientists in Basic Research (Grant No. YSBR-084). The calculations were performed at Hefei Advanced Computing Center.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

-
- [1] C. A. F. Vaz, J. Hoffman, C. H. Ahn, and R. Ramesh, Magnetoelectric coupling effects in multiferroic complex oxide composite structures, *Adv. Mater.* **22**, 2900 (2010).
 - [2] J. D. Burton and E. Y. Tsymbal, Prediction of electrically induced magnetic reconstruction at the manganite/ferroelectric interface, *Phys. Rev. B* **80**, 174406 (2009).
 - [3] Y. W. Yin, J. D. Burton, Y. -M. Kim, A. Y. Borisevich, S. J. Pennycook, S. M. Yang, T. W. Noh, A. Gruverman, X. G. Li, E. Y. Tsymbal, and Q. Li, Enhanced tunnelling electroresistance effect due to a ferroelectrically induced phase transition at a magnetic complex oxide interface, *Nat. Mater.* **12**, 397 (2013).
 - [4] C. A. F. Vaz, J. Hoffman, Y. Segal, J. W. Reiner, R. D. Grober, Z. Zhang, C. H. Ahn, and F. J. Walker, Origin of the magnetoelectric coupling effect in $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3/\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ multiferroic heterostructure, *Phys. Rev. Lett.* **104**, 127202 (2010).
 - [5] R. O. Cherifi, V. Ivanovskaya, L. C. Phillips, A. Zobelli, I. C. Infante, E. Jacquet, V. Garcia, S. Fusil, P. R. Briddon, N. Guiblin, A. Mougin, A. A. Ünal, F. Kronast, S. Valencia, B. Dkhil, A. Barthélemy, and M. Bibes, Electric-field control of magnetic order above room temperature, *Nat. Mater.* **13**, 345 (2014).
 - [6] L. L. Tao and E. Y. Tsymbal, Perspectives of spin-textured ferroelectrics, *J. Phys. D Appl. Phys.* **54**, 113001 (2021).
 - [7] A. Manchon, H. C. Koo, J. Nitta, S. M. Frolov, and R. A. Duine, New perspectives for Rashba spin-orbit coupling, *Nat. Mater.* **14**, 871 (2015).
 - [8] E. I. Rashba, Properties of semiconductors with an extremum loop .I. Cyclotron and combinational resonance in a magnetic field perpendicular to the plane of the loop, *Sov. Phys. Solid State* **2**, 1109 (1960).
 - [9] G. Dresselhaus, Spin-orbit coupling effects in zinc blende structures, *Phys. Rev.* **100**, 580 (1955).
 - [10] V. M. Edelstein, Spin polarization of conduction electrons induced by electric current in two-dimensional asymmetric electron systems, *Solid State Commun.* **73**, 233 (1990).
 - [11] A. Johansson, Theory of spin and orbital Edelstein effects, *J. Phys.: Condens. Matter* **36**, 423002 (2024).
 - [12] A. Manchon and S. Zhang, Theory of nonequilibrium intrinsic spin torque in a single nanomagnet, *Phys. Rev. B* **78**, 212405 (2008).
 - [13] I. Mihal Miron, K. Garello, G. Gaudin, P. Zermatten, Marius V. Costache, S. Auffret, S. Bandiera, B. Rodmacq, A. Schuhl, and P. Gambardella, Perpendicular switching of a single ferromagnetic layer induced by in-plane current injection, *Nature (London)* **476**, 189 (2011).
 - [14] I. Mihal Miron, G. Gaudin, S. Auffret, B. Rodmacq, A. Schuhl, S. Pizzini, J. Vogel, and P. Gambardella, Current-driven spin

- torque induced by the Rashba effect in a ferromagnetic metal layer, *Nat. Mater.* **9**, 230 (2010).
- [15] A. Manchon, J. Železný, I. M. Miron, T. Jungwirth, J. Sinova, A. Thiaville, K. Garello, and P. Gambardella, Current-induced spin-orbit torques in ferromagnetic and antiferromagnetic systems, *Rev. Mod. Phys.* **91**, 035004 (2019).
- [16] S. Datta and B. Das, Electronic analog of the electro-optic modulator, *Appl. Phys. Lett.* **56**, 665 (1990).
- [17] H. C. Koo, J. H. Kwon, J. Eom, J. Chang, S. H. Han, and M. Johnson, Control of spin precession in a spin-injected field effect transistor, *Science* **325**, 1515 (2009).
- [18] D. Di Sante, P. Barone, R. Bertacco, and S. Picozzi, Electric control of the giant Rashba effect in bulk GeTe, *Adv. Mater.* **25**, 509 (2013).
- [19] M. Liebmann, C. Rinaldi, D. Di Sante, J. Kellner, C. Pauly, R. N. Wang, J. E. Boschker, A. Giussani, S. Bertoli, M. Cantoni, L. Baldrati, M. Asa, I. Vobornik, G. Panaccione, D. Marchenko, J. Sanchez-Barriga, O. Rader, R. Calarco, S. Picozzi, R. Bertacco, and M. Morgenstern, Giant Rashba-type spin splitting in ferroelectric GeTe(111), *Adv. Mater.* **28**, 560 (2016).
- [20] L. L. Tao, T. R. Paudel, A. A. Kovalev, and E. Y. Tsymlal, Reversible spin texture in ferroelectric HfO₂, *Phys. Rev. B* **95**, 245141 (2017).
- [21] L. L. Tao and E. Y. Tsymlal, Persistent spin texture enforced by symmetry, *Nat. Commun.* **9**, 2763 (2018).
- [22] Siti Amalia Sasmito, Muhammad Anshory, Ibnu Jihad, and Moh. Adhib Ulil Absor, Reversible spin textures with giant spin splitting in two-dimensional GaXY ($X = \text{Se, Te}$; $Y = \text{Cl, Br, I}$) compounds for a persistent spin helix, *Phys. Rev. B* **104**, 115145 (2021).
- [23] Luiz Gustavo Davense da Silveira, P. Barone, and S. Picozzi, Rashba-Dresselhaus spin-splitting in the bulk ferroelectric oxide BiAlO₃, *Phys. Rev. B* **93**, 245159 (2016).
- [24] L. L. Tao and J. Wang, Strain-tunable ferroelectricity and its control of Rashba effect in KTaO₃, *J. Appl. Phys.* **120**, 234101 (2016).
- [25] J. He, D. Di Sante, R. Li, X.-Q. Chen, J. M. Rondinelli, and C. Franchini, Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide, *Nat. Commun.* **9**, 492 (2018).
- [26] R. Arras, J. Gosteau, H. J. Zhao, C. Paillard, Y. Yang, and L. Bellaiche, Rashba-like spin-orbit and strain effects in tetragonal PbTiO₃, *Phys. Rev. B* **100**, 174415 (2019).
- [27] J. Varignon, J. Santamaria, and M. Bibes, Electrically switchable and tunable Rashba-type spin splitting in covalent perovskite oxides, *Phys. Rev. Lett.* **122**, 116401 (2019).
- [28] H. Djani, A. C. Garcia-Castro, W.-Y. Tong, P. Barone, E. Bousquet, S. Picozzi, and P. Ghosez, Rationalizing and engineering Rashba spin-splitting in ferroelectric oxides, *npj Quantum Mater.* **4**, 51 (2019).
- [29] H. J. Zhao, P. Chen, C. Paillard, R. Arras, Y.-W. Fang, X. Li, J. Gosteau, Y. Yang, and L. Bellaiche, Large spin splittings due to the orbital degree of freedom and spin textures in a ferroelectric nitride perovskite, *Phys. Rev. B* **102**, 041203(R) (2020).
- [30] A. Stroppa, D. Di Sante, P. Barone, M. Bokdam, G. Kresse, C. Franchini, M.-H. Whangbo, and S. Picozzi, Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites, *Nat. Commun.* **5**, 5900 (2014).
- [31] M. Kim, J. Im, A. J. Freeman, J. Ihm, and H. Jin, Switchable $S = 1/2$ and $J = 1/2$ Rashba bands in ferroelectric halide perovskites, *Proc. Natl. Acad. Sci. USA* **111**, 6900 (2014).
- [32] M. Kepenekian, R. Robles, C. Katan, D. Saporì, L. Pedesseau, and J. Even, Rashba and Dresselhaus effects in hybrid organic-inorganic perovskites: From basics to devices, *ACS Nano* **9**, 11557 (2015).
- [33] E. Plekhanov, P. Barone, D. Di Sante, and S. Picozzi, Engineering relativistic effects in ferroelectric SnTe, *Phys. Rev. B* **90**, 161108(R) (2014).
- [34] A. Narayan, Class of Rashba ferroelectrics in hexagonal semiconductors, *Phys. Rev. B* **92**, 220101(R) (2015).
- [35] H. Ai, X. Ma, X. Shao, W. Li, and M. Zhao, Reversible out-of-plane spin texture in a two-dimensional ferroelectric material for persistent spin helix, *Phys. Rev. Mater.* **3**, 054407 (2019).
- [36] M. A. U. Absor and F. Ishii, Intrinsic persistent spin helix state in two-dimensional group-IV monochalcogenide MX monolayers ($M = \text{Sn or Ge}$ and $X = \text{S, Se, or Te}$), *Phys. Rev. B* **100**, 115104 (2019).
- [37] C. M. Acosta, A. Fazzio, G. M. Dalpian, and A. Zunger, Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality, *Phys. Rev. B* **102**, 144106 (2020).
- [38] Q. Yang, J. Hu, Y.-W. Fang, Y. Jia, R. Yang, S. Deng, Y. Lu, O. Dieguez, L. Fan, D. Zheng, X. Zhang, Y. Dong, Z. Luo, Z. Wang, H. Wang, M. Sui, X. Xing, J. Chen, J. Tian, and L. Zhang, Ferroelectricity in layered bismuth oxide down to 1 nanometer, *Science* **379**, 1218 (2023).
- [39] Y. Jia, Q. Yang, Y.-W. Fang, Y. Lu, M. Xie, J. Wei, J. Tian, L. Zhang, and R. Yang, Giant tunnelling electroresistance in atomic-scale ferroelectric tunnel junctions, *Nat. Commun.* **15**, 693 (2024).
- [40] P. E. Blöchl, Projector augmented-wave method, *Phys. Rev. B* **50**, 17953 (1994).
- [41] G. Kresse and D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, *Phys. Rev. B* **59**, 1758 (1999).
- [42] G. Kresse and J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [43] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [44] L. Vega and F. Viñes, Generalized gradient approximation adjusted to transition metals properties: Key roles of exchange and local spin density, *J. Comput. Chem.* **41**, 2598 (2020).
- [45] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/12t3-n7r1> for lattice parameters and symmetry analysis of Bi₆O₉. Deeper insights into the band anti-crossing and band splitting can be found in the orbital-projected band structures. More detailed strain dependence of spin-orbit coupling parameters and associated explanations are provided. Analysis of the ferroelectricity-modulated electronic structures is included as well.
- [46] V. Wang, N. Xu, J.-C. Liu, G. Tang, and W.-T. Geng, VASPKIT: A user-friendly interface facilitating high-throughput computing and analysis using VASP code, *Comput. Phys. Commun.* **267**, 108033 (2021).

- [47] N. Vonnruti and U. Aschauer, Anion order and spontaneous polarization in LaTiO_2N oxynitride thin films, [Phys. Rev. Lett. **120**, 046001 \(2018\)](#).
- [48] C. Mera Acosta, E. Ogoshi, A. Fazzio, G. M. Dalpian, and A. Zunger, The Rashba scale: Emergence of band anticrossing as a design principle for materials with large Rashba coefficient, [Matter **3**, 145 \(2020\)](#).
- [49] Y. A. Bychkov and E. I. Rashba, Properties of a 2D electron gas with lifted spectral degeneracy, *Sov. Phys. JETP Lett.* **39**, 78 (1984).
- [50] 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 \(2012\)](#).