Switching Rashba spin-splitting by reversing electric-field direction

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The manipulation of the Rashba spin-splitting is crucial for the development of nanospintronic technology. Here, it is proposed that the Rashba spin-splitting can be turned on and off by reversing electric-field direction. By the first-principles calculations, our proposal is illustrated by a concrete example of Janus monolayer RbKNaBi. The designed RbKNaBi possesses dynamical, thermal, and mechanical stabilities, and is a large-gap quantum Hall insulator (QSHI) with Rashba spin-splitting near the Fermi level. A small built-in electric field is predicted due to very small electronegativity difference between the bottom and top atoms, which is very key to switch Rashba spin-splitting through the experimentally available electric field intensity. Due to out-of-plane structural asymmetry, the Janus monolayer has distinctive behaviors by applying external electric field \( E \) with the same magnitude but different directions (\( z \) or \( -z \)). Our results reveal that the Rashba energy (\( E_R \)) and Rashba constant (\( \alpha_R \)) are increased by the positive \( E \), while a negative \( E \) suppresses the Rashba splitting to disappear, and then appears again. In a certain \( E \) region (0.15 V/Å to 0.25 V/Å), switching Rashba spin-splitting can be achieved by only reversing electric-field direction. Besides, the piezoelectric strain coefficients \( d_{11} \) and \( d_{31} \) (5.52 pm/V and –0.41 pm/V) are predicted, which are higher than or compared with those of many 2D materials. By piezoelectric effect, the strain can also be used to tune Rashba spin-splitting of RbKNaBi. In Janus RbKNaBi monolayer, the combination of piezoelectricity and Rashba spin-splitting with topological insulating phase can promote the integration of various physical phenomena. Moreover, a possible spintronic device is proposed to realize the function of spintronic switch. Our proposed manipulation of the Rashba spin-splitting may make a special contribution to semiconductor spintronics.

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I. INTRODUCTION

Spintronics has attracted considerable attention, which can transmit information using spins rather than charges by manipulating the spin degree of freedom of electrons [1,2]. The semiconductor spintronic devices are compatible with the integration technologies of conventional semiconductor nanoelectronic devices. Generating spin currents is necessary for semiconductor spintronic devices, which can be achieved by spin-orbit coupling (SOC) [3]. The SOC-induced spin-splitting exists in noncentrosymmetric structures, mainly including two types: the Rashba effect induced by the structure inversion asymmetry [4–6] and the Dresselhaus effect induced by the bulk inversion asymmetry [3]. Here, we concentrate on Rashba spin-splitting in two-dimensional (2D) materials.

When an electron moves across an electric field \( \vec{E} \), it experiences an effective magnetic field \( \vec{B}_{\text{eff}} \sim \vec{E} \times \vec{\rho}/mc^2 \) in its rest-frame. The effective magnetic field can induce a momentum-dependent Zeeman energy \( H_{\text{SOC}} \sim \mu_B (\vec{E} \times \vec{\rho} \cdot \vec{\sigma}/mc^2 \). In crystals, the electric field \( \vec{E} \) is the gradient of the crystal potential. For 2D Janus materials, there is a built-in electric field \( \vec{E}_b \) along the \( z \) direction (\( \vec{E} = E_z \hat{\vec{z}} \), and the spin degeneracy of the energy spectrum is lifted, which can be described by the Rashba Hamiltonian [4,5],

\[
H_R = \frac{\alpha_R}{\hbar} (\vec{z} \times \vec{\rho}) \cdot \vec{\sigma}
\]

where \( \alpha_R \) is proportional to \( E \). The spin-splitting of the energy spectrum is called Rashba spin-splitting. The Rashba semiconductors have been predicted in many 2D Janus materials [7–12]. However, there is a growing class of materials, where Rashba SOC is instead cubic in wave vector [13]. When including cubic terms, besides in-plane spin polarization \( S_x \) and \( S_y \), a sizable spin polarization \( S_z \) in the out-of-plane direction can also be observed, which is beyond the simple linear Rashba model in Eq. (1).

It is a natural idea to turn on and off Rashba spin-splitting through an external electric field. As shown in Fig. 1(a), a 2D Janus material with a built-in electric field \( E_v \) possesses Rashba spin-splitting. By applying an appropriate positive electric field \( E_p \) along \( z \) direction, the Rashba spin-splitting is enhanced. However, when the applied electric field is reversed (\( E_n = -E_p \), the Rashba spin-splitting will disappear. To accomplish our proposal practically, a 2D Janus material should lack a built-in electric field with low cost, which is why we concentrate on Rashba spin-splitting in Janus monolayer.
FIG. 1. (a) A 2D Janus material with a built-in electric field $E_b$ possesses Rashba spin-splitting. When an appropriate positive electric field $E_p$ along $z$ direction is applied, the Rashba spin-splitting is enhanced. However, the applied electric field is reversed ($\vec{E}_n = -\vec{E}_p$), and the Rashba spin-splitting will disappear. For Janus monolayer RbKNaBi, (b) Top view and (c) side view of crystal structure, and the primitive cell (rectangle supercell) is marked by red (black) frames. (d) The phonon band dispersions. (e) The temperature and total energy fluctuations as a function of simulation time at 300 K.

meet these conditions: (1) there is a Rashba spin-splitting, and it is better to be at the $\Gamma$ point; (2) the electronegativity difference between the bottom and top atoms is small, which will induce small built-in electric field; (3) there are heavy elements, which may produce observable Rashba spin-splitting and remedy for small built-in electric field.

The MoSSe is a representative 2D Janus material, which has been synthesized experimentally [14,15]. However, the magnitude of the inherent electric field of MoSSe is very large (0.856 V/Å) [16]. It has been proved that the Rashba spin-splitting of MoSSe still maintains by applying the external electric field of $-0.5$ V/Å [17]. Recently, the large-gap QSHIs K$_2$NaBi and Rb$_2$NaBi monolayers are predicted with Na$_3$Bi-like crystal structure [18], and they have sandwich structures. The Na atoms are connected with Bi atoms forming a graphene-like sheet in the $ab$ plane, while the K/Rb atoms are above and below NaBi layer. In this paper, we construct a Janus RbKNaBi material by replacing one of two K/Rb layers with Rb/K atoms in monolayer K$_2$NaBi/Rb$_2$NaBi. The artificial RbKNaBi meets the three conditions mentioned above to switch Rashba spin-splitting by reversing electric-field direction. By the first-principles calculations, our idea is illustrated in Janus monolayer RbKNaBi as a QSHI. It is found that the increasing positive external electric field can enhance Rashba energy ($E_R$) and Rashba constant ($\alpha_R$). However, the increasing negative external electric field firstly quenches Rashba spin-splitting, and then recover it again. In a certain electric field region, simply reversing electric-field direction can switch Rashba spin-splitting. Finally, the piezoelectric properties of RbKNaBi are studied, and the strain-induced electric field by piezoelectric effect can be used to tune Rashba spin-splitting of RbKNaBi. Our proposed manipulation of the Rashba spin-splitting can be used for future spintronic devices.

The rest of the paper is organized as follows. In the next section, we shall give our computational details and methods. In the next few sections, we shall present crystal structure and structural stability, electronic structures along with electric field effects, and piezoelectric properties of Janus monolayer RbKNaBi. Finally, we shall give our discussion and conclusion.

II. COMPUTATIONAL DETAIL

Within density functional theory (DFT) [19], the first-principles calculations are carried out using the projected augmented wave (PAW) method with a kinetic cutoff energy of 500 eV, as implemented in the Vienna ab initio simulation package (VASP) [20–22]. The generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof [23] is adopted as the exchange-correlation potential. The total energy convergence criterion of $10^{-8}$ eV and residual force of less than 0.0001 eV Å$^{-1}$ on each atom are set to obtain accurate results. A vacuum spacing of larger than 16 Å along the $z$ direction is included to avoid interactions between two neighboring images. The SOC is incorporated for band structure calculations.

The phonon dispersions are performed using a finite difference approach with a supercell of $5 \times 5 \times 1$, as implemented in Phonopy code [24]. We calculate the elastic stiffness
tensor $C_{ij}$ and piezoelectric stress coefficients $e_{ij}$ by using strain-stress relationship (SSR) and density functional perturbation theory (DFPT) method [25], respectively. The 2D elastic coefficients $C_{ij}^{2D}$ and piezoelectric stress coefficients $e_{ij}^{2D}$ have been renormalized by the the length of unit cell along $z$ direction $(L_z)$: $C_{ij}^{2D} = L_z C_{ij}^{3D}$ and $e_{ij}^{2D} = L_z e_{ij}^{3D}$. A $\Gamma$-centered 12 $\times$ 12 $\times$ 1 k-point meshes in the Brillouin zone (BZ) is adopted to calculate $C_{ij}$ and electronic structures, and a 8 $\times$ 12 $\times$ 1 Monkhorst-Pack k-point meshes for $e_{ij}$. The WannierTools code [26] is used to investigate topological properties of RbKNaBi, based on the tight-binding Hamiltonians constructed from maximally localized Wannier functions, as implemented in Wannier90 code [27]. The PYPROCAR code is used to obtain the constant energy contour plots of the spin texture [28].

III. CRYSTAL STRUCTURE AND STRUCTURAL STABILITY

As shown in Figs. 1(b) and 1(c), the RbKNaBi monolayer shares the honeycomb crystal with the space group of $P\bar{3}m1$ (No.156). The Na, K, and Rb atoms are all bonded to the surrounding three Bi atoms, and Na and Bi atoms form a layer, while K and Rb atoms form two more layers. The symmetry of RbKNaBi is lower than that of K$_2$NaBi/Rb$_2$NaBi with the space group of $P\bar{6}m2$ (No.187). The RbKNaBi and K$_2$NaBi/Rb$_2$NaBi all lack the spatial inversion symmetry. Besides, the RbKNaBi also lacks horizontal mirror symmetry, which will induce out-of-plane piezoelectricity and Rashba effect. The Janus monolayer RbKNaBi can be constructed by replacing one of two K/Rb layers with Rb/K atoms in monolayer K$_2$NaBi/Rb$_2$NaBi. The optimized lattice parameters $a$ of RbKNaBi is 5.587 Å, which is between ones of K$_2$NaBi (5.548 Å) and Rb$_2$NaBi (5.629 Å).

The phonon spectra, $ab$ initio molecular dynamics (AIMD) simulations, and elastic constants $C_{ij}$ are calculated to confirm the stability of RbKNaBi. As shown in Fig. 1(d), no imaginary vibrational frequency can be observed, which clearly suggests that the RbKNaBi is dynamically stable. Moreover, both linear and flexural modes can be observed around the $\Gamma$ point, which shares the general features of 2D materials [29,30]. The AIMD simulation is performed by using the canonical (NTV) ensemble with a 4 ps with a time step of 1 fs. As shown in Fig. 1(e), the total energy and temperature fluctuate in the simulation time, but the average energy and temperature remain almost invariant. The final atomic configuration shows no obvious distortion of the geometric structure after 8000 steps of AIMD simulation, which can allow returning to its initiating structure by optimizing this final configuration. These results indicate its thermal stability of RbKNaBi at room temperature.

Due to $P\bar{3}m1$ symmetry, the 2D elastic tensor with using Voigt notation can be reduced into

$$C = \begin{pmatrix}
C_{11} & C_{12} & 0 \\
C_{12} & C_{11} & 0 \\
0 & 0 & (C_{11} - C_{12})/2
\end{pmatrix}. \quad (2)$$

The calculated two independent elastic constants $C_{11} = 18.40 \text{ Nm}^{-1}$ and $C_{12} = 5.01 \text{ Nm}^{-1}$, which meet the Born criteria of mechanical stability [31]: $C_{11} > 0$ and $C_{11} - C_{12} > 0$, confirming its mechanical stability. The shear modulus $G^{2D}$ equals to $C_{66} = (C_{11} - C_{12})/2 (6.70 \text{ Nm}^{-1})$. We calculate the direction-dependent Young’s modulus $C_{2D}(\theta)$ [32],

$$C_{2D}(\theta) = \frac{C_{12}C_{22} - C_{12}^2}{C_{11} \sin^4 \theta + A \sin^2 \theta \cos^2 \theta + C_{22} \cos^4 \theta} \quad (3)$$

where $A = (C_{11}C_{22} - C_{12}^2)/(C_{66} - 2C_{12})$. Calculated results show that the RbKNaBi is mechanically isotropic due to $P\bar{3}m1$ symmetry. The $C_{2D}$ of RbKNaBi is 17.04 Nm$^{-1}$, which is between ones of K$_2$NaBi (18.83 Nm$^{-1}$) and Rb$_2$NaBi (16.44 Nm$^{-1}$) [18]. The RbKNaBi monolayer demonstrates larger mechanical flexibility than those of other well-known 2D materials (graphene and MoS$_2$) [33,34]. It is found that the Poisson’s ratio $\nu_{2D}(\theta)$ is independent of direction, and can be simply expressed as

$$\nu_{2D} = \frac{C_{12}}{C_{11}}. \quad (4)$$

The calculated $\nu_{2D}$ is 0.272.

Intrinsic polar electric field is responsible for the emergence of out-of-plane piezoelectricity and Rashba effect. The difference in atomic size and electronegativity of K and Rb atoms leads to inequivalent Bi-K and Bi-Rb bond lengths (3.727 and 3.855 Å), and K-Bi-K and Rb-Bi-Rb bond angles (97.12 and 92.90$^{\circ}$), giving rise to a net electric field pointing from the K layer to the Rb layer. To identify the inherent electric field further, the planar average of the electrostatic potential energy is plotted in Fig. 2. The mirror asymmetry produces an electrostatic potential gradient ($\Delta \Phi$) of about 0.29 eV, which is related to the work function change of the structure. The magnitude of the net vertical electric field is estimated to be 0.20 eV/Å, which is determined by the slope of the plane-averaged electrostatic potential between K and Rb atoms’ minima. The predicted net vertical electric field is smaller than that of Janus MoSSe (0.856 eV/Å) [16], implying a weak vertical polarization. The small built-in electric field makes for switching Rashba spin-splitting by reversing electric-field direction.
at the actively. The band inversion induced by SOC can be clearly observed in the Fermi level for RbKNaBi.

IV. ELECTRONIC STRUCTURES AND ELECTRIC FIELD EFFECTS

Monolayer K$_2$NaBi and Rb$_2$NaBi are predicted to be large-gap QSHIs [18]. The nontrivial topological properties may be broken by building Janus structure from a QSHI, for example Janus SrAlGaSe$_4$ and MoSSe as derivatives of QSHIs SrGa$_2$Se$_4$ and 1T’-MoS$_2$ [35,36]. Next, we investigate the electronic properties of RbKNaBi from GGA and GGA + SOC, and the Bi-$s$, $p_x + p_z$, and $p_z$ projected band structures are plotted in Fig. 3. The GGA results show that RbKNaBi has a direct band gap of 0.110 eV with valence band maximum (VBM) and conduction band minimum (CBM) at the $\Gamma$ point. However, the GGA + SOC results show an indirect band gap of 0.229 eV, and the VBM has a slight deviation from the $\Gamma$ point. The calculated gap within SOC is close to those of K$_2$NaBi (0.18 eV) and Rb$_2$NaBi (0.22 eV) [18]. Without considering SOC, Bi-$p_x + p_z$ orbitals contribute to the VBM, while the CBM is dominated by Bi-$s$ states. When including SOC, an inversion of Bi-$s$ and Bi-$p_x + p_z$ states can be observed in the band structures, suggesting that monolayer RbKNaBi is a QSHI. On the other hand, the SOC can lift the degenerate spins due to relativistic effects. For Janus structures, the mirror asymmetry can produce built-in electric field, leading to Rashba spin-splitting (see Fig. 4). The strength of the Rashba effect can be quantized by the Rashba energy ($E_R$) and Rashba constant ($\alpha_R$), and the $\alpha_R = 2E_R/k_z$ with $k_z$ for the Rashba momentum (see Fig. 1 in the Supplemental Material [37]). The calculated $E_R = 1.3$ meV and $\alpha_R = 0.274$ eVÅ. To further confirm nontrivial topological properties of RbKNaBi, we calculate the $Z_2$ topological invariant. For a material with inversion symmetry, we can calculate $Z_2$ topological invariant by the product of parities of all occupied states at four time-reversal-invariant-momentum points in the 2D BZ. However, for RbKNaBi with broken spatial inversion symmetry, the $Z_2$ can be obtained by the calculation of Wannier charge center (WCC) [38]. If $Z_2$ equals 1, a material is a topologically nontrivial, while $Z_2 = 0$ means trivial state. As plotted in Fig. 5(a), the evolution lines of WCC cross an odd number of times by an arbitrary reference line, giving rise to $Z_2 = 1$, which indicates that monolayer RbKNaBi is a QSHI. The projected edge spectra along the [100] direction is calculated, which indicates that monolayer RbKNaBi is a QSHI. The projected edge spectra against the interference of the thermally activated (QSH) effect, because the large gap can stabilize the helical edge states against the interference of the thermally activated carriers. Experimentally, the larger topological gap has been measured in bismuthine on a SiC substrate [39]. A given material can be transformed through proximity effects whereby it acquires properties of its neighbors, for example, becoming magnetic, topologically nontrivial, or with an enhanced SOC [40]. The monolayer RbKNaBi possesses strong SOC, which can be used to produce spin-orbit proximity effects with potential applications in spintronics.

A perpendicular electric field is used to explore the manipulation of the Rashba spin-splitting of RbKNaBi. There are different atomic species on its upper and lower facets for Janus RbKNaBi, implying that applying $+z$ and $-z$ directional electric field are not equivalent. The energy band structures as a function of electric field $E$ are calculated by using GGA + SOC. Some representative energy band structures are plotted in Fig. 6, and the energy band gap vs $E$ are shown in Fig. 7. In considered positive $E$ range, the gap firstly increases with increasing $E$, and then has a sudden drop at $E = 0.30$ V/Å. However, the negative $E$ has small effects on gap. In considered both positive and negative $E$ ranges, the RbKNaBi is always a QSHI, and the calculated WCC
evolutions at representative positive and negative $E = 0.20$ V/Å are plotted in Fig. 2 in the Supplemental Material [37].

Next, we mainly investigate electric field effects on Rashba spin-splitting of RbKNaBi. The calculated $E_R$ as a function of both positive and negative $E$ are presented in Fig. 3 in the Supplemental Material [37]. For positive case, the $E_R$ increases with increasing $E$. However, for negative situation, the $E_R$ firstly decreases with increasing $E$, and become almost zero in a certain $E$ region, and then increases. This is due to a competition between the external electric field and internal electric field. To clearly see the disappeared Rashba spin-splitting, the enlarged valence bands centered at the $\Gamma$ point near the Fermi level at representative positive and negative $E = 0.20$ V/Å are plotted in Fig. 8. The calculated $\alpha_R$ vs $E$ along both positive and negative directions are presented in Fig. 7. The overall trend of $\alpha_R$ vs $E$ is consistent with that of $E_R$ vs $E$. It is clearly seen that the Rashba spin-splitting of RbKNaBi is nonexistent, when $E$ is between negative $0.15$ V/Å and $0.25$ V/Å. In this region, the Rashba spin-splitting will be opened by reversing electric field direction (from negative $E$ to positive $E$). Experimentally, the large electric fields have been realized [41–44]. Recently, an intense electric field larger than $0.4$ V/Å can be produced in 2D materials by dual ionic gating [44]. This switch operation can expand the range of possible applications in future spintronic technology.

Besides, the constant energy (at an energy surface $0.16$ eV below the Fermi level) spin-resolved 2D contours for the spin texture centered at the $\Gamma$ point are plotted in Fig. 9 under both positive and negative $E = 0.2$ eV/Å. For positive case, the $S_z$ components have a 90° of rotation as compared to $S_x$ counterpart. The concentric spin-texture circles mean the purely 2D Rashba spin-splitting (an isotropic splitting). Only in-plane $S_x$ and $S_y$ spin components are present in the Rashba spin-splitting bands, while the out-of-plane $S_z$ component is non-existent, which further confirms that the spin-splitting under positive $E = 0.2$ eV/Å has an isotropic 2D Rashba nature. For negative situation, no Rashba spin-splitting bands can be observed. Only out-of-plane $S_z$ spin component is present, while in-plane $S_x$ and $S_y$ components vanish. It is clearly
FIG. 8. For RbKNaBi monolayer, the enlarged valence bands centered at the \( \Gamma \) point near the Fermi level at representative \( E = 0.20 \text{ V}/\text{Å} \) with positive (a) and negative (b) electric field.

seen that the out-of-plane \( S_z \) spin component has three-fold rotational symmetry.

V. PIEZOELECTRIC PROPERTIES

When a strain or stress is applied on a non-centrosymmetric material, the electric dipole moments can be induced and produce electricity, called piezoelectric effect. The piezoelectric response of a material can be described by third-rank piezoelectric stress tensor \( e_{ijk} \) and strain tensor \( d_{ijk} \). The relaxed piezoelectric tensors \( e_{ijk} \) and \( d_{ijk} \) include the ionic and electronic contributions,

\[
e_{ijk} = \frac{\partial P_i}{\partial \varepsilon_{jk}} = e_{elc}^{ijk} + e_{ion}^{ijk} \tag{5}
\]

and

\[
d_{ijk} = \frac{\partial P_i}{\partial \sigma_{jk}} = d_{elc}^{ijk} + d_{ion}^{ijk} \tag{6}
\]

in which \( P_i \), \( \varepsilon_{jk} \), and \( \sigma_{jk} \) are polarization vector, strain, and stress, respectively, and the superscripts \( elc \) and \( ion \) is used to denote electronic and ionic contributions. The \( e_{elc}^{ijk} \) and \( d_{elc}^{ijk} \) are also called clamped-ion piezoelectric coefficients, while \( e_{ion}^{ijk} \) and \( d_{ion}^{ijk} \) mean relax-ion cases. The \( e_{ijk} \) is related with \( d_{ijk} \) by elastic tensor \( C_{mnjk} \),

\[
e_{ijk} = \frac{\partial P_i}{\partial \varepsilon_{jk}} = \frac{\partial P_i}{\partial \sigma_{mn}} \cdot \frac{\partial \sigma_{mn}}{\partial \varepsilon_{jk}} = d_{mn} C_{mnjk}. \tag{7}
\]

With respect to K2NaBi and Rb2NaBi, for RbKNaBi, the introduction of Janus structure results in a lower degree of \( C_3 \)v symmetry, and both the in-plane and out-of-plane piezoelectric effects are allowed, when a uniaxial in-plane strain is applied. By using Voigt notation, the 2D piezoelectric stress and strain tensors can be expressed as [45,46]

\[
e = \begin{pmatrix} e_{11} & -e_{11} & 0 \\ 0 & 0 & -e_{11} \\ e_{31} & e_{31} & 0 \end{pmatrix}, \tag{8}
\]

\[
d = \begin{pmatrix} d_{11} & -d_{11} & 0 \\ 0 & 0 & -2d_{11} \\ d_{31} & d_{31} & 0 \end{pmatrix}. \tag{9}
\]

FIG. 9. For RbKNaBi monolayer, the spin projected constant energy contour plots of spin texture calculated in a \( k_x-k_y \) plane centered at the \( \Gamma \) point at an energy surface 0.16 eV below the Fermi level with positive (top plate) and negative (bottom plate) electric field \( E = 0.20 \text{ V}/\text{Å} \). In the color scale, red means spin-up states while blue means spin-down states.

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It is found that only out-of-plane piezoelectric response can exist \( e_{11}/d_{11} = 0 \), but \( e_{31}/d_{31} \neq 0 \), when applying a biaxial in-plane strain. In other words, the pure out-of-plane piezoelectric response can be realized by imposed biaxial strain. Here, the two independent \( d_{11} \) and \( d_{31} \) can be derived by \( e_{ij} = d_{ij}C_{jk} \),

\[
d_{11} = \frac{e_{11}}{C_{11} - C_{12}} \quad \text{and} \quad d_{31} = \frac{e_{31}}{C_{11} + C_{12}}.
\]

(10)

We use the orthorhombic supercell [see Fig. 1(b)] to calculate the \( e_{11}/e_{31} \) of RbKNaBi. The predicted \( e_{11}/e_{31} \) is \( 0.74 \times 10^{-10}/-0.095 \times 10^{-10} \) C/m with ionic part \( 0.51 \times 10^{-10}/-0.024 \times 10^{-10} \) C/m and electronic part \( 0.23 \times 10^{-10}/-0.071 \times 10^{-10} \) C/m. For both \( e_{11} \) and \( e_{31} \), the electronic and ionic parts have superposed contributions. Based on Eq. (10), the predicted \( d_{11}/d_{31} \) is \( 5.52/-0.41 \) pm/V. The predicted \( d_{11} \) and \( d_{31} \) (absolute value) are higher than or compared with those of familiar 2D materials [45,46].

The \( E \) along \( z \) direction can also be induced with a biaxial in-plane strain by piezoelectric effect, and then tune Rashba spin-splitting of RbKNaBi. When in-plane vibration is applied to RbKNaBi, the Rashba effect will be modulated periodically. (Here, the direct effect of strain on band structure is not considered.) As shown in Fig. 10(a), the compressive strain induce negative electric field, which can reduce Rashba spin-splitting. However, Fig. 10(b) shows that the tensile strain induce positive electric field, which can enhance Rashba spin-splitting.

The monolayer K\(_2\)NaBi and Rb\(_2\)NaBi possess horizontal mirror symmetry, and only in-plane \( d_{11} \) can exist, when a uniaxial in-plane strain is applied. For comparison, we also calculate the piezoelectric coefficients of K\(_2\)NaBi and Rb\(_2\)NaBi, and the related data are listed in Table I. It is found that the \( d_{11} \) of the three monolayers are very close, and the \( d_{11} \) of RbKNaBi monolayer fall in between those of the K\(_2\)NaBi and Rb\(_2\)NaBi monolayers, as expected. The coexistence of piezoelectricity and nontrivial topological insulating phase, namely piezoelectric quantum spin Hall insulator (PQSHI), has potential advantages toward the development of high-speed and dissipationless electronic devices. Combining their nontrivial electronic structures, K\(_2\)NaBi, Rb\(_2\)NaBi, and RbKNaBi all are PQSHIs.

### VI. DISCUSSIONS AND CONCLUSIONS

Some suggestions on experimental synthesis aspects of RbKNaBi are discussed. Firstly, the dynamically stable bulk compounds K\(_2\)NaBi and Rb\(_2\)NaBi are thermodynamically stable against disproportionation into the competing phases [47]. Secondly, by exfoliating these Na\(_3\)Bi-like alkali bismide three-dimensional Dirac semimetals K\(_2\)NaBi and Rb\(_2\)NaBi, their monolayer structures are also dynamically, thermally and mechanically stable [18]. Finally, similar to Janus monolayer MoSSe from MoS\(_2\) [14,15], the RbKNaBi can be synthesized experimentally with similar experimental techniques based on K\(_2\)NaBi or Rb\(_2\)NaBi monolayer.

The SOC effects (Rashba spin-splitting) can be reversibly turned on and off by reversing electric-field direction, which provides a switch for the subsequent development of spin devices to control the passage of electrons (see Fig. 11). For example, two ferromagnetic electrodes in the same direction are set for the component. With an appropriate negative applied electric field, the injected electrons pass through the RbKNaBi channel and keep the spin orientation unchanged [Fig. 11(a)]. When the external electric field direction is reversed, the spin of electrons in the channel will rotate un-

### Table I

For monolayer K\(_2\)NaBi, RbKNaBi, and Rb\(_2\)NaBi, the elastic constants \( C_{ij} \) (Nm\(^{-1}\)), piezoelectric stress coefficient \( e_{ij} \) along with electronic part \( e_{ij} \), and ionic part \( e_{ij} \) (10\(^{-10}\) C/m), and piezoelectric strain coefficient \( d_{ij} \) (pm/V).

| Name          | \( C_{11} \) | \( C_{12} \) | \( e_{11} \) | \( e_{12} \) | \( e_{11} \) | \( e_{12} \) | \( e_{31} \) | \( e_{31} \) | \( d_{11} \) | \( d_{31} \) |
|---------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| K\(_2\)NaBi   | 19.46       | 5.29        | 0.15        | 0.66        | 0.81        | –           | –           | –           | 5.69        | –           |
| RbKNaBi       | 18.41       | 5.02        | 0.23        | 0.51        | 0.74        | –0.071      | –0.024      | –0.095      | 5.52        | –0.41       |
| Rb\(_2\)NaBi  | 17.08       | 4.51        | 0.293       | 0.348       | 0.641       | –           | –           | –           | 5.10        | –           |
under the effect of SOC, and will be blocked by the derived electrode [Fig. 11(b)]. This possible spintronic device realizes the function of spintronic switch.

In summary, we have demonstrated that Rashba spin-splitting can be reversibly turned on and off by reversing electric-field direction in RbKNaBi. Calculated results show that the $E_R$ and $\alpha_R$ are increased by the positive $E$, while a negative $E$ suppresses the Rashba splitting to disappear, and then appears again. In a certain electric field region, simply reversing electric-field direction can achieve switching Rashba spin-splitting. Besides, it is proved that RbKNaBi is a QSHI and possesses excellent piezoelectric properties, which makes RbKNaBi become a multifunctional 2D material. Our findings can inspire more works about electric-field-tuned switch of Rashba spin-splitting.

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