Piezoelectric properties and carrier mobilities of Janus monolayer XTeI (X=Sb and Bi): a first-principle study

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The absence of both the inversion symmetry and out-of-plane mirror symmetry together with spin-orbit coupling (SOC) can induce novel electronic and piezoelectric properties. In this work, the piezoelectric properties and carrier mobilities of Janus monolayer XTeI (X=Sb and Bi) are studied by density functional theory (DFT). By using generalized gradient approximation (GGA) plus SOC, they are found to be indirect gap semiconductors with the Rashba spin splitting. The piezoelectric tensors of Janus monolayer XTeI (X=Sb and Bi) are reported by using density functional perturbation theory (DFPT). Due to lacking both the inversion symmetry and out-of-plane mirror symmetry for Janus monolayer XTeI (X=Sb and Bi), both in-plane and out-of-plane piezoelectric effects can be observed, and the large piezoelectric coefficients are predicted (e.g. $d_{11} = 12.95 \text{ pm/V}$ for SbTeI and $d_{11} = 8.20 \text{ pm/V}$ for BiTeI), which are comparable and even higher than ones of many other two-dimensional (2D) materials and other well-known bulk piezoelectric materials, especially for out-of-plane piezoelectric coefficients. With GGA+SOC, the high electron carrier mobilities are obtained, and the electron mobility of BiTeI along armchair direction reaches up to about $1319 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$. The carrier mobility shows a rather pronounced anisotropy between electron and hole/armchair and zigzag directions. Our works imply Janus monolayer XTeI (X=Sb and Bi) have potential applications in flexible electronics and piezoelectric devices, and can stimulate further experimental works.

I. INTRODUCTION

Compared to their bulk counterparts, 2D materials can show some unique or surprising properties, like high mechanical strength, high photocatalytic activity, remarkable optical and magnetic properties. Due to potential nanoscale piezoelectric applications, the piezoelectricity in 2D materials has attracted growing interest, which can be used in sensors, actuators and energy sources. A piezoelectric material must be non-centrosymmetric, and should have a band gap for prohibiting current leakage. For 2D materials, the reduction in dimensionality leads to that their inversion symmetry is often eliminated, allowing them to become piezoelectric. Due to the inversion asymmetry in the 2H phase, the monolayer MoS$_2$ as a typical example have been proved to possess piezoelectricity experimentally ($\epsilon_{11} = 2.9 \times 10^{-10} \text{ C/m}$). A large in-plane piezoelectricity and additional out-of-plane piezoelectricity have been predicted in 2D Janus transition metal dichalcogenides (TMD), which can directly break the inversion symmetry and out-of-plane mirror symmetry. Recently, the existence of vertical dipoles has been experimentally proved in the Janus MoSSe monolayer, which shows an intrinsic vertical piezoelectric response. In theory, the piezoelectric properties of lots of 2D materials have been reported, like metal dichalcogenides, group IIA and IIB metal oxides, group III-V semiconductors and Janus TMD.

Janus monolayer SbTeI and BiTeI have been predicted theoretically with a low formation energy, and they are dynamically stable. The bulk SbTeI or BiTeI has a layered structure along its crystallographic c axis, and a Bi or Sb atom is sandwiched between one Te and one I, forming a triple layer. Within each triple layer, these atoms have strong chemical bonding, but the adjacent triple layers are weakly coupled via the van der Waals interactions. Thus, Janus monolayer SbTeI and BiTeI can be exfoliated from their bulks. The Rashba spin splitting in monolayer SbTeI or BiTeI has been reported with a sizable Rashba coupling parameter of 1.39 eVÅ or 1.97 eVÅ, and they are potentially useful for spintronics, like spin-polarized field effect transistor. Recently, we have predicted that Janus monolayer SbTeI and BiTeI may be potential 2D thermoelectric materials due to very low lattice thermal conductivities. How-
TABLE I. For SbTeI (BiTeI) monolayer, the lattice constants \(a_0\) (Å), the elastic constants \(C_{ij}\) (Nm\(^{-1}\)), shear modulus \(G_{2D}\) (Nm\(^{-1}\)), Young’s modulus \(C_{2D}\) (Nm\(^{-1}\)), Poisson’s ratio \(\nu\), the GGA+SOC gaps (eV) and the Rashba energy \(E_R\) (meV).

| Name   | \(a_0\) (Å) | \(C_{11} = C_{22}\) | \(C_{12}\) | \(G_{2D}\) | \(\nu\) | \(\text{Gap}\) (eV) | \(E_R\) (meV) |
|--------|-------------|---------------------|------------|-----------|--------|----------------|------------|
| SbTeI  | 4.32 (4.42) | 28.52 (26.91)       | 7.72 (7.93)| 10.4 (9.49)|        |                 |            |
| BiTeI  | 26.43 (24.57)| 0.271 (0.295)       | 0.89 (0.67)| 17.2 (40.1)|        |                 |            |

ever, to the best of our knowledge, no studies have been reported on piezoelectric properties of Janus monolayer SbTeI and BiTeI. In this work, inspiring from their special Janus structure of monolayer SbTeI or BiTeI, their piezoelectric properties along with carrier mobilities are studied by density functional theory (DFT). Calculated results show they have the large piezoelectric coefficients (e.g., \(d_{11}=12.95\) pm/V for SbTeI and \(d_{11}=8.20\) pm/V for BiTeI), which are comparable and even higher than ones of many other 2D materials and other well-known bulk piezoelectric materials, especially for out-of-plane piezoelectric coefficients with respect to other ones of 2D materials. The high electron carrier mobilities are also predicted, for example about 1319 cm\(^2\)V\(^{-1}\)s\(^{-1}\) for the electron mobility of BiTeI along armchair direction. These results make us believe that Janus monolayer SbTeI and BiTeI may be potential 2D piezoelectric materials, and can stimulate further experimental synthesis of these monolayers.

II. COMPUTATIONAL DETAIL

Based on DFT\(^{21}\), our calculations are performed using the projected augmented wave (PAW) method with a kinetic cutoff energy of 500 eV, as implemented in the VASP package\(^{22-24}\). The popular GGA of Perdew, Burke and Ernzerhof (GGA-PBE)\(^{25}\) is used as the exchange-correlation potential, and the SOC was included self-consistently. For the Janus monolayer SbTeI and BiTeI, a vacuum spacing of more than 18 Å along the z direction is included to avoid interactions between two neighboring images. The total energy convergence criterion is set to \(10^{-8}\) eV. The geometry optimization was considered to be converged with the residual force on each atom being less than 0.001 eV Å\(^{-1}\). To obtain the piezoelectric properties of the Janus monolayer SbTeI and BiTeI, the elastic stiffness tensor \(C_{ij}\) are calculated by using the finite difference method (FDM), and the piezoelectric stress coefficients \(e_{ij}\) are calculated by DFPT method\(^{26}\) by the VASP package. 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 (\(L_z\)): \(C_{ij}^{2D} = L_z C_{ij}\) and \(e_{ij}^{2D} = L_z e_{ij}\).

### III. ELECTRONIC STRUCTURES

The geometric structure of the Janus XTeI (X=Sb and Bi) is plotted in Figure 1, which consists of of three atomic layers with X sandwiched between the Te and I layers. The structure is similar to Janus TMD monolayer PtSSe\(^{27}\) and SaSSe\(^{29}\). Both rhombus primitive cell and rectangle supercell are shown, and calculating carrier mobilities and piezoelectric coefficients need to use rectangle supercell. The armchair and zigzag directions of the rectangular supercell are defined as x and y directions, respectively. Their symmetry is \(P3m_1\), which lacks the reflection symmetry with respect to the central X atoms. The lattice constant of the Janus monolayer SbTeI and BiTeI are 4.32 Å and 4.42 Å, which agree well previous theoretical values\(^{14,15}\). It have been proved that the SOC has very important effects on their electronic structures\(^{13-15}\), thus only GGA+SOC energy bands of monolayer SbTeI and BiTeI are plotted in Figure 2. The Janus monolayer SbTeI (BiTeI) is found to be a semiconductors with an indirect band gap of 0.89 eV (0.67 eV) with GGA+SOC. The conduction band minimum (CBM) is located at slightly away from the \(\Gamma\) point along the \(\Gamma-K\) or \(\Gamma-M\) paths, and the valence band maximum (VBM) is between the \(\Gamma\) and \(K\) or \(M\) points. The Rashba-like and Zeeman-like band splitting can be observed, which is due to the absence of vertical mirror symmetry combined with the SOC effect. The Rashba spin splitting in the lowest conduction band at the high-symmetric \(\Gamma\) point can be clearly seen, and their Rashba energy, defined as the band crossing point of the conduction bands at the \(\Gamma\) point minus the energy of the CBM, are 17.2 meV and 40.1 meV, respectively, which are consistent with the previously reported values\(^{13-15}\).

### IV. PIEZOELECTRIC PROPERTIES

For both in-plane and out-of-plane directions, SbTeI and BiTeI monolayers clearly lack an inversion center, which means both the in-plane and out-of-plane piezo-
electricity can be produced, when a tension along x axis is applied. The third-rank piezoelectric stress tensors $e_{ijk}$ and strain tensor $d_{ijk}$ from the sum of ionic and electronic contributions are defined as:

$$ e_{ijk} = \frac{\partial P_i}{\partial \varepsilon_{jk}} = e^{elc}_{ijk} + e^{ion}_{ijk} \quad (1) $$

and

$$ d_{ijk} = \frac{\partial P_i}{\partial \sigma_{jk}} = d^{elc}_{ijk} + d^{ion}_{ijk} \quad (2) $$

In which $P_i$, $\varepsilon_{jk}$ and $\sigma_{jk}$ are polarization vector, strain and stress, respectively. For 2D materials, the plane stress and plane strain conditions are assumed ($\varepsilon_{jk}=0$ or $\sigma_{jk}=0$ for $i=3$ or $j=3$). Due to a $3m$ point-group symmetry of SbTeI and BiTeI monolayers, by employing Voigt notation, the piezoelectric stress and strain tensors become:

$$ e = \begin{pmatrix} e_{11} & -e_{11} & 0 \\ 0 & 0 & -e_{11} \\ e_{31} & e_{31} & 0 \end{pmatrix} \quad (3) $$

$$ d = \begin{pmatrix} d_{11} & -d_{11} & 0 \\ 0 & 0 & -2d_{11} \\ d_{31} & d_{31} & 0 \end{pmatrix} \quad (4) $$

where $e/d_{11}$ and $e/d_{31}$ represent the in-plane and out-plane piezoelectric stress/strain components, respectively. The $e_{ij}$ can be calculated by DFPT, and derive the values of $d_{ij}$ using the relation:

$$ e = dC \quad (5) $$

and the elastic tensor $C$ can be expressed as:

$$ C = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & (C_{11} - C_{12})/2 \end{pmatrix} \quad (6) $$

The $C_{ij}$ can be attained by FDM. Here, the $d_{11}$ and $d_{31}$ are derived by Equation 3, Equation 4, Equation 5 and Equation 6:

$$ d_{11} = \frac{e_{11}}{C_{11} - C_{12}} \quad and \quad d_{31} = \frac{e_{31}}{C_{11} + C_{12}} \quad (7) $$

In general, a piezoelectric material should be a semiconductor for prohibiting current leakage, which has been proved from energy bands structures from Figure 2. The elastic stiffness coefficients of $C_{11}$ and $C_{12}$ of SbTeI and BiTeI monolayers are firstly calculated, and the shear modulus $G_{2D}$, Young’s modulus $C_{2D}$ and Poisson’s ratio $\nu$ are attained from calculated $C_{ij}$, which are listed in Table I. These elastic coefficients $C_{ij}$ satisfy the Born criteria of 2D hexagonal structure, proving their mechanical stabilities. These values are obviously smaller than those of other 2D materials, like monolayer TMDs like $\alpha$-quartz ($d_{11}=2.3$ pm/V), wurtzite-AlN ($d_{33}=5.1$ pm/V) and wurtzite-GaN.
(d_{31}=3.1 \text{ pm/V}), and are found to be comparable to or even superior than other 2D materials\cite{7,9,11,12,29,30}, such as MoS\(_2\), WS\(_2\), ZnO, MoSSe and MoSTe. The related data are listed Table II. These imply that the SbTeI and BiTeI monolayers may have large in-plane piezoelectric effects with a uniaxial strain being applied.

For 2D materials, a large out-of-plane piezoelectric response is highly desired, since it is compatible with the nowadays bottom/top gate technologies. The calculated out-of-plane piezoelectric strain coefficient (d_{31}) has large value of -0.37 pm/V for SbTeI monolayer, and 0.66 pm/V for BiTeI monolayer. The out-of-plane piezoelectricity d_{31} of BiTeI monolayer is obviously higher than ones of other 2D materials, like functionalized h-BN (0.13 pm/V)\cite{31}, MoSSe (0.29 pm/V)\cite{29}, MoSTe (0.4 pm/V)\cite{40}, Janus group-III materials (0.46 pm/V)\cite{52} and α-In\(_2\)Se\(_3\) (0.415 pm/V)\cite{33}. It is noted that the e_{31} and d_{31} of MoSSe and MoSTe are very different between ref.\cite{7} and ref.\cite{29,30}, which are likely due to different computational method.

In ref.\cite{29,30}, the e_{ij} are calculated by DFPT, while these are attained by evaluating the change of unit-cell polarization after imposing small strain in ref.\cite{7}. It is clearly seen that the e_{11} are very close for different method, but the e_{31} by polarization-strain relation is smaller by 1 order of magnitude compared to one by DFPT. The large out-of-plane piezoelectric effect makes SbTeI and BiTeI monolayers have potential applications on ultrathin piezoelectric devices.

V. CARRIER MOBILITY

To evaluate the performance of monolayer SbTeI and BiTeI for great potential in piezoelectric and electronic application, the carrier mobilities of their electron/hole transport can be calculated by the deformation potential (DP) theory proposed by Bardeen and Shockley\cite{34}. In this theory, the expression of the carrier mobility of a 2D material (\(\mu_{2D}\)) is given:

\[
\mu_{2D} = \frac{e\hbar^2 C_{2D}}{K_BTm^*m_dE_t^2}
\]  

where \(e\), \(\hbar\) and \(K_B\) are the electron charge, the reduced Planck constant and the Boltzmann constant; the \(T\) and \(m^*\) are temperature and effective mass in the transport direction, and \(m_d = \sqrt{m_xm_y}\) is the average effective mass. The \(C_{2D}\) is the elastic modulus derived from elastic constants \(C_{ij}\), and the relationship between them is\cite{28}:

\[
C_{2D} = \frac{C_{11}^2 - C_{12}^2}{C_{11}}
\]  

In addition, \(E_t\) represents the DP constant of the VBM for a hole or the CBM for an electron along the transport direction, which is defined by \(E_t = \Delta E/\delta\), where \(\Delta E\) is the energy shift of the band edge of CBM or VBM with respect to the vacuum level. These data are calculated with strain from -0.01 to 0.01, and the step \(\delta=0.005\). When the \(\mu_{2D}\) is attained, the relaxation time \(\tau\) of a hole at VBM or an electron at CBM along the transport direction can be calculated by:

\[
\tau = \frac{\mu_{2D}m^*/e}{\Delta E}
\]
The rectangular supercell with armchair and zigzag being defined as $x$ and $y$ directions in Figure 1 is used to study the carrier mobilities of SbTeI and BiTeI monolayers, and the 300 K (room temperature) is used in the mobility calculations. It is noteworthy that calculating effective masses and the DP constant need consider SOC. Firstly, the effective masses of CBM and VBM along armchair and zigzag directions, are calculated, and they are shown in Table III. The calculated elastic modulus ($C_{2D}$), effective mass ($m^*$) using GGA+SOC, deformation potential ($E_l$), carrier mobility ($\mu_{2D}$) [300 K] and relaxation time ($\tau$) [300 K] of SbTeI and BiTeI monolayers. 

| Carrier type | $C_{2D}$ (Nm$^{-1}$) | $m^*$ | $E_l$ (eV) | $\mu_{2D}$ (cm$^2$V$^{-1}$s$^{-1}$) | $\tau$ (s) |
|--------------|----------------------|-------|-----------|----------------------------------|------------|
| SbTeI        |                      |       |           |                                  |            |
| Electrons    | x                    | 26.43 | 0.21      | -3.61                            | 739.74     | $8.88 \times 10^{-14}$ |
|              | y                    | 26.43 | 0.36      | -4.24                            | 311.70     | $6.43 \times 10^{-14}$ |
| Holes        | x                    | 26.43 | -1.86     | -2.99                            | 34.97      | $3.70 \times 10^{-14}$ |
|              | y                    | 26.43 | -0.50     | -2.06                            | 272.59     | $7.80 \times 10^{-14}$ |
| BiTeI        |                      |       |           |                                  |            |
| Electrons    | x                    | 24.57 | 0.19      | -2.62                            | 1319.24    | $1.40 \times 10^{-13}$ |
|              | y                    | 24.57 | 0.52      | -3.04                            | 351.18     | $1.04 \times 10^{-13}$ |
| Holes        | x                    | 24.57 | -1.36     | -2.06                            | 102.92     | $7.95 \times 10^{-14}$ |
|              | y                    | 24.57 | -0.57     | -1.66                            | 376.58     | $1.22 \times 10^{-13}$ |

The band energies of SbTeI and BiTeI are smaller than ones of MoSSe and MoSTe, and the effective masses of electron are smaller than ones of holes. Thus, the effective masses and the DP constant need consider SOC. 

VI. DISCUSSIONS AND CONCLUSION 

From Table II, the $e_{11}$ of Janus monolayer SbTeI and BiTeI are found to be comparable to or even smaller than ones of MoS$_2$, WS$_2$, ZnO, MoSSe and MoSTe$^{7,9,29,30}$, but their $d_{11}$ are larger than ones of other 2D materials, except for ZnO. To find out underlying reasons, the elastic constants $C_{ij}$, shear modulus $G_{2D}$, Young’s modulus $C_{2D}$ of Janus monolayer SbTeI and BiTeI along with ones of MoS$_2^9$, WS$_2^9$, ZnO$^9$, MoSSe$^7$ and MoSTe$^7$ are listed in Table IV. Based on Equation 7, the $d_{11}$ is inversely proportional to $G_{2D}$ [$G_{2D}=(C_{11}−C_{12})/2$]. It is clearly seen that $G_{2D}$ of Janus monolayer SbTeI and BiTeI are smaller than ones of other 2D materials listed in Table IV, which leads to larger $d_{11}$. It is also noted that $G_{2D}$ of monolayer ZnO is relatively small, along with relatively large $e_{11}$, which gives rise to large $d_{11}$ ($8.65$ pm/V). The $\tau$ can be calculated from effective masses and carrier mobilities, which is useful for attaining the electronic transport properties of their electronic transport properties.
FIG. 4. (Color online) With respect to the vacuum energy, the GGA+SOC band energies of the VBM and CBM of BiTeI monolayer as a function of lattice dilation along both x and y directions. The red solid lines are linear fitting curves, and the fitted slopes are given, corresponding to the DP.

1 eV for BiTeI. The specific structural symmetry along with flexible mechanical properties induce large in-plane piezoelectric coefficient ($d_{11}=12.95 \text{ pm/V}$ for SbTeI and $d_{11}=8.20 \text{ pm/V}$ for BiTeI) and an additional out-of-plane piezoelectric coefficient ($d_{31}=-0.37 \text{ pm/V}$ for SbTeI and $d_{31}=0.66 \text{ pm/V}$ for BiTeI). Their carrier mobilities are attained with pronounced anisotropy, and the hole mobilities are higher than electron ones. The hole carrier mobility of the BiTeI monolayer along the armchair direction could be as high as 1319 cm$^2$V$^{-1}$s$^{-1}$. These findings can stimulate experimental works to explore piezoelectric and electronic applications of Janus monolayer SbTeI and BiTeI.

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