Spin-valley-coupled quantum spin Hall insulator with topological Rashba-splitting edge states in Janus monolayer CSb$_{1.5}$Bi$_{1.5}$

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Abstract

Achieving combination of spin and valley polarized states with topological insulating phase is pregnant to promote the fantastic integration of topological physics, spintronics and valleytronics. In this work, a spin-valley-coupled quantum spin Hall insulator (svc-QSHI) is predicted in Janus monolayer CSb$_{1.5}$Bi$_{1.5}$ with dynamic, mechanical and thermal stabilities. Calculated results show that the CSb$_{1.5}$Bi$_{1.5}$ is a direct band gap semiconductor with and without spin–orbit coupling, and the conduction-band minimum and valence-band maximum are at valley point. The inequivalent valleys have opposite Berry curvature and spin moment, which can produce a spin-valley Hall effect. In the center of Brillouin zone, a Rashba-type spin splitting can be observed due to missing horizontal mirror symmetry. The topological characteristic of CSb$_{1.5}$Bi$_{1.5}$ is confirmed by the $Z_2$ invariant and topological protected conducting helical edge states. Moreover, the CSb$_{1.5}$Bi$_{1.5}$ shows unique Rashba-splitting edge states. Both energy band gap and spin-splitting at the valley point are larger than the thermal energy of room temperature (25 meV) with generalized gradient approximation level, which is very important at room temperature for device applications. It is proved that the spin-valley-coupling and nontrivial quantum spin Hall state are robust again biaxial strain. Our work may provide a new platform to achieve integration of topological physics, spintronics and valleytronics.

Keywords: valley, spin, topological insulator

Supplementary material for this article is available online
(Some figures may appear in colour only in the online journal)

1. Introduction

Since the valley-dependent effects are discovered in MoS$_2$ monolayer with missing inversion symmetry, the field of valleytronics is truly flourishing [1–3]. For hexagonal two-dimensional (2D) materials like monolayer MoS$_2$, the conically shaped valleys at $-K$ and $K$ corners are inequivalent, and the spin polarizations are opposite, as the two points are connected by the time reversal symmetry operation. The combination of inversion symmetry breaking and SOC can remove spin degeneracy, and then gives rise to valley-contrastingspin splitting, which is the foundation for spin-valleytronics. With an applied in-plane electric field, the charge carriers with opposite valley and spin indexes will attain opposite anomalous transverse velocity, and then a simultaneous spin and valley Hall effect is produced [4, 5].

On the other hand, the topological insulator (TI) has spin-momentum-locked conducting edge states and insulating properties in the bulk, whose charge and spin transport...
in the edge states are quantized dissipationless [6, 7]. These bring possibilities for low-dissipation electronic devices. For 2D materials, the TI is also called as QSH insulator (QSHI) characterized by counter-propagating edge currents with opposite spin polarization, which is firstly predicted in graphene [8]. Experimentally confirmed QSHIs include the HgTe/CdTe and InGaAs/GaSb quantum wells [9, 10], and many other 2D materials have been proposed as QSHIs by the first-principles calculations [11–16]. To this end, it is a natural idea to achieve the integration of QSHI with spin-valleytronics (namely, svc-QSHI).

Several AB3 type atomic sheets have been experimentally synthesized, for example, BC3 nanosheets [17]. Recently, 2D AB3 monolayers have also been theoretically reported [18–21]. The CP1 monolayer can be used as anode for sodium-ion batteries [18], and the massless Dirac–Fermions can be achieved in CA3 monolayer [19]. In addition to this, the QSHIs and topological Rashba-splitting edge states in monolayer CX3 (X = Sb and Bi) with inversion symmetry have been predicted [21]. The MoS2 with 1T phase is a QSHI, and the corresponding Janus structures MoSe can still possess nontrivial topology tuned by strain [22]. Compared to MoS2, the MoSe will lose inversion symmetry. Inspired from this, we construct Janus monolayer CSb1.5Bi1.5 based on monolayer CX3 (X = Sb and Bi). By first principles simulations, we show that the CSb1.5Bi1.5 is a svc-QSHI with topological Rashba-splitting edge states. The svc-QSHIs have been proposed in some composite monolayers [23–25], like functionalized SbAs monolayers and Janus functionalized β-BiAs monolayer. The topological phases like the QSH or quantum anomalous Hall one have also been predicted in some materials with Janus structure [26–29]. Calculated results show these novel features are robust again biaxial strain. These results make CSb1.5Bi1.5 an appealing original quantum material for topological physics, spintronics and valleytronics.

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 stabilities, and electronic structures of CSb1.5Bi1.5. Finally, we shall give our conclusions.

2. Computational detail

Within density functional theory (DFT) [30], we perform the first-principles calculations using the projected augmented wave (PAW) method, as implemented in the VASP package [31–33]. We use GGA of Perdew et al [34] as the exchange–correlation potential. To confirm topological properties of CSb1.5Bi1.5, we also adopt the Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional [35] for band structure and topology invariant calculations. The cutoff energy for plane-wave expansion is 500 eV with the total energy convergence criterion being $10^{-7}$ eV. To avoid interactions between two neighboring images, the vacuum region along the z direction is set to be larger than 18 Å. The SOC is incorporated for band structure calculations. The Brillouin zone is sampled by using a $12 \times 12 \times 1$ K-point meshes for geometry optimization, elastic coefficients and self-consistent electronic structure calculations. The geometry optimization is considered to be converged, when the residual force on each atom is less than 0.0001 eV Å$^{-1}$.

Phonon dispersion spectrum is attained by the Phonopy code [36] based on finite displacement method using a $5 \times 5 \times 1$ supercell of size $4 \times 4 \times 1$ for more than 5000 fs with a time step of 1 fs. The Z2 invariants are used to investigate topological properties of Janus monolayer CSb1.5Bi1.5 as implemented by the Wannier90 and WannierTools codes [37, 38], where a tight-binding Hamiltonian with the maximally localized Wannier functions is fitted to the first-principles band structures. We use PYPYCAR code to obtain the constant energy contour plots of the spin texture [39].

3. Crystal structure and structural stability

Based on DFT calculations, the optimized lattice parameters of CSb1.5Bi1.5 is 7.772 Å, which is between ones of CSb1 (7.58 Å) and CBi1 (7.96 Å) [21]. As shown in figure 1 with top and side views, each C atom forms three C–Sb or C–Bi bonds with three neighboring Sb or Bi atoms, and each Sb/Bi atom forms two Sb–Bi bonds and one C–Sb/Bi bond with neighboring Bi/Sb and C atoms, respectively. The symmetry of CSb1.5Bi1.5 with space group P$3m1$ (No. 156) is lower than that of CSb1/CBi1 monolayer with space group P$3m1$ (No. 164) due to the lack of space inversion symmetry. Monolayer CSb1/CBi1 is composed of two C atomic layers sandwiched between Sb/Bi atomic layers. Similar to Janus monolayer MoSSe from MoS2 [40, 41], the CSb1.5Bi1.5 can be constructed by replacing one of two Sb/Bi layers with Bi/Sb atoms.

Figure 1. The crystal structure of CSb1.5Bi1.5: top view (a) and side view (b). The rhombus primitive cell is shown by black frames in (a). (c) The Brillouin zone with high-symmetry points labeled.
in monolayer CSb\textsubscript{3}/CBi\textsubscript{3}. For the CSb\textsubscript{1.5}Bi\textsubscript{1.5}, the inequivalent C–Sb and C–Bi bond lengths (Sb–C–Sb and Bi–C–Bi bond angles) will be induced due to the difference in atomic sizes and electronegativities of Sb and Bi atoms, and they are 2.131 Å and 2.217 Å (115.442° and 115.154°), which gives rise to a built-in electric field. The symmetry reduction will induce Rashba spin splitting, valley degree of freedom and piezoelectric polarizations.

To confirm the stability of CSb\textsubscript{1.5}Bi\textsubscript{1.5}, phonon spectra, AIMD simulations and elastic constants \(C_{ij}\) are carried out. Figure 2 shows that all phonon branches have no imaginary frequency in the entire Brillouin zone, suggesting its dynamical stability. It is noted that two in-plane acoustic branches show linear dispersions, while the ZA branch corresponding to the out-of-plane vibrations displays a quadratic dispersion. These conform to quadratic dispersion of ZA phonon branch, when a 2D material is free of stress [42, 43]. The optical branches are well separated from acoustic branches with a gap of 0.29 THz, which prohibits the scattering between acoustic and optical phonon modes. The vibration of the O atoms may be experimentally achieved by the bottom-up approaches such as molecular beam epitaxy [21], because the epitaxial BC\textsubscript{3} sheet with a similar structure has been successfully synthesized [17]. Similar to Janus monolayer MoSSe from MoS\textsubscript{2} [40, 41], the CSb\textsubscript{1.5}Bi\textsubscript{1.5} can be synthesized experimentally with similar experimental techniques based on CSb\textsubscript{3}/CBi\textsubscript{3} monolayer.

Using Voigt notation, the 2D elastic tensor with space group \(P3m1\) can be reduced into:

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

The two independent elastic constants of monolayer CSb\textsubscript{3}/CBi\textsubscript{3} are \(C_{11} = 26.01\) Nm\textsuperscript{-1} and \(C_{12} = 9.13\) Nm\textsuperscript{-1}. The shear modulus \(G_{2D}\) equals to \(G_{66}\), which can be attained by \((C_{11}-C_{12})/2\), and the corresponding value is 8.44 Nm\textsuperscript{-1}. The calculated \(C_{ij}\) satisfy the Born criteria of mechanical stability of a material with hexagonal symmetry [44]: \(C_{11} > 0\) and \(C_{66} > 0\), confirming its mechanical stability. The Young’s modulus \(C_{2D}(\theta)\) can be calculated by the following equation [45]:

\[
C_{2D}(\theta) = \frac{C_{11}C_{22} - C_{12}^2}{C_{11}\sin^4\theta + A\sin^2\theta\cos^2\theta + C_{22}\cos^2\theta}\tag{2}
\]

where \(A = (C_{11}C_{22} - C_{12}^2)/C_{66} - 2C_{12}\). The CSb\textsubscript{3}/Bi\textsubscript{3} is mechanically isotropic due to hexagonal symmetry, and the \(C_{2D}\) is 22.81 Nm\textsuperscript{-1}, which is obviously smaller than those of other 2D materials [46–48], suggesting that monolayer CSb\textsubscript{1.5}Bi\textsubscript{1.5} is more flexible than other 2D materials. The Poisson’s ratio \(\nu_{2D}(\theta)\) is also isotropic, and can be simply written as:

\[
\nu_{2D} = \frac{C_{12}}{C_{11}}.\tag{3}
\]

The calculated \(\nu_{2D}\) of CSb\textsubscript{3}/Bi\textsubscript{1.5} is 0.351. The related data are summarized in table 1.

Next, we provide some suggestions on experimental aspects. Firstly, the CSb\textsubscript{3}/CBi\textsubscript{3} monolayer may be experimentally achieved by the bottom-up approaches such as the molecular beam epitaxy [21], because the epitaxial BC\textsubscript{3} sheet with a similar structure has been successfully synthesized [17]. Similar to Janus monolayer MoS\textsubscript{2} [40, 41], the CSb\textsubscript{1.5}Bi\textsubscript{1.5} can be synthesized experimentally with similar experimental techniques based on CSb\textsubscript{3}/CBi\textsubscript{3} monolayer.

### Table 1

| \(a_0\) | \(d_1\) | \(d_2\) | \(\theta_1\) | \(\theta_2\) | \(t\) |
|---|---|---|---|---|---|
| 7.772 | 2.131 | 2.217 | 115.442 | 115.154 | 1.901 |
| \(C_{11}/C_{22}\) | \(C_{12}\) | \(G_{2D}\) | \(C_{2D}\) | \(\nu_{2D}\) |
| 26.01 | 9.13 | 8.44 | 22.81 | 0.351 |
4. Electronic structures

The energy band structures of CSb$_{1.5}$Bi$_{1.5}$ with both GGA and GGA + SOC are plotted in figure 4. In the absence of SOC, one observes that CSb$_{1.5}$Bi$_{1.5}$ is a direct band-gap semiconductor with both CBM and VBM at K point with a gap of 39.9 meV. This is different from that of CSb$_{3}$/CBi$_{3}$ with gapless Dirac points at K points due to symmetry reduction. When considering SOC, one observes that CSb$_{1.5}$Bi$_{1.5}$ is still a direct band-gap semiconductor with a gap of 40.1 meV. Based on the projected band states to atomic orbitals, the states near the band edges are dominated by the C-p, orbitals and the Sh/Bi-p orbitals (see figure 2 of ESI). The main SOC effect is to give rise to a spin splitting of the GGA bands. From the symmetry perspective, the inversion symmetry breaking lifts the spin degeneracy at each generic k point. For CSb$_{3}$/CBi$_{3}$, no spin degeneracy is removed within SOC due to existing inversion symmetry [21]. The spin-splitting at the K point is as large as 139 meV ($\Delta C$) and 229 meV ($\Delta V$) for the lowermost conduction band (LCB) and uppermost valence band (UVB), respectively. These splitting energies are significantly greater than the thermal energy of room temperature (25 meV), which is highly desirable for avoiding spin-flip scattering in spintronics applications.

It should be noted that the conically shaped conduction (valence) band valleys of CSb$_{1.5}$Bi$_{1.5}$ at K and $-K$ corners are inequivalent but related by time-reversal symmetry. We redraw the energy band structures with the projection of spin operator $\hat{S}_z$, including $-K$ high symmetry point (see figure 5). It is clearly seen that the spin polarizations at K and $-K$ are opposite, which means that the low-energy states in the K and $-K$ valleys can be distinguished by their spin index. Once the K and $-K$ valleys are separated with a valley polarization, 100% out-of-plane spin polarization can be realized in transport. The missing inversion symmetry will make these valleys acquire a valley-contrasting Berry curvature $\Omega_z(k)$:

$$\Omega_z(k) = \nabla_k \times i\langle \mu_{\text{orb},k} | \nabla_k \mu_{\text{orb},k} \rangle$$

in which $\mu_{\text{orb},k}$ is the lattice periodic part of the Bloch wave functions. The distribution of Berry curvature in the momentum space for monolayer CSb$_{1.5}$Bi$_{1.5}$ is plotted in figure 5. It is clearly seen that two obvious peaks at both K and $-K$ valleys but with opposite sign appear, and the distribution of $\Omega_z(k)$ exhibits a three-fold rotational symmetry. It is not possible to distinguish these two kinds of valleys from energy, but can discern them by their opposite Berry curvatures and out-of-plane spin moments. This will lead to spin-valley-coupled transport properties. When the in-plane electric field is applied, the valley Hall and spin Hall effects would occur simultaneously due to the valley index being coupled with spin (the charge carriers of different valleys flow to the opposite transverse edges due to $\nu \sim E \times \Omega_z(k)$), resulting in both valley and spin polarization along the edges, namely spin-valley Hall effect.

Moreover, due to the lack of the horizontal mirror symmetry, the CSb$_{1.5}$Bi$_{1.5}$ should have Rashba effect, which can be observed at K point. Anisotropic Rashba splitting can also be observed at M point in Pt-based Janus monolayers PtXY (X, Y = S, Se, or Te) [49], and the Rashba-like spin splitting along three momentum directions can be achieved in trigonal layered PtBi$_2$ [50]. To examine the Rashba effect, the in-plane spin-textures are calculated, and figure 6 shows the spin projected constant energy (0.25 eV above the Fermi level) contour plots of the spin textures calculated in k$_x$–k$_y$ plane centered at the K point. It is clearly seen that the pair of spin-splitting bands for both $S_z$ and $S_\perp$ spin components have opposite spin orientation. The pure 2D Rashba spin splitting at the conduction bands around K point near the Fermi level is observed due to existing conentric spin-texture circles. It is found that only in-plane $S_z$ and $S_\perp$ spin components are present in the Rashba spin split bands with missing out-of-plane $S_\parallel$ component. The in-plane spin moments of two rings have opposite chirality. The large ring is anticlockwise, while the small ring is clockwise (see figure 6).

The monolayer CSb$_{3}$/CBi$_{3}$ is predicted to be a QSHI [21]. It is natural to confirm the topological properties of CSb$_{1.5}$Bi$_{1.5}$, which can be characterized by the $Z_2$ topological invariant. For a material with space inversion symmetry, the $Z_2$ can be calculated by calculating the parities of the occupied valence bands by using Fu and Kanes method [51], like monolayer CSb$_{3}$/CBi$_{3}$ [21]. The universal method is to calculate the Wannier charge centers (WCCs), which is used for monolayer CSb$_{1.5}$Bi$_{1.5}$. The evolution of WCCs for monolayer CSb$_{1.5}$Bi$_{1.5}$ is plotted in figure 7. Taking an arbitrary horizontal line (e.g. WCC = 0.13) as reference, one can see that...
the number of crossings between the reference line and the evolution of WCCs is odd, which verifies that \(Z_2 = 1\). This means that the CSb_{1.5}Bi_{1.5} is a QSHI. Furthermore, a QSHI should exhibit topological protected conducting helical edge states. The Green’s-function method is used to calculate the edge states on (100) edge based on the tight-binding Hamiltonian, which are shown in figure 7. It is clearly seen that there is a pair of gapless non-trivial edge states, which connect the conduction and valence bands. The edge states exhibit two quadratic dispersive branches with opposite spin. The Dirac point is pushed above the Fermi level, and the Rashba-like splitting states can be observed. Similar phenomenon can be found in monolayer CSb_{3} \cite{21}.

In practical application, a substrate is likely to introduce strain to a 2D material due to lattice mismatch. A biaxial in-plane strain is used to study the robustness of the related physical properties of CSb_{1.5}Bi_{1.5} against the strain effects. We use \(a/a_0\) (0.94–1.06) to simulate biaxial in-plane strain, where \(a\) and \(a_0\) represent the in-plane lattice constants with and without strain, respectively. The strained energy band structures with both GGA and GGA + SOC are plotted in figures 3 and 4 of ESI. Except for 0.94 strain, they all show direct band-gap semiconductors with both CBM and VBM at \(K\) point. For 0.94 strain, GGA results show a metal, but GGA + SOC results demonstrate an indirect band-gap semiconductor with CBM and VBM at \(\Gamma\) and \(K\) points. The energy band gaps with both GGA and GGA + SOC and spin-splittings at the \(K\) point for LCB and UVB as a function of strain are plotted in figures 5 and 6 of ESI. These gaps (except for 0.94 strain) and spin-splittings are greater than the thermal energy of room temperature (25 meV), which is necessary to readily access and manipulate valleys for memory and logic applications. Finally, we calculate \(Z_2\) at all strain points to confirm topological properties of strained monolayer CSb_{1.5}Bi_{1.5}, and only show the evolution of WCCs at 0.94 and 1.06 strains in figure 7 of ESI. The calculated results show that the WCCs can be crossed only one time by an arbitrary horizontal line, which means \(Z_2 = 1\). These confirm that all strained monolayer CSb_{1.5}Bi_{1.5} are TIs. These imply that the spin-valley coupling and nontrivial topological state are robust against the biaxial strain.

5. Discussion and conclusion

The CSb_{1.5} and CBi_{3} monolayers are QSHIs with HSE06 + SOC \cite{21}. The percentage of Sb/Bi atoms and lattice constants of Janus monolayer CSb_{1.5}Bi_{1.5} are between ones of CSb_{3} and CBi_{3} monolayers, and it should also be QSHI with HSE06 + SOC. To confirm this, the energy band structures and WCCs of CSb_{1.5}Bi_{1.5} with HSE06 + SOC are plotted in figure 8 of ESI. The calculated gap is about 0.284 eV, which is larger than one (0.04 eV) with GGA + SOC. The WCCs show that the CSb_{1.5}Bi_{1.5} is still a QSHI with \(Z_2 = 1\).

In summary, our calculated results demonstrate that svc-QSHI with spin and valley polarized states can emerge in the CSb_{1.5}Bi_{1.5}. Particularly, the CSb_{1.5}Bi_{1.5} monolayer hosts Rashba-splitting edges states, which can be measured.
by angle-resolved photoemission spectroscopy. Furthermore, we demonstrate that the spin-valley-coupling and topological properties are perfectly preserved, when a suitable biaxial strain is applied. In view of the recent experimental progress in AB₃ type atomic sheets [17] and Janus monolayers [40, 41], our findings can promote further experimental exploration for intriguing svc-QSHI.

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