Two-Dimensional Janus Antimony Selenium Telluride with Large Rashba Spin Splitting and High Electron Mobility

Lei Zhang, Yuantong Gu, and Aijun Du*

ABSTRACT: Janus two-dimensional materials with large Rashba spin splitting and high electron mobility are rarely reported but highly desired for nanoscale spintronics. Herein, using density functional theory calculations, we predicted Janus Sb$_2$Se$_x$Te$_{3-x}$ ($x = 1$ or 2) monolayers simultaneously harboring these fascinating properties. The predicted monolayers are indirect semiconductors with great dynamical, thermal, and mechanical stability. The spin–orbital coupling (SOC) and the out-of-plane asymmetry lead to Rashba spin splitting at the conduction band minimum (CBM), which can be effectively tuned by the small uniaxial strain. The strong band dispersion at the CBM leads to small electron spin splitting at the conduction band minimum (CBM), which can be effectively tuned by the small uniaxial strain. Moreover, Janus Sb$_2$Se$_x$Te$_{3-x}$ monolayers possess great light absorption capability within the visible and infrared regions of solar light. Our findings highlight promising candidates for high-speed spintronic devices and may motivate more research efforts on carrier transport and SOC effects in Janus group V and VI monolayers.

INTRODUCTION

Ever since the discovery of graphene, the 2D world has expanded extensively with numerous novel 2D materials fabricated or predicted. An emerging class of 2D materials, Janus materials, has received great research attention recently due to the absence of inversion symmetry along the out-of-plane direction. Various Janus 2D materials have been proposed such as Janus transition metal dichalcogenides (TMDs) and Janus group III monochalcogenides M$_x$XY ($M = Ga$ or In; $X/Y = S$, Se, or Te), displaying versatile properties including magnetism, piezoelectricity, ferroelectricity, valley polarization, and Rashba-type spin splitting. The Rashba effect describes the momentum-dependent splitting of spin bands that results from the spin–orbital coupling (SOC) in structural inversion asymmetric systems. The Rashba effect offers unique gate tunability over spin precession, which has been experimentally demonstrated in BiTeBr heterostructures, SrTiO$_3$/Sr$_2$TiO$_3$ interfaces, showing promising applications in novel spintronic devices like spin injectors and spin field-effect transistors. The intrinsic inversion asymmetry in Janus 2D materials offers an ideal platform to explore the Rashba SOC down to the 2D regime. However, the low carrier mobility can limit the practical applications of Janus 2D materials. For example, the electron mobility of Janus TMDs only ranges from $\sim$70 to $\sim$245 cm$^2$ V$^{-1}$ s$^{-1}$, considerably smaller than black phosphorus with a high electron mobility over 2200 cm$^2$ V$^{-1}$ s$^{-1}$, which hinders their applications in high-speed and fast-response electronic/spintronic devices. Hence, it is of great interest to explore new Janus 2D materials with a strong Rashba effect and high electron mobility.

Previous reports have demonstrated the high electron mobility in centrosymmetric 2D group V and VI layers and most of them contain heavy elements; thus, a strong Rashba effect can be expected if inversion asymmetry is introduced by Janus structural design. In this work, by first-principles calculations, we proposed 2D Janus antimony selenium telluride (Sb$_2$Se$_x$Te$_{3-x}$) simultaneously harboring strong Rashba SOC and high electron mobility. Their centrosymmetric bulk counterparts have been experimentally synthesized and display a layered morphology. Especially, for Sb$_2$Se$_x$Te, there is one experimentally fabricated layered allotrope with intrinsic Janus layers, indicating the high possibility of achieving these Janus monolayers in experiments. The Janus Sb$_2$Se$_x$Te$_{3-x}$ monolayers possess robust structures with great dynamical, thermal, and mechanical stability. The lateral asymmetry leads to Rashba spin splitting at the conduction band bottom with large $\alpha_R$ that can be tuned by external strain. They are indirect semiconductors with moderate band gaps (0.90 eV for Sb$_2$Se$_x$Te and Sb$_2$Se$_x$Te$_2$, respectively) and display great light absorption capability. Moreover, the electron mobility of these monolayers surpasses 2000 cm$^2$ V$^{-1}$ s$^{-1}$ and reaches up to 6816.63 cm$^2$ V$^{-1}$ s$^{-1}$. The Rashba effect can be tuned by external strain. They are indirect semiconductors with moderate band gaps (0.90 eV for Sb$_2$Se$_x$Te and Sb$_2$Se$_x$Te$_2$, respectively) and display great light absorption capability. Moreover, the electron mobility of these monolayers surpasses 2000 cm$^2$ V$^{-1}$ s$^{-1}$ and reaches up to 6816.63 cm$^2$ V$^{-1}$ s$^{-1}$. The Rashba effect describes the momentum-dependent splitting of spin bands that results from the spin–orbital coupling (SOC) in structural inversion asymmetric systems. The Rashba effect offers unique gate tunability over spin precession, which has been experimentally demonstrated in BiTeBr heterostructures, SrTiO$_3$/Sr$_2$TiO$_3$ interfaces, showing promising applications in novel spintronic devices like spin injectors and spin field-effect transistors. The intrinsic inversion asymmetry in Janus 2D materials offers an ideal platform to explore the Rashba SOC down to the 2D regime. However, the low carrier mobility can limit the practical applications of Janus 2D materials. For example, the electron mobility of Janus TMDs only ranges from $\sim$70 to $\sim$245 cm$^2$ V$^{-1}$ s$^{-1}$, considerably smaller than black phosphorus with a high electron mobility over 2200 cm$^2$ V$^{-1}$ s$^{-1}$, which hinders their applications in high-speed and fast-response electronic/spintronic devices. Hence, it is of great interest to explore new Janus 2D materials with a strong Rashba effect and high electron mobility.

 Received: August 27, 2021
Accepted: November 5, 2021
Published: November 18, 2021
These novel properties make Janus 2D Sb$_2$Te$_{3-x}$Se$_x$ promising candidates for nanoscale spintronics and electronics.

**RESULTS AND DISCUSSION**

The Janus Sb$_2$Te$_{3-x}$Se$_x$ monolayers possess a rhombohedral geometry with a $P3_1m1$ space group, as shown in Figure 1a,c. Each monolayer consists of five atomic layers following the stacking sequences of Se-Sb-Se-Sb-Te and Se-Sb-Te-Sb-Te for Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$, respectively. The lattice parameter and thickness of Sb$_2$SeTe$_2$ are larger than those of Sb$_2$Se$_2$Te due to the larger atomic radius of Te (see Table 1). The cohesive energies are calculated to be $-3.04$ and $-2.93$ eV/atom for Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$, respectively, suggesting the strong bonding characteristics of these monolayers. To further understand the bonding nature of Janus Sb$_2$Te$_{3-x}$Se$_x$ monolayers, the electron localization function (ELF) is calculated and shown in Figure 1b,d. The red (1.0), green (0.5), and blue (0.0) regions correspond to fully localized electrons, fully delocalized electrons, and very low charge density, respectively. It is clear that the value of ELF is high around the atomic sites while the value is close to 0.5 in the bonding regions. It is known that in the case of a covalent bond, the lone-pair electrons are localized around the atoms and the electrons constituting the bonds are delocalized. Hence, the Sb-Se and Sb-Te atoms are bonded by forming covalent bonds, which is similar to the bonding nature of Bi$_2$Te$_2$Se and Bi$_2$Te$_3$Se.  

The phonon spectra of Sb$_2$Te$_{3-x}$Se$_x$ are shown in Figure 2a,b. Clearly, there is no negative frequency in the spectra, which demonstrates the dynamical stability of these monolayers. Their thermal stability is also confirmed by the AIMD (ab initio molecular dynamics) simulations of 5 ps performed at 300 K (as shown in Figure S1), where the structures and total energy only fluctuate slightly during the simulations. Moreover, the calculated elastic constants of Janus Sb$_2$Te$_{3-x}$Se$_x$ (Table 1) fulfill the Born mechanical stability criteria and suggest their mechanical stability. The in-plane Young’s modulus ($Y$) and Poisson’s ratio ($v$) as a function of in-plane angle ($\theta$) can be determined by the following two equations, respectively:

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



![Figure 1](image1.png)

*(a, c) Top and side views of Janus Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$ monolayers, respectively. (b, d) ELF of Janus Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$ monolayers, respectively.*

![Figure 2](image2.png)

*(a, b) Phonon spectra of Janus Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$ monolayers, respectively. The inset represents the Brillouin zone marking the high symmetry k-points. (c) Young’s modulus and Poisson’s ratio of Janus Sb$_2$Te$_{3-x}$Se$_x$ monolayers as functions of the in-plane angle $\theta$.)*

|                | lattice parameters (Å) | thickness (Å) | $C_{11}$ (N/m) | $C_{12}$ (N/m) | $C_{66}$ (N/m) |
|----------------|------------------------|--------------|----------------|---------------|---------------|
| Sb$_2$Se$_2$Te | 4.12                   | 9.73         | 70.71          | 18.01         | 26.37         |
| Sb$_2$SeTe$_2$| 4.21                   | 9.83         | 64.50          | 18.10         | 23.17         |
where $A = (C_{11}C_{22} - C_{12}^2)/C_{66} - 2C_{12}$ and $B = C_{11} + C_{22} - (C_{11}C_{22} - C_{12}^2)/C_{66}$. The calculated direction-dependent $Y$ and $\nu$ are shown in Figure 2c. The $Y(\nu)$ values of Janus Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$ monolayers are calculated to be 66.15 N/m (0.25) and 59.38 N/m (0.28), respectively, along all directions, suggesting that these Janus monolayers are mechanically isotropic. Noticeably, the $Y$ values of Janus Sb$_2$Se$_2$Te$_{1-x}$ monolayers are far smaller than those of graphene (335 N/m) $^{46}$ and MoS$_2$ ($180 \pm 60$ N/m) $^{47}$, offering the opportunity to tune their electronic structures by applying strain.

Having confirmed the stability of Janus Sb$_2$Se$_x$Te$_{1-x}$ monolayers, we then focus on their electronic structures. Figure 3 shows the band structures calculated by the HSE06 functional with/without the inclusion of SOC and band structures with SOC by the HSE06 functional for Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$, respectively. The insets are the zoomed-in views of the conduction band minimum around the gamma point. The calculated direction-dependent $Y$ and $\nu$ are shown in Figure 2c. The $Y(\nu)$ values of Janus Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$ monolayers are calculated to be 66.15 N/m (0.25) and 59.38 N/m (0.28), respectively, along all directions, suggesting that these Janus monolayers are mechanically isotropic. Noticeably, the $Y$ values of Janus Sb$_2$Se$_2$Te$_{1-x}$ monolayers are far smaller than those of graphene (335 N/m) $^{46}$ and MoS$_2$ ($180 \pm 60$ N/m) $^{47}$, offering the opportunity to tune their electronic structures by applying strain.

Having confirmed the stability of Janus Sb$_2$Se$_x$Te$_{1-x}$ monolayers, we then focus on their electronic structures. Figure 3 shows the band structures calculated by the HSE06 functional with/without the inclusion of SOC and band structures with SOC by the HSE06 functional for Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$, respectively. The insets are the zoomed-in views of the conduction band minimum around the gamma point. Bands are mainly composed of the in-plane $S_x$ and $S_y$ spin components, with a negligible out-of-plane $S_z$ component. The in-plane spin orientation is found perpendicular to the direction of the $k$ vectors, which is a typical signature of Rashba-type spin splitting. $^{27}$ The Rashba parameter $\alpha_R$ which evaluates the strength of the Rashba effect, can then be obtained from the formula $\alpha_R = 2E_R/k_R$ based on a linear Rashba model, where $E_R$ and $k_R$ represent the Rashba energy and Rashba momentum, respectively, as indicated in Figure 4d. The $\alpha_R$ along the arm-chair ($\alpha_R^{\text{arm}}$) and zig-zag ($\alpha_R^{\text{zag}}$) directions are calculated separately. The calculated values of $\alpha_R^{\text{arm}}$ are 1.53 and 1.00 eV Å while the calculated values of $\alpha_R^{\text{zag}}$ are 1.52 and 1.12 eV Å for Janus Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$ monolayers, respectively. Clearly, the $\alpha_R$ values of Janus Sb$_2$Se$_2$Te$_{1-x}$ monolayers are far smaller than those of Janus transition metal dichalcogenides ($0.08-0.51$ eV Å) $^{27}$ Janus TiBr$_3$ (0.15 eV Å) $^{30}$ and Janus Te$_2$Se (0.39 eV Å) $^{31}$ and comparable to those of Janus TiS$_2$Se (1.08 eV Å) $^{29}$ Janus SbTe (1.39 eV Å) $^{32}$ and Janus Pbi (1.56 eV Å) $^{33}$ suggesting the promising applications of Janus Sb$_2$Se$_2$Te$_{1-x}$ monolayers in spintronic devices like spin-polarized field-effect transistors. $^{27,28}$

We then explored the effect of uniaxial strain along the arm-chair ($\epsilon_{\text{arm}}$) and zig-zag ($\epsilon_{\text{zag}}$) directions on the Rashba SOC in our systems. The negative values indicate compressive strain, while the positive values represent tensile strain. As shown in Figure 5, we can find that there is a general trend where an increase in uniaxial strain would lead to the decrease in $E_R$ and $k_R$ along the strain direction and the increase in $E_R$ and $k_R$ along the vertical direction. Generally, a larger $E_R$ is desirable for stabilizing electron spin while a larger $k_R$ will benefit the phase offset for different spin channels, which are favorable for spin transport. Through applying uniaxial strain, the stability of electron spin and phase offset can then be enhanced (suppressed) along the strain direction but suppressed (enhanced) along the vertical direction, which may favor the anisotropic spin transport.

When uniaxial strain is applied, the $\alpha_R$ for both Janus Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$ monolayers becomes anisotropic, as shown in Figure 6. The strength of $\alpha_R$ can be tuned more significantly if they lie in the same direction with the external

$$v(\theta) = \frac{C_{12}\sin^4 \theta - B\sin^2 \theta \cos^2 \theta + C_{12}\cos^4 \theta}{C_1\sin^4 \theta + A\sin^2 \theta \cos^2 \theta + C_{12}\cos^4 \theta}$$

Figure 3. (a, b) Orbital resolved band structures calculated without SOC and band structures with SOC by the HSE06 functional for Sb$_2$Se$_2$Te and Sb$_2$SeTe$_2$, respectively. The insets are the zoomed-in view of the conduction band minimum around the gamma point.
while the (1.13 eV Å) and the minimum at di directions, respectively. (c, d) αx and kx of Janus Sb2SeTe2 monolayers under different uniaxial strains applied along the arm-chair and zig-zag directions, respectively. (a, b) αy and ky of Janus Sb2SeTe2 monolayers under different uniaxial strains applied along the arm-chair and zig-zag directions, respectively.

Figure 5. (a, b) εy and ky of Janus Sb2SeTe2 monolayers under different uniaxial strains applied along the arm-chair and zig-zag directions, respectively. (c, d) εx and kx of Janus Sb2SeTe2 monolayers under different uniaxial strains applied along the arm-chair and zig-zag directions, respectively.

Figure 6. (a, b) αy of Janus Sb2SeTe2 monolayers under different uniaxial strains applied along the arm-chair and zig-zag directions, respectively. (c, d) αx of Janus Sb2SeTe2 monolayers under different uniaxial strains applied along the arm-chair and zig-zag directions, respectively.

uniaxial strain. For Janus Sb2SeTe2, the αarm - chair reaches the maximum at the equilibrium state (1.53 eV Å) and the minimum at εarm - chair = 4% (1.15 eV Å), while the αzig - zig reaches the maximum at εarm - chair = −2% (1.54 eV Å) and the minimum at εzig - zig = −4% (1.20 eV Å). For Janus Sb2SeTe2, the αarm - chair reaches the maximum at the equilibrium state (1.12 eV Å) and the minimum at εarm - chair = 4% (0.67 eV Å), while the αzig - zig reaches the maximum at the equilibrium state (1.12 eV Å) and the minimum at εzig - zig = 3% (0.65 eV Å). The strong Rashba SOC tunable by external strain makes Janus Sb2SeTe2 monolayers promising candidates for nanoscale spintronic devices.

The conduction band near the CBM displays rather strong dispersive along the G-M and K-G paths, which correspond, respectively, to the arm-chair and zig-zag directions in the real space, indicating the small effective mass along with these directions. Fitting these bands (with SOC) using a free electron model, the effective carrier mass of 2D Sb2SeTe2 (Sb2SeTe2) is calculated to be 0.14 (0.15) m0 along the arm-chair direction and 0.15 (0.15) m0 along the zig-zag direction. These values are comparable to other high-mobility semiconductors such as black phosphorene (0.14–0.18 m0)35 and AlGaAs (0.1 m0),48 inspiring us to explore the electron mobility of these monolayers.

The electron mobility (μ) is calculated based on the phonon-limited scattering model, in the formula, as shown below, which incorporates the anisotropy of the deformation potential:49

\[
\mu = \frac{e\hbar}{k_B T (m_e/(2\pi)^{1/2})(\varepsilon_0^2 + \varepsilon_1^2 + 4\varepsilon_2^2)^{1/2}}
\]

where e is the electron charge, \(\hbar\) is the reduced Plank constant, \(k_B\) is the Boltzmann constant, and T is the temperature. \(C_{2D}\) and m are the elastic constant and effective mass of the electron along the transport direction. E is the deformation potential of the CBM in the transport direction, calculated by E = ΔV/Δ(l), where l is the lattice constant along the transport direction and ΔV is the change of CBM positions upon deformation Δl. The subscripts x and y mark the directions (arm-chair/zig-zag directions). The three parameters effective mass, elastic constants, and deformation potential are the most relevant factors in determining the mobility, as we can see in eq 3. We show these parameters together with the electron mobility in Table 2. The calculated electron mobilities along the arm-chair (zig-zag) direction are 2310.98 (2253.25) and 5414.73 (6816.63) cm2 V−1 s−1 for Janus Sb2Se2Te and Sb2SeTe2 monolayers, respectively. These values are larger than or comparable to many reported Janus 2D materials including Janus MXY (M = Mo or W; X/Y = S, Se, or Te; and X ≠ Y) (70–245 cm2 V−1 s−1),34 Janus MXY (M = Ti, Zr, or Hf; X = S or Se; Y = O or S; X ≠ Y) (1–430 cm2 V−1 s−1),50 Janus PtSSE (1546.52 cm2 V−1 s−1),51 Janus PtXO (X = S or Se) (2164.95 cm2 V−1 s−1),52 and Janus In2SO (3428 cm2 V−1 s−1),53 offering great potential for high-speed electronic devices.43

Janus Sb2SeTe2 monolayers with moderate band gaps are expected to exhibit excellent optical properties. Figure 7 shows the optical absorption spectra of Janus Sb2SeTe2 monolayers calculated by the GW-BSE method with the inclusion of SOC and excitonic effects. Both monolayers possess great light absorbance in the whole visible light range. The light absorption onsets are determined to be around 1350 and 1670 nm for Sb2SeTe2 and Sb2SeTe2, respectively, which lie within the infrared region of solar light. The strong absorption at the long-wavelength range may be

Table 2. In-Plane Stiffness (C), Effective Mass of Charge Carriers (m), Deformation Potential (E) (as Shown in Figure S4), and Electron Mobility (μ) of Sb2Se2Te2 and Sb2SeTe2 Monolayers at 300 K

|                | C (N/m) | E (eV) | m (m0) | μ (cm²V⁻¹s⁻¹) |
|----------------|---------|--------|--------|--------------|
| Sb2SeTe2    |         |        |        |              |
| arm-chair    | 70.71   | 5.85   | 0.14   | 2310.98      |
| zig-zag      | 70.71   | 5.36   | 0.15   | 2253.25      |
| Sb2SeTe2    |         |        |        |              |
| arm-chair    | 64.50   | 3.89   | 0.15   | 5414.73      |
| zig-zag      | 64.50   | 2.42   | 0.15   | 6816.63      |
attributed to the transition from the occupied s orbital of Sb and p orbital of Te to the unoccupied p orbital of Sb based on the electronic structures in Figure 3. Because the infrared region accounts for more than half of the solar energy, these two monolayers show promising applications in photovoltaic devices such as high-efficiency light-absorbers.

**CONCLUSIONS**

In summary, we have investigated the electronic structure and electron mobility of Janus Sb₂Se₂Te and Sb₂Se₃ monolayers by DFT calculations. They exhibit great dynamical, thermal, and mechanical stability. It is found that Janus 2D Sb₂Se₂Te and Sb₂Se₃ are indirect semiconductors with band gaps of 0.90 and 0.85 eV, respectively. The inversion asymmetry of the Janus structures leads to Rashba spin splitting at the CBM, and the large Rashba spin splitting and high electron mobility in these two monolayers show promising applications in photovoltaic devices such as high-efficiency light-absorbers.

**COMPUTATIONAL METHODS**

The DFT calculations were performed by using the Vienna Ab-initio Simulation Package (VASP). The exchange–correlation interaction was described by the generalized gradient approximation (GGA) of the Perdew–Burke–Ernzerhof (PBE)-type functional. The projector augmented wave (PAW) method was applied to treat the electron–core interactions. The van der Waals (vdW) dispersion was included by the Grimme method (DFT-D3). The cutoff energy for plane waves was set to 400 eV, and a $9 \times 9 \times 1$ k-point mesh was applied to sample the first Brillouin zone. A vacuum space around 18 Å was used to exclude the influence of neighboring images induced by the periodic boundary conditions. The structures were fully relaxed until the residual forces and the energy were converged to 0.005 eV/Å and $1 \times 10^{-6}$ eV, respectively. The electronic structure was calculated by the Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional with the SOC effect taken into consideration. The optical absorption spectrum was obtained by using single-shot GW (G0W0) with the Bethe–Salpeter equation (BSE) approach, which includes many-body effects.

**ASSOCIATED CONTENT**

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.1c04680.

A AIMD results; band structures calculated by the GW method; projection of spin components at a constant energy contour; linear fitting of deformation potential; and light absorbance calculated with different vacuum thicknesses (PDF).

**AUTHOR INFORMATION**

**Corresponding Author**

Aijun Du — School of Chemistry and Physics and Centre for Materials Science, Queensland University of Technology, Brisbane, QLD 4000, Australia; @orcid.org/0000-0002-3369-3283; Email: aijun.du@qut.edu.au

**Authors**

Lei Zhang — School of Chemistry and Physics and Centre for Materials Science, Queensland University of Technology, Brisbane, QLD 4000, Australia

Yuantong Gu — School of Mechanical, Medical and Process Engineering, Queensland University of Technology, Brisbane, QLD 4000, Australia

Complete contact information is available at: https://pubs.acs.org/doi/10.1021/acsomega.1c04680

**Notes**

The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**

We acknowledge generous grants of high-performance computing resources provided by the NCI National Facility and the Pawsey Supercomputing Centre through the National Computational Merit Allocation Scheme supported by the Australian Government and the Government of Western Australia. A.D. also greatly appreciates the financial support of the Australian Research Council under Discovery Project (DP170103598, DP210100721, and DP210100331).

**REFERENCES**

(1) Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A. Electric Field Effect in Atomically Thin Carbon Films. Science 2004, 306, 666–669.

(2) Mak, K. F.; Lee, C.; Hone, J.; Shan, J.; Heinz, T. F. Atomically Thin MoS₂: A New Direct-Gap Semiconductor. Phys. Rev. Lett. 2010, 105, 136805.

(3) Gong, C.; Li, L.; Li, Z.; Ji, H.; Stern, A.; Xia, Y.; Cao, T.; Bao, W.; Wang, C.; Wang, Y.; Qiu, Z. Q.; Cava, R. J.; Louie, S. G.; Xia, J.; Zhang, X. Discovery of Intrinsic Ferromagnetism in Two-Dimensional Van Der Waals Crystals. Nature 2017, 546, 265.

(4) Huang, B.; Clark, G.; Navarro-Moratalla, E.; Klein, D. R.; Cheng, R.; Seyler, K. L.; Zhong, D.; Schmidgall, E.; McGuire, M. A.; Cobden,
(42) Ruan, Y.; Huang, L.; Yang, Y.; Xu, G.; Zhong, K.; Huang, Z.; Zhang, J.-M. Robustness of the Electronic Structure and Charge Transfer in Topological Insulator Bi2Te2Se and Bi2Se3:Te Thin Films under an External Electric Field. *Phys. Chem. Chem. Phys.* 2020, 22, 3867–3874.

(43) Mouhat, F.; Coudert, F.-X. Necessary and Sufficient Elastic Stability Conditions in Various Crystal Systems. *Phys. Rev. B* 2014, 90, 224104.

(44) Peng, R.; Ma, Y.; He, Z.; Huang, B.; Kou, L.; Dai, Y. Single-Layer Ag2S: A Two-Dimensional Bidirectional Auxetic Semiconductor. *Nano Lett.* 2019, 19, 1227–1233.

(45) Zhang, L.; Tang, C.; Zhang, C.; Gu, Y.; Du, A. First-Principles Prediction of Ferroelasticity Tuned Anisotropic Auxeticity and Carrier Mobility in Two-Dimensional AgO. *J. Mater. Chem. C* 2021, 9, 3155–3160.

(46) Şahin, H.; Cenangirov, S.; Topsakal, M.; Bekaroluğ, E.; Aksu, E.; Senger, R. T.; Ciraci, S. Monolayer Honeycomb Structures of Group-IV Elements and III-V Binary Compounds: First-Principles Calculations. *Phys. Rev. B* 2009, 80, 155453.

(47) Bertolazzi, S.; Brivio, J.; Kis, A. Stretching and Breaking of Ultrathin MoS2. *ACS Nano* 2011, 5, 9703–9709.

(48) Walukiewicz, W.; Ruda, H. E.; Lagowski, J.; Gatos, H. C. Electron Mobility in Modulation-Doped Heterostructures. *Phys. Rev. B* 1984, 30, 4571–4582.

(49) Lang, H.; Zhang, S.; Liu, Z. Mobility Anisotropy of Two-Dimensional Semiconductors. *Phys. Rev. B* 2016, 94, 235306.

(50) Chen, W.; Hou, X.; Shi, X.; Pan, H. Two-Dimensional Janus Transition Metal Oxides and Chalcogenides: Multifunctional Properties for Photocatalysts, Electronics, and Energy Conversion. *ACS Appl. Mater. Interfaces* 2018, 10, 35289–35295.

(51) Peng, R.; Ma, Y.; Huang, B.; Dai, Y. Two-Dimensional Janus PtSe2 for Photocatalytic Water Splitting under the Visible or Infrared Light. *J. Mater. Chem. A* 2019, 7, 603–610.

(52) Shen, H.; Zhang, Y.; Wang, G.; Ji, W.; Xue, X.; Zhang, W. Janus PtXO (X = S, Se) Monolayers: The Visible Light Driven Water Splitting Photocatalysts with High Carrier Mobilities. *Phys. Chem. Chem. Phys.* 2021, 23, 21825–21832.

(53) Vu, T. V.; Nguyen, C. V.; Phuc, H. V.; Lavrentev, A. A.; Khyzhuin, O. Y.; Hieu, N. V.; Obeid, M. M.; Rai, D. P.; Tong, H. D.; Hieu, N. N. Theoretical Prediction of Electronic, Transport, Optical, and Thermoelectric Properties of Janus Monolayers InXO (X = S, Se, Te). *Phys. Rev. B* 2021, 103, No. 085422.

(54) Rajabali, M.; Esfandiari, M.; Rajabali, S.; Vakili-Tabatabaei, M.; Mohajerzadeh, S.; Mohajerzadeh, S. High-Performance Photoreactor-Based Transistors Using a Novel Exfoliation-Free Direct Crystallization on Silicon Substrates. *Adv. Mater. Interfaces* 2020, 7, 2000774.

(55) Kresse, G.; Furthmüller, J. Efficiency of Ab-Initio Total Energy Calculations for Metals and Semiconductors Using a Plane-Wave Basis Set. *Comput. Mater. Sci.* 1996, 4, 15–50.

(56) Kresse, G.; Furthmüller, J. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Phys. Rev. B* 1996, 54, 11169–11186.

(57) Kresse, G.; Hafner, J. Ab Initio Molecular-Dynamics Simulation of the Liquid-Metal–Amorphous-Semiconductor Transition in Germanium. *Phys. Rev. B* 1994, 49, 14251–14269.

(58) Perdew, J. P.; Ernzerhof, M.; Burke, K. Rationale for Mixing Exact Exchange with Density Functional Approximations. *J. Chem. Phys.* 1996, 105, 9982–9985.

(59) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* 1996, 77, 3865.

(60) Kresse, G.; Joubert, D. From Ultrasoft Pseudopotentials to the Projector Augmented-Wave Method. *Phys. Rev. B* 1999, 59, 1758–1775.

(61) Grimme, S. Semiempirical Gga-Type Density Functional Constructed with a Long-Range Dispersion Correction. *J. Comput. Chem.* 2006, 27, 1787–1799.

(62) Krukau, A. V.; Vydrov, O. A.; Izmaylov, A. F.; Scuseria, G. E. Influence of the Exchange Screening Parameter on the Performance of Screened Hybrid Functionals. *J. Chem. Phys.* 2006, 125, 224106.