Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Hexagonal warping effect in the Janus group-VIA binary monolayers with large Rashba spin splitting and piezoelectricity

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POSCAR for STe_2

```
janus-STe2
   1.00000000000000
     4.1143932840923965    0.0000000000000000    0.0000000000000000
    -2.0571966419950698    3.5631691051114833    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0000000000000000
   Te   Se
    2    1
Direct
  0.0000000000000000 -0.0000000000000000  0.5050366693966156
  0.6666667300000029  0.3333333409999995  0.4111593086469315
  0.3333333409999995  0.6666666830000025  0.5838039739564491

  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
```

POSCAR for $SeTe_2$

```
janus-SeTe2
   1.00000000000000
     4.1143932840923965    0.0000000000000000    0.0000000000000000
    -2.0571966419950698    3.5631691051114833    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0000000000000000
   Te   Se
    2    1
Direct
  0.0000000000000000 -0.0000000000000000  0.5050366693966156
  0.6666667300000029  0.3333333409999995  0.4111593086469315
  0.3333333409999995  0.6666666830000025  0.5838039739564491

  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
```

POSCAR for Se_2Te

```
janus-Se2Te
   1.00000000000000
     3.8818440697551000    0.0000000000000000    0.0000000000000000
    -1.9409220348293115    3.3617691579502660    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0000000000000000
   Se   Te
    2    1
```

Direct
0.0000001664869984 0.9999998335118718 0.5045256278404865
0.3333329332017030 0.6666671127966097 0.5795145576671500
0.6666669593113070 0.3333331116915232 0.4159597874923647

0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00

INCAR for optimized structures

Global Parameters
ISTART = 0 (Read existing wavefunction; if there)
#ISPIN = 2 (Spin polarised DFT)
ICHARG = 2 (Non-self-consistent: GGA/LDA band structures)
LREAL = .FALSE. (Projection operators: automatic)
ENCUT = 500 (Cut-off energy for plane wave basis set, in eV)
PREC = Accurate (Precision level)
LWAVE = .F. (Write WAVECAR or not)
LCHARG = .F. (Write CHGCAR or not)
ADDGRID= .TRUE. (Increase grid; helps GGA convergence)
# LVTOT = .TRUE. (Write total electrostatic potential into LOCPOT or not)
# LVHAR = .TRUE. (Write ionic + Hartree electrostatic potential into LOCPOT or not)
# NELECT = (No. of electrons: charged cells; be careful)
# LPLANE = .TRUE. (Real space distribution; supercells)
# NPAR = 4 (Max is no. nodes; don't set for hybrids)
# NWRITE = 2 (Medium-level output)
# KPAR = 2 (Divides k-grid into separate groups)
# NGX = 500 (FFT grid mesh density for nice charge/potential plots)
# NGY = 500 (FFT grid mesh density for nice charge/potential plots)
# NGZ = 500 (FFT grid mesh density for nice charge/potential plots)
ISIF = 3 (Stress/relaxation: 2-Ions, 3-Shape/Ions/V, 4-Shape/Ions)
Electronic Relaxation
ISMEAR = 0 (Gaussian smearing; metals:1)
SIGMA = 0.05 (Smearing value in eV; metals:0.2)
NELM = 60 (Max electronic SCF steps)
NELMIN = 6 (Min electronic SCF steps)
EDIFF = 1E-08 (SCF energy convergence; in eV)
# GGA = PS (PBEsol exchange-correlation)
Ionic Relaxation
NSW = 100 (Max electronic SCF steps)
IBRION = 2 (Algorithm: 0-MD; 1-Quasi-New; 2-CG)

#ISIF = 2 (Stress/relaxation: 2-Ions, 3-Shape/Ions/V, 4-Shape/Ions)
EDIFFG = -1E-03 (Ionic convergence; eV/AA)
# ISM = 2 (Symmetry: 0=none; 2=GGA; 3=hybrids)
Spin-Orbit Coupling Calculation
LSORBIT = .TRUE. (Activate SOC)
GGA_COMPAT = .FALSE. (Apply spherical cutoff on gradient field)
VOSKOWN = 1 (Enhances the magnetic moments and the magnetic energies)
LMAXMIX = 4 (For d elements increase LMAXMIX to 4, f: LMAXMIX = 6)
! SAXIS = 0 0 1 (Direction of the magnetic field)
! MAGMOM = 0 0 3 (Set this parameters manually, Local magnet

To gain further insight into the influence of the in-plane biaxial strain on the electronic band structures, we calculate the band structures various with different strains ranging from -6% to 6%, as shown in Fig. S2. The blue positive percent sign indicates tensile strain and the negative percent sign indicates compressive strain. The band gap (E_g) of the systems under different strains is also directly highlighted in the corresponding figure. It is easily found that the band structures can be altered by strain engineering.

To reveal the mechanical property of Janus Group-VIA monolayers, Young's modulus (Y) and shear modulus (G), and Poisson's ratio (v) of Janus STe2, SeTe2, and Se2Te monolayers are presented in Fig. S3. In Fig. S3(a), the solid line shows Young's modulus (Y) and the dashed line shows the shear modulus (G). Different materials are distinguished by different colors. Fig. S3(b) represents the Poisson's ratio (v) of Janus STe_2, $SeTe_2$, and Se_2Te monolayers. It is found that Young's modulus (Y), shear modulus (G), and Poisson's ratio (v) are in-plane isotropy.

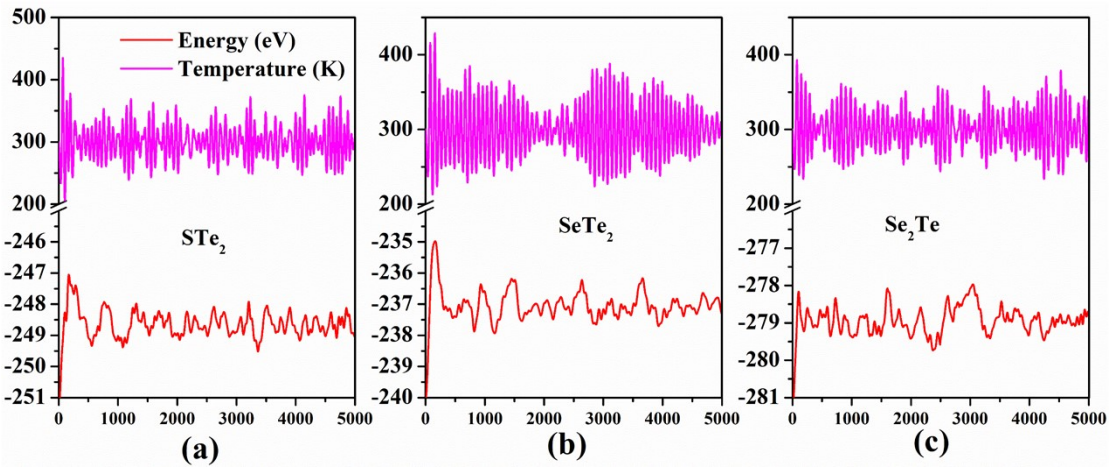
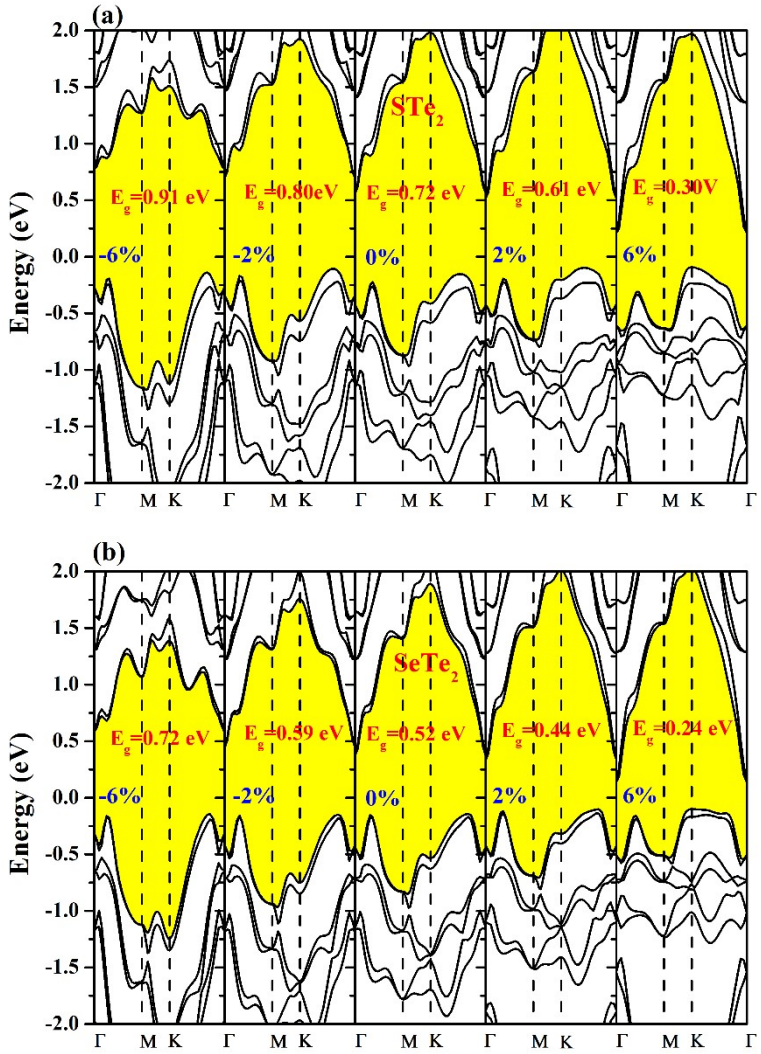


Fig.S1 (Color online) The ab initio molecular dynamics (AIMD) simulations at the temperature of 300 K with a time of 5 ps.



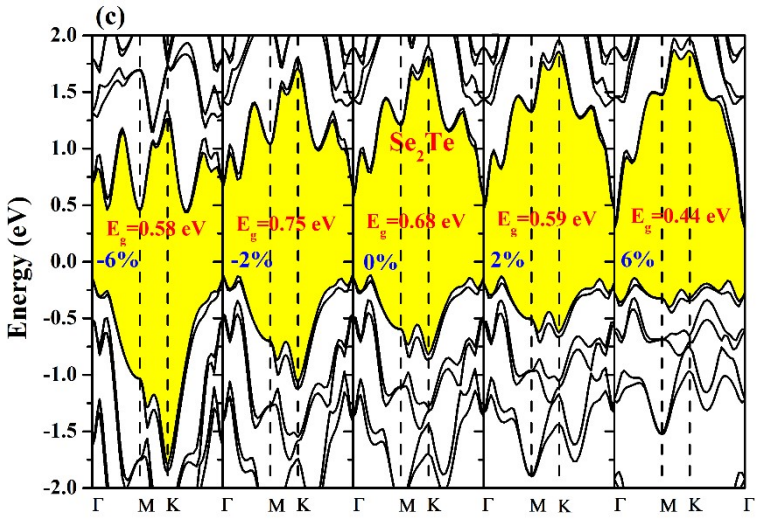


Fig.S2 (Color online) Strain-dependent electronic band structure of (a) STe_2, (b) $SeTe_2$, and (c) Se_2Te monolayers, as well as the value of band-gap. Positive and negative values represent tensile and compressive strains, respectively.

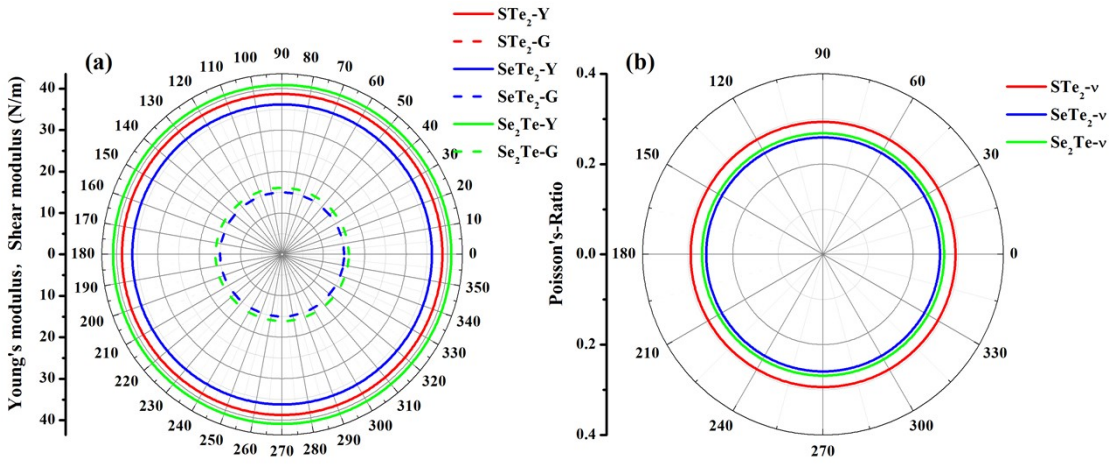


Fig. S3 (Color online) The calculated (a) Young's modulus (Y) and shear modulus (G), (b) Poisson's ratio (ν) of Janus STe_2, $SeTe_2$, and Se_2Te monolayers.