Supplement Material for the publication

First principles study on the stability, electronic and optical properties of 2D SbXY(X=Se/Te, Y=I/Br) Janus layers

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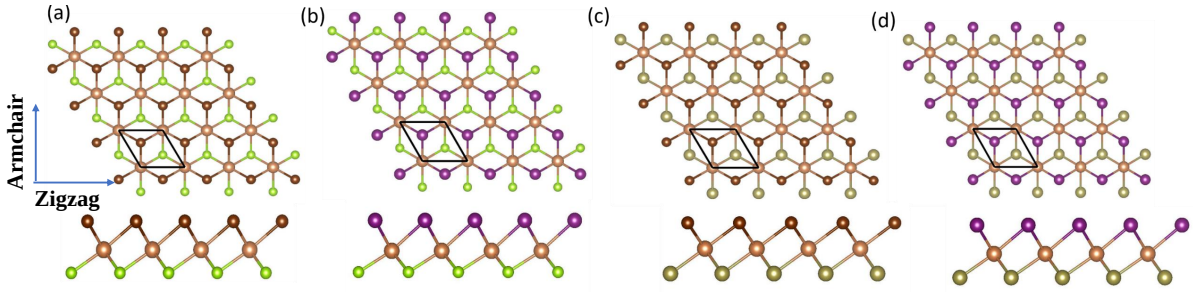
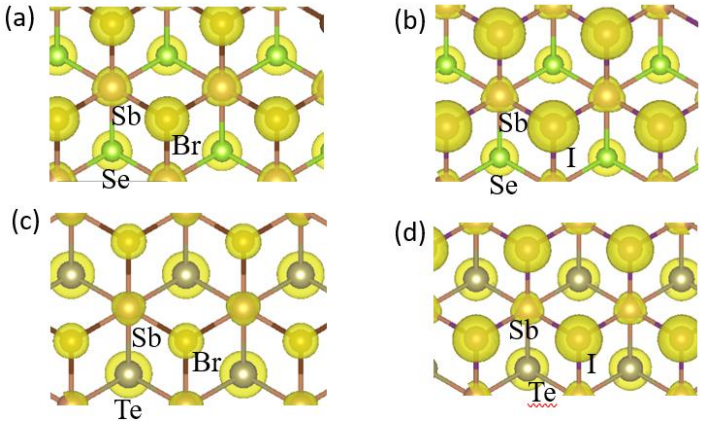
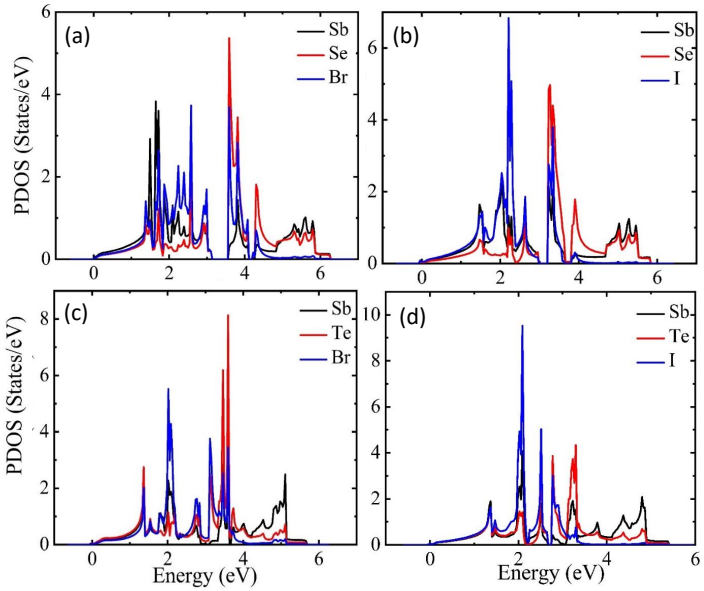


SFig. 1: The top and lateral views of geometrically optimized SbSeBr (a), SbSeI (b), SbTeBr (c), SbTeI (d) Janus structures. The golden, brown, violet, green, and bronze colours represent Sb, Br, I, Se, and Te respectively.



SFig. 2: The electron localization function of SbSeBr (a), SbSeI (b), SbTeBr (c), SbTeI (d). The yellow colour represents regions with electron accumulation.



SFig. 3: The phonon density of states of SbSeBr (a) SbSeI (b), SbTeBr (c) and SbTeI (d) Janus structures.

STab. 1: The calculated elastic constants, Young's modulus, Bulk modulus, and Poisson's ratio of SbXY (X=I/Br, Y=Se/Te) Janus structures.

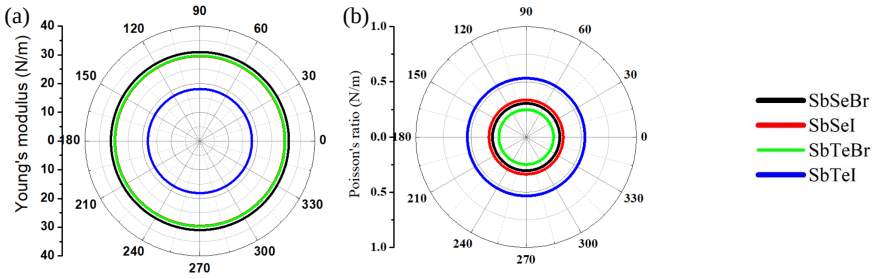
Structure	C11 (N/m)	C12 (N/m)	Y (N/m)	B (N/m)	ν
SbSeBr	34.14	10.40	30.97	22.27	0.30
SbSeI	33.36	11.22	29.59	22.29	0.33
SbTeBr	31.58	7.82	29.64	19.70	0.24
SbTeI	25.29	13.47	18.11	19.38	0.53

The elastic moduli of the 2D structure like Youngs modulus($Y(\theta)$), Poissons ratio ($\nu(\theta)$) and calculated in dependence on the in-plane polar angle θ using the equation given below:

$$Y(\theta) = \frac{C_{11}C_{12} - C_{12}^2}{C_{11}sin^4\theta + Asin^2\theta cos^2\theta + C_{22}cos^2\theta} \tag{1}$$

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

where $A = C_{11}C_{12} - C_{12}^2/(C_{66} - 2C_{12})$ and $B = C_{11} + C_{22} - (2C_{11}C_{12} - C_{12}^2)/C_{66}$.



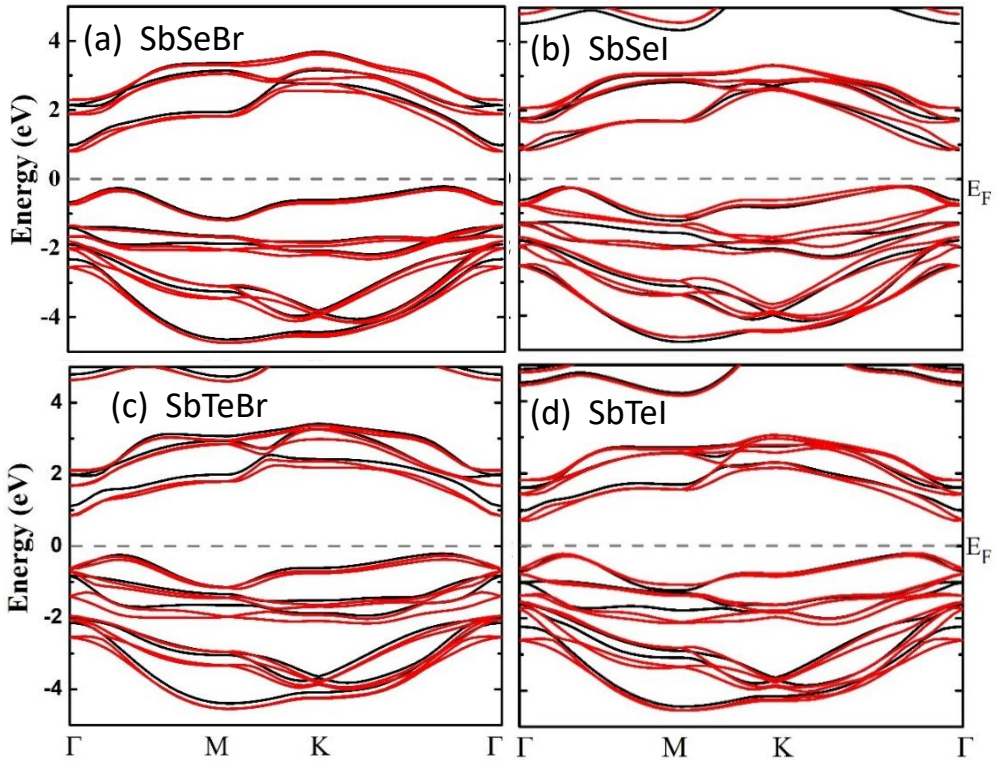
SFig. 4: The polar diagram for the in-plane variation (x-y) of Young's modulus and Poisson's ratio of SbXY (X=Se/Te, Y=Br/I) Janus structures.

STab. 2: The calculated total energy of Janus and their parent structures.

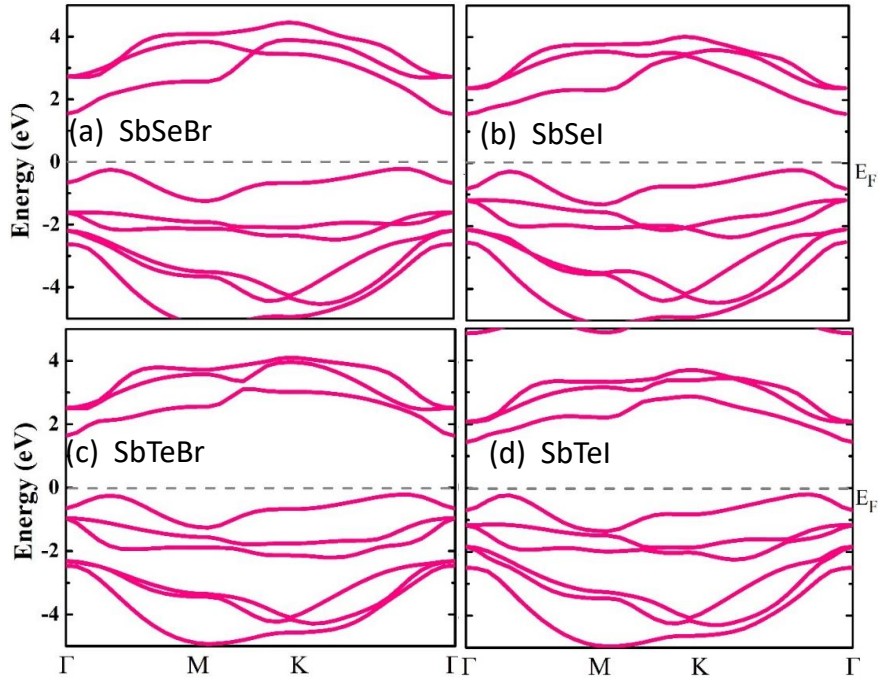
Structure	Total Energy (eV)
SbSeBr	-10.91
SbSeI	-10.48
SbTeBr	-10.40
SbTeI	-9.98
$SbSe_2$	-11.92
$SbTe_2$	-10.86
$SbBr_2$	-8.39
SbI_2	-7.59

STab. 3: The calculated chemical potential of the ground state of Sb, Se, Te, I and Br is given in the table. The ground state of Sb is found to be in a trigonal (R3m) structure. The chalcogenides Se and Te are in trigonal (P3_121) structure and the halides I and Br are in orthorhombic (Cmce) structure.

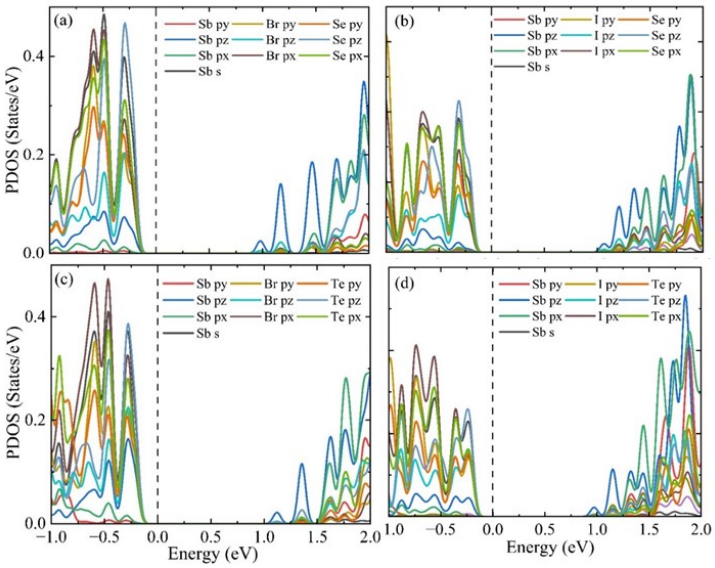
Material	Crystal system	Chemical potential(eV)
Sb	Trigonal(R3m)	-4.43
I	Orthorhombic(Cmce)	-1.60
Br	Orthorhombic(Cmce)	-1.58
Te	Trigonal(P3_121)	-3.35
Se	Trigonal(P3_121)	-3.66



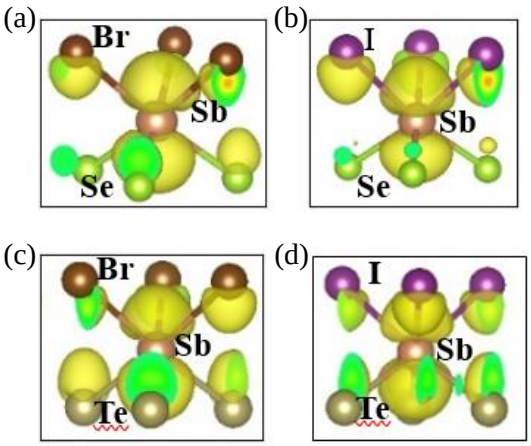
SFig. 5: The electronic band structure of SbSeBr (a) SbSeI (b), SbTeBr (c) and SbTeI (d) Janus structures at GGA(black) and GGA+SOC results (red). The dashed line represents Fermi energy level



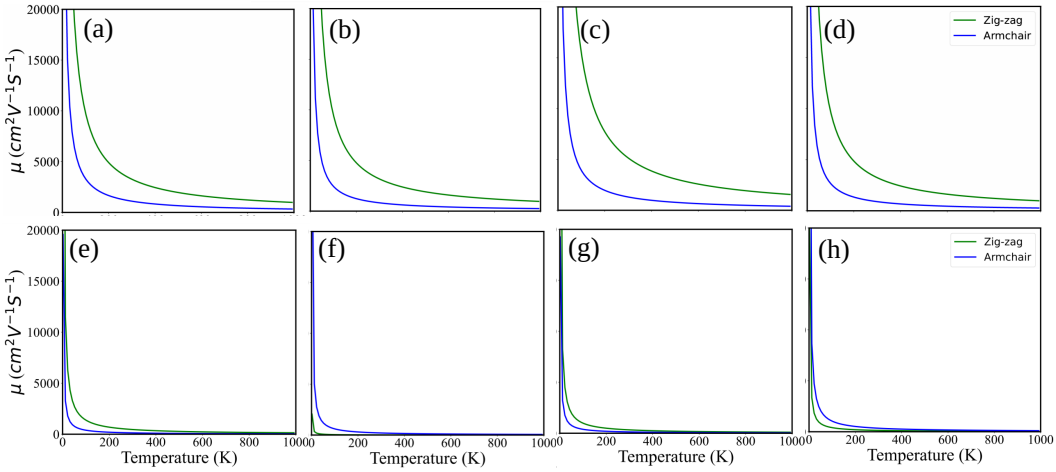
SFig. 6: The electronic band structure of SbSeBr (a) SbSeI (b), SbTeBr (c) and SbTeI (d) Janus structures calculated using hybrid functional HSE. The dashed line represents Fermi energy level.



SFig. 7: The electronic density of states of SbSeBr (a) SbSeI (b), SbTeBr (c) and SbTeI (d) Janus structures at GGA level.



SFig. 8: The partial charge density calculated at the CBM of SbSeBr (a) SbSeI (b), SbTeBr (c), and SbTeI (d) Janus structures. The yellow colour represents electron accumulation. The green areas solely denote cross sections of yellow areas with the plane of the picture.



SFig. 9: Illustration of mobility variation of charge carriers with temperature. The mobility of electrons and holes in the SbSeBr (a) and (e), SbSeI (b) and (f), SbTeBr (c) and (g), SbTeI (d) and (h) are presented.

STab. 4: The excitonic binding energy (E_b) calculated along x and y direction and the dielectric constant (ϵ_r) of SbXY Janus structures using classical Mott-Wannier model.

	E_b (eV)		
Structure	x	y	ϵ_r
SbSeBr	0.047	0.048	3.76
SbSeI	0.062	0.042	4.32
SbTeBr	0.036	0.036	4.26
SbTeI	0.044	0.036	4.89