

## Supporting Information

# Tuning of the electronic, photocatalytic and optical properties of Janus $XWAZ_2$ ( $X=S, Se, Te$ ; $A = Si, Ge$ ; $Z=N, P, As$ ) monolayers *via* strain and external electric field

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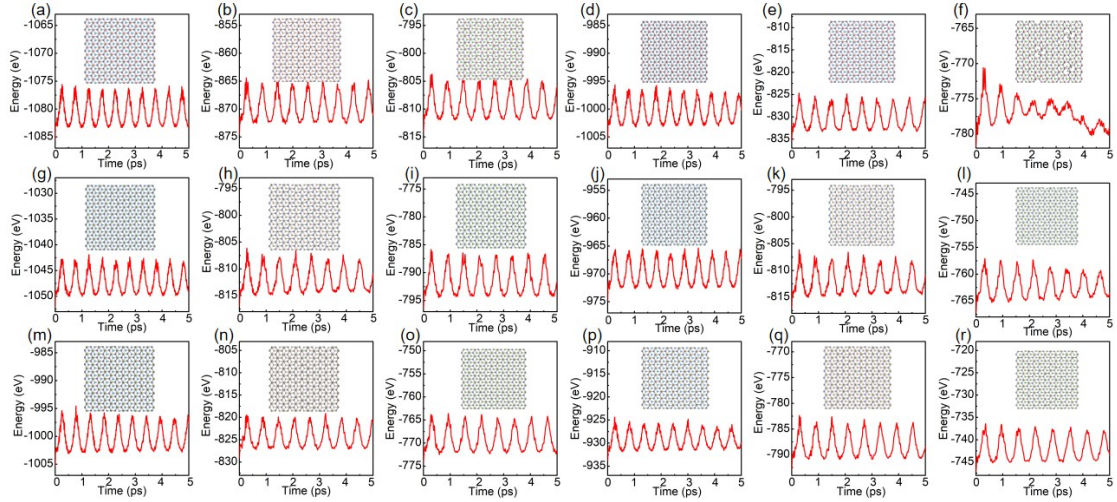


Fig S1 Variation of the energy as a function of time for the Janus (a)SWSiN<sub>2</sub>, (b)SWSiP<sub>2</sub>, (c)SWSiAs<sub>2</sub>, (d)SWGeN<sub>2</sub>, (e)SWGeP<sub>2</sub>, (f)SWGeAs<sub>2</sub>, (g)SeWSiN<sub>2</sub>, (h)SeWSiP<sub>2</sub>, (i)SeWSiAs<sub>2</sub>, (j)SeWGeN<sub>2</sub>, (k)SeWGeP<sub>2</sub>, (l)SeWGeAs<sub>2</sub>, (m)TeWSiN<sub>2</sub>, (n)TeWSiP<sub>2</sub>, (o)TeWSiAs<sub>2</sub>, (p)TeWGeN<sub>2</sub>, (q)TeMoGeP<sub>2</sub> and (r)TeWGeAs<sub>2</sub> monolayer monolayers at 300K. The insets are the top view of the structure at the end of the AIMD simulation.

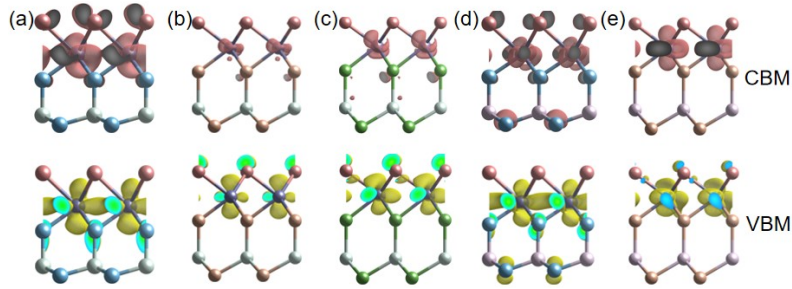


Fig S2 The charge density of the CBM and VBM of (a)SWSiN<sub>2</sub>, (b)SWSiP<sub>2</sub>, (c)SWSiAs<sub>2</sub>, (d)SWGeN<sub>2</sub>, and (e)SWGeP<sub>2</sub> monolayers. The CBM and VBM are marked in red and yellow, respectively. The isosurface values of SWAZ<sub>2</sub> monolayers are taken as 0.015 eÅ<sup>-3</sup>.

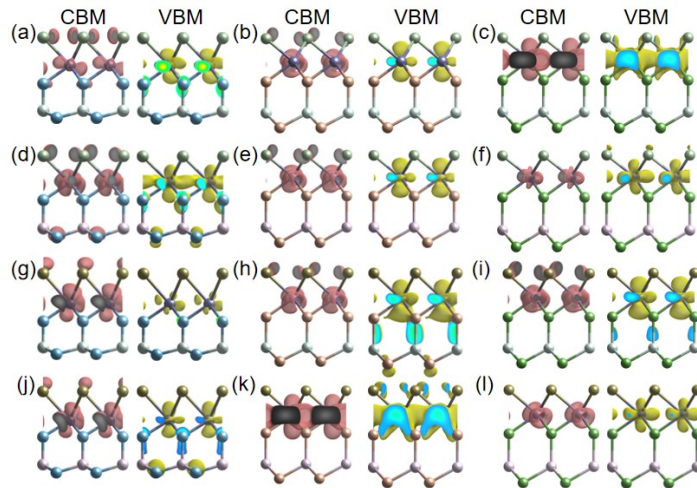


Fig S3 The charge density of the CBM and VBM of (a)SeWSiN<sub>2</sub>, (b)SeWSiP<sub>2</sub>, (c)SeWSiAs<sub>2</sub>, (d)SeWGeN<sub>2</sub>, (e)SeWGeP<sub>2</sub>, (f)SeWGeAs<sub>2</sub>, (g)TeWSiN<sub>2</sub>, (h)TeWSiP<sub>2</sub>, (i)TeWSiAs<sub>2</sub>, (j)TeWGeN<sub>2</sub>, (k)TeMoGeP<sub>2</sub> and (l)TeWGeAs<sub>2</sub> monolayers. The CBM and VBM are marked in red and yellow, respectively. The isosurface values of SWAZ<sub>2</sub> monolayers are taken as 0.015 eÅ<sup>-3</sup>.

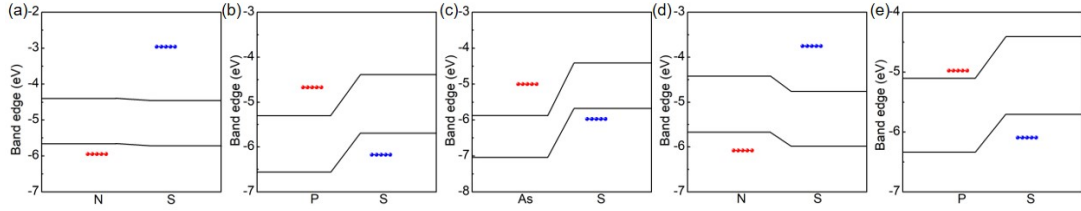


Fig S4 Band alignments with regard to the vacuum level of pristine (a) SWSiN<sub>2</sub>, (b) SWSiP<sub>2</sub>, (c) SWSiAs<sub>2</sub>, (d) SWGeN<sub>2</sub> and (e) SWGeP<sub>2</sub> under the HSE06 functional.

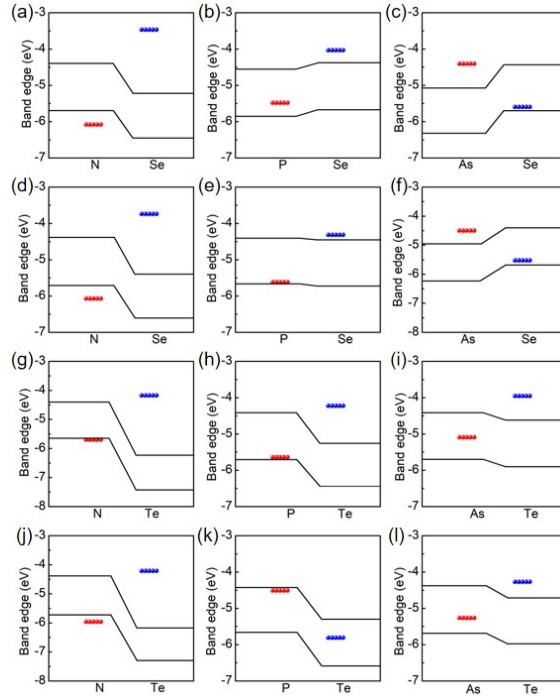


Fig S5 Band alignments with regard to the vacuum level of pristine (a) SeWSiN<sub>2</sub>, (b) SeWSiP<sub>2</sub>, (c) SeWSiAs<sub>2</sub>, (d) SeWGeN<sub>2</sub>, (e) SeWGeP<sub>2</sub>, (f) SeWGeAs<sub>2</sub>, (g) TeWSiN<sub>2</sub>, (h) TeWSiP<sub>2</sub>, (i) TeWSiAs<sub>2</sub>, (j) TeWGeN<sub>2</sub>, (k) TeMoGeP<sub>2</sub> and (l) TeWGeAs<sub>2</sub> monolayers under the HSE06 functional.

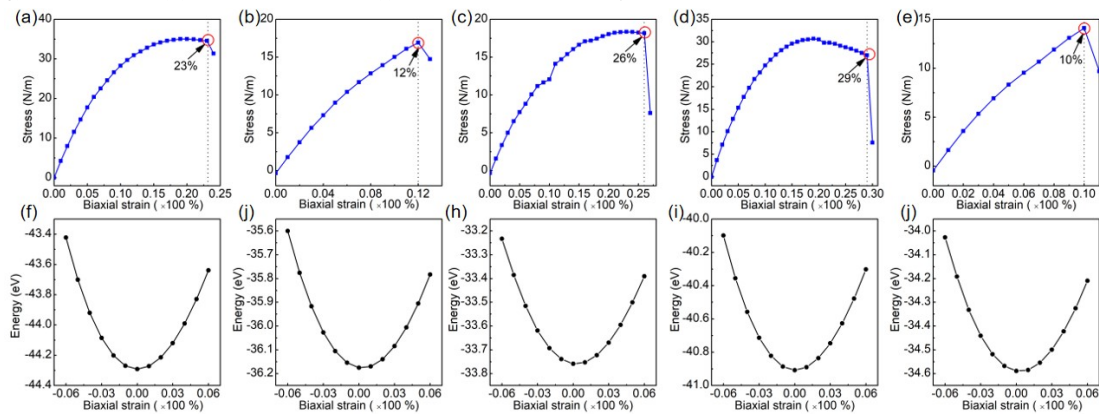


Fig S6 (a-e) Strain-stress curve and (f-j) energy-strain curves for 2D Janus SWSiN<sub>2</sub>, SWSiP<sub>2</sub>, SWSiAs<sub>2</sub>, SWGeN<sub>2</sub> and SWGeP<sub>2</sub> monolayers.

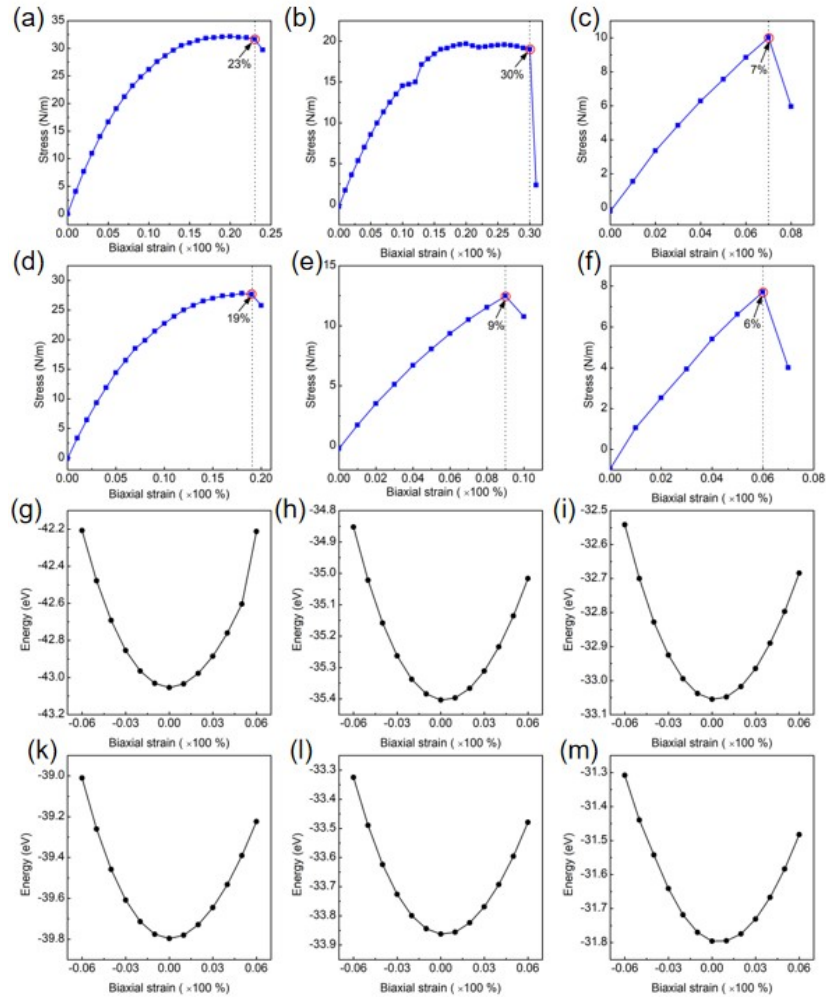


Fig S7 (a-f) Strain-stress curve and (g-m) energy-strain curves for 2D Janus  $\text{SeWSiN}_2$ ,  $\text{SeWSiP}_2$ ,  $\text{SeWSiAs}_2$ ,  $\text{SeWGeN}_2$ ,  $\text{SeWGeP}_2$ , and  $\text{SeWGeAs}_2$  monolayers.

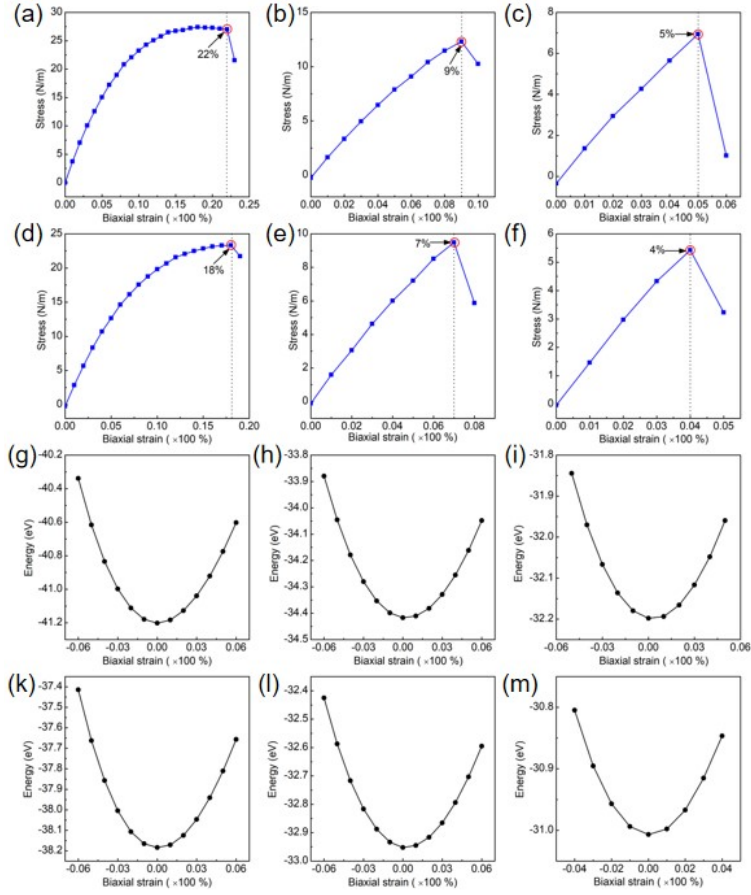


Fig S8 (a-f) Strain-stress curve and (g-m) energy-strain curves for 2D Janus TeWSiN<sub>2</sub>, TeWSiP<sub>2</sub>, TeWSiAs<sub>2</sub>, TeWGeN<sub>2</sub>, TeWGeP<sub>2</sub>, and TeWGeAs<sub>2</sub> monolayers.

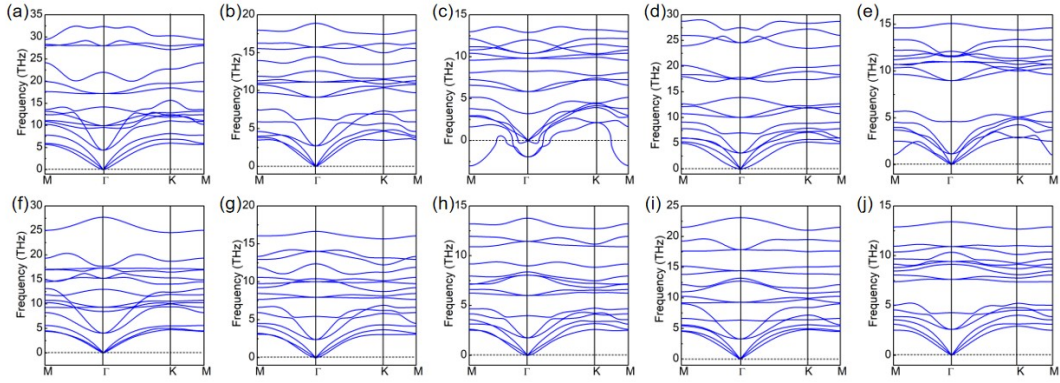


Fig S9 Phonon spectrum of SWSiN<sub>2</sub>, SWSiP<sub>2</sub>, SWSiAs<sub>2</sub>, SWGeN<sub>2</sub>, and SWGeP<sub>2</sub> monolayers under strain of (a-e) -6% and (f-j) +6%, respectively.



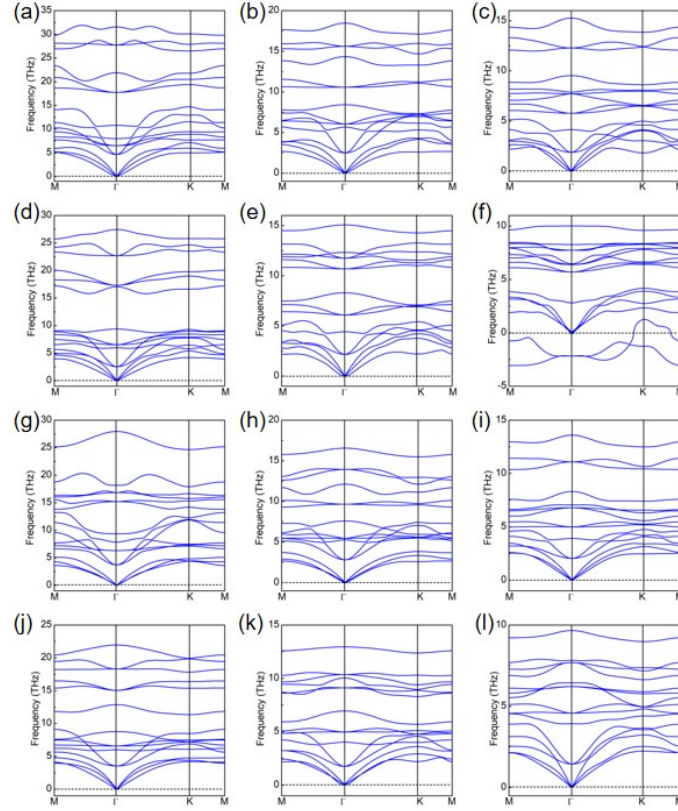


Fig S10 Phonon spectrum of  $\text{SeWSiN}_2$ ,  $\text{SeWSiP}_2$ ,  $\text{SeWSiAs}_2$ ,  $\text{SeWGeN}_2$ ,  $\text{SeWGeP}_2$  and  $\text{SeWGeAs}_2$  monolayers under strain of (a-f) -6% and (g-l) +6%, respectively.

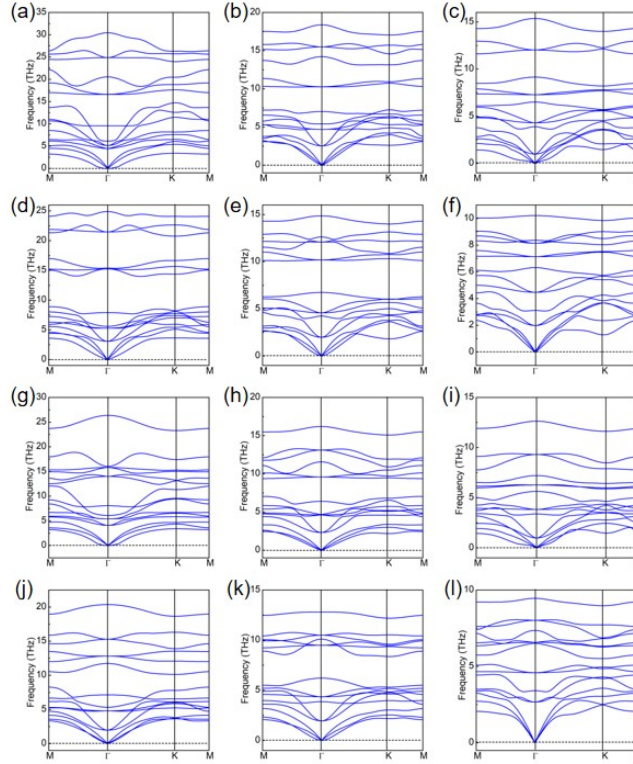


Fig S11 Phonon spectrum of  $\text{TeWSiN}_2$ ,  $\text{TeWSiP}_2$ ,  $\text{TeWGeN}_2$ , and  $\text{TeWGeP}_2$  monolayers under strain of (a, b, d, e) -6% and (g, h, j, k) +6%, respectively.  $\text{TeWSiAs}_2$  monolayer under strain of (c) -5% and (i) +5%.  $\text{TeWGeAs}_2$  monolayer under strain of (f) -4% and (l) +5%.

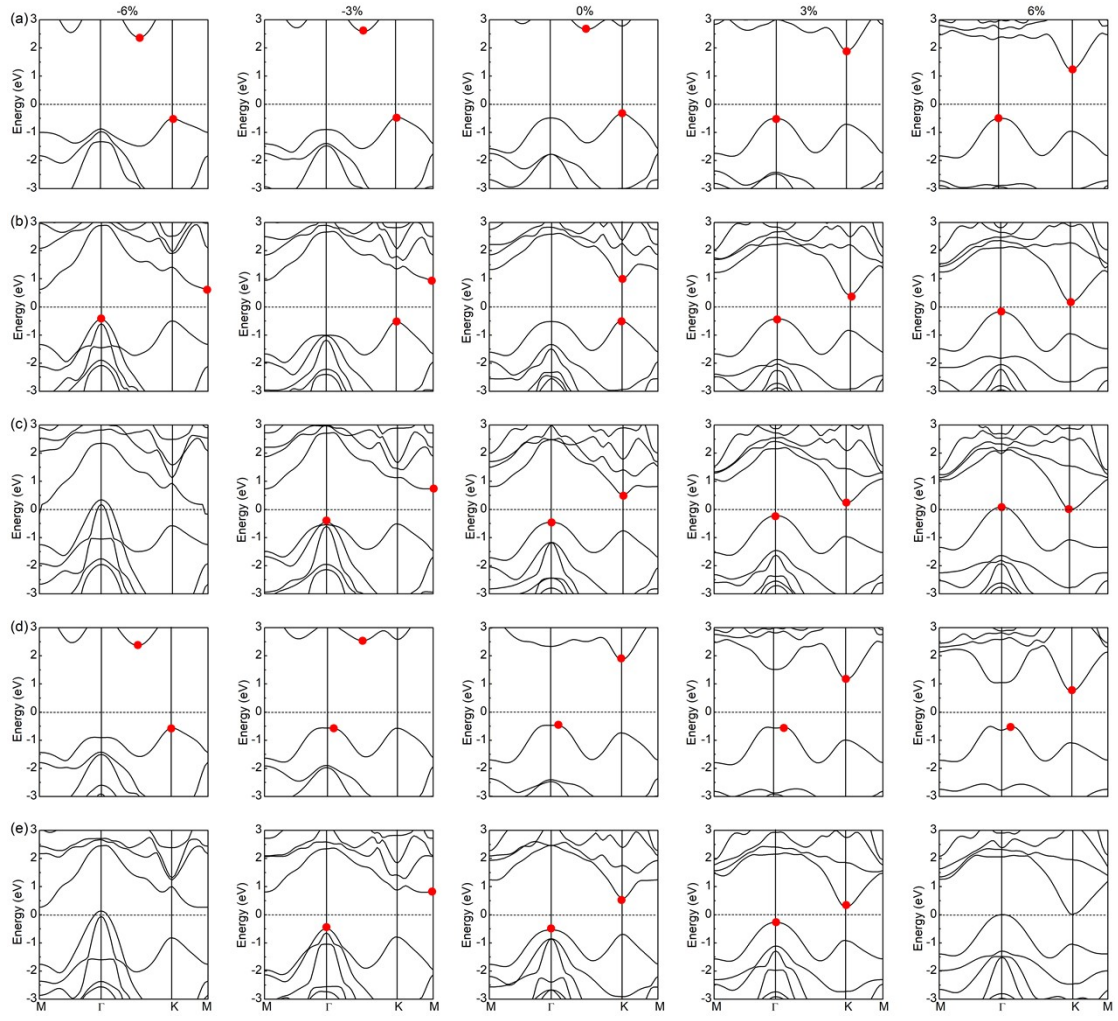


Fig S12 Band structure under biaxial strain of 2D Janus (a) SWSiN<sub>2</sub>, (b) SWSiP<sub>2</sub>, (c) SWSiAs<sub>2</sub>, (d) SWGeN<sub>2</sub> and (e) SWGeP<sub>2</sub> monolayers.

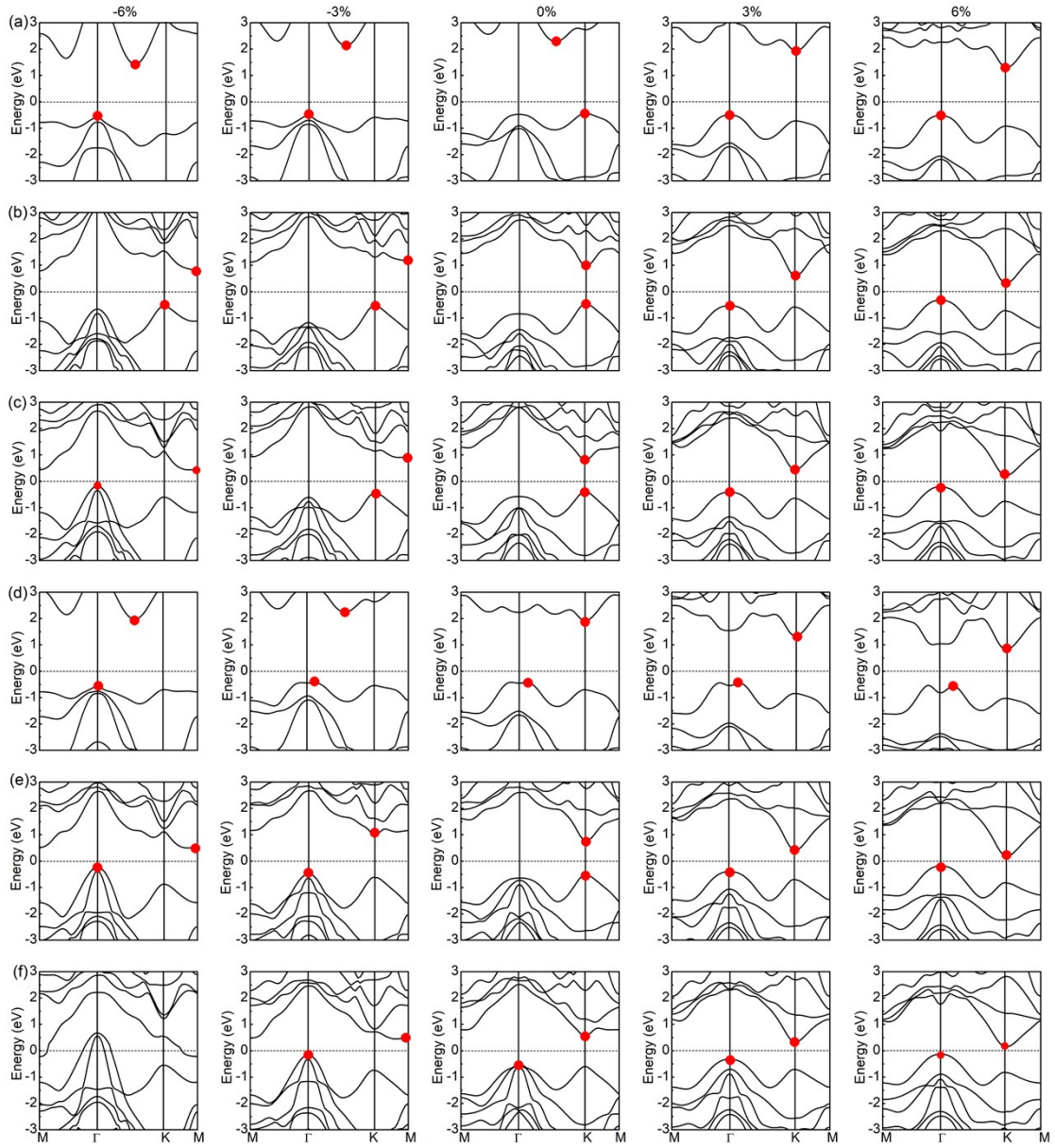


Fig S13 Band structure under biaxial strain of 2D Janus (a) SeWSiN<sub>2</sub>, (b) SeWSiP<sub>2</sub>, (c) SeWSiAs<sub>2</sub>, (d) SeWGeN<sub>2</sub>, (e) SeWGeP<sub>2</sub> and (f) SeWGeAs<sub>2</sub> monolayers.



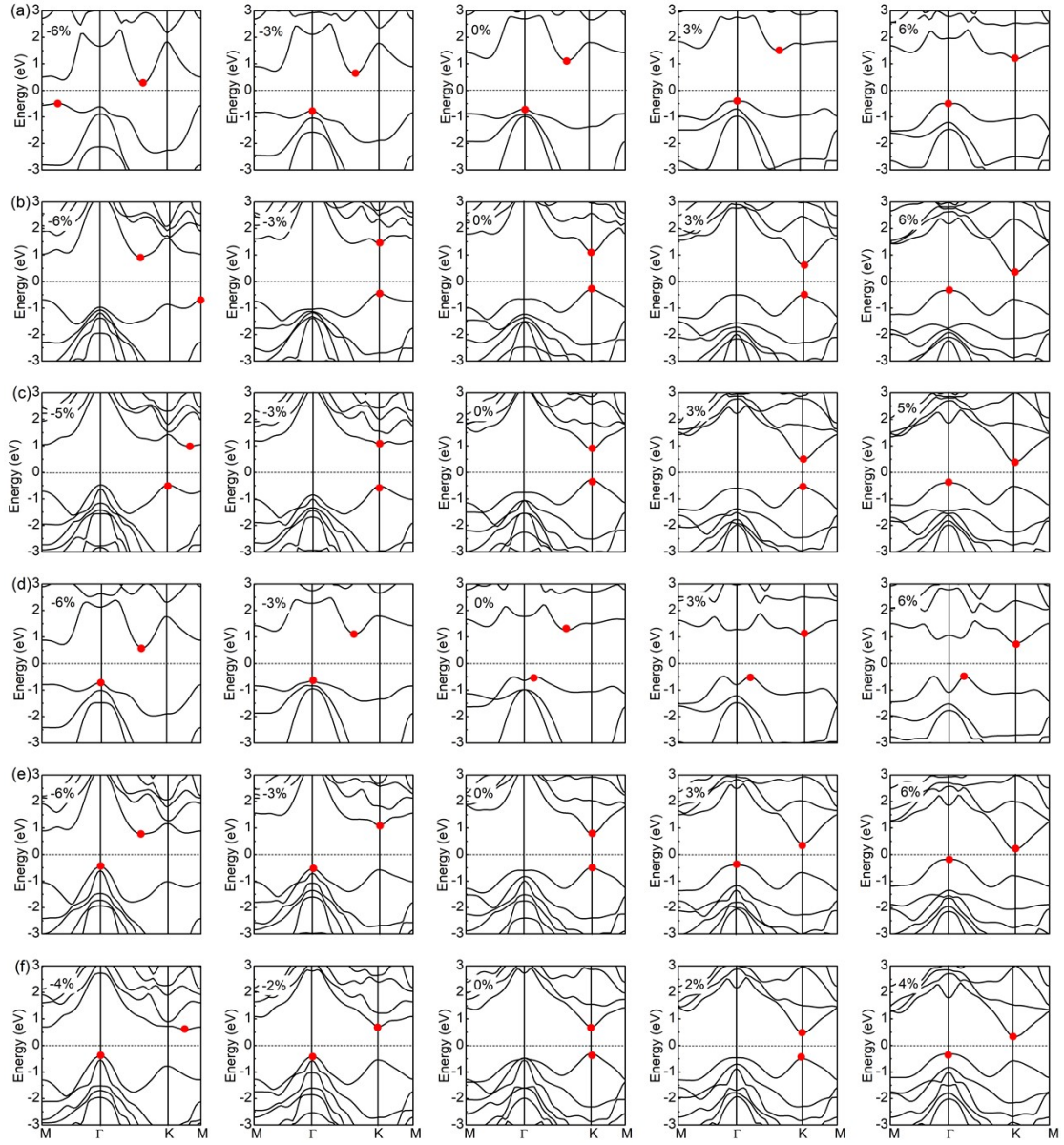


Fig S14 Band structure under biaxial strain of 2D Janus (a) TeWSiN<sub>2</sub>, (b) TeWSiP<sub>2</sub>, (c) TeWSiAs<sub>2</sub>, (d) TeWGeN<sub>2</sub>, (e) TeWGeP<sub>2</sub> and (f) TeWGeAs<sub>2</sub> monolayers.

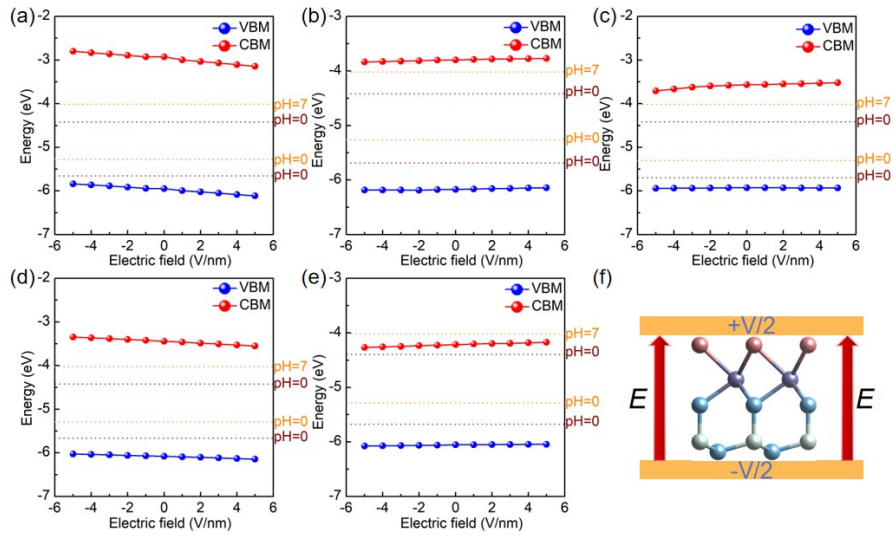


Fig S15 Band alignments of Janus (a) SWSiN<sub>2</sub>, (b) SWSiP<sub>2</sub>, (c) SWSiAs<sub>2</sub>, (d) SWGeN<sub>2</sub>, and (e) SWGeP<sub>2</sub> under external electric field. (f) The top view of Janus XWAZ<sub>2</sub> (X=S, Se, Te; A=Si, Ge; Z=N, P, As) under external electric field.

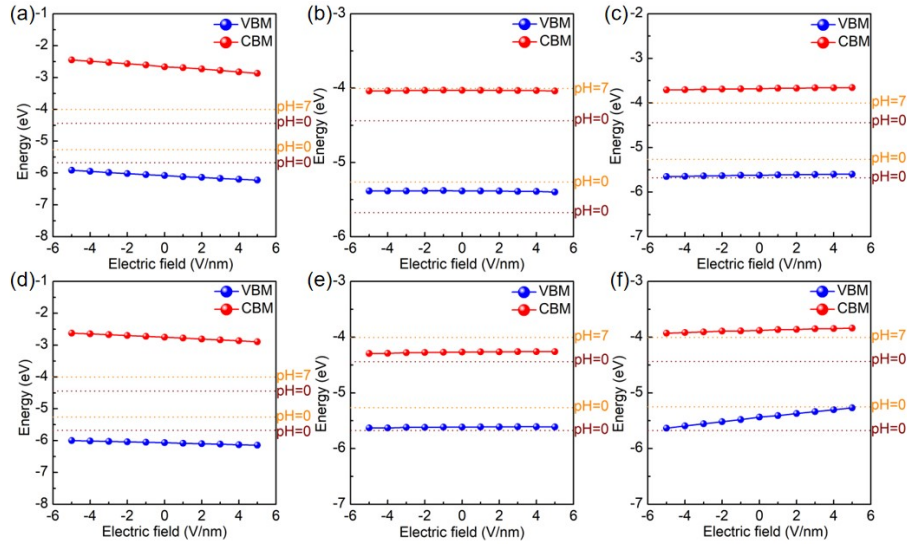


Fig S16 Band alignments of Janus (a) SeWSiN<sub>2</sub>, (b) SeWSiP<sub>2</sub>, (c) SeWSiAs<sub>2</sub>, (d) SeWGeN<sub>2</sub>, (e) SeWGeP<sub>2</sub>, and (f) SeWGeAs<sub>2</sub> under external electric field.

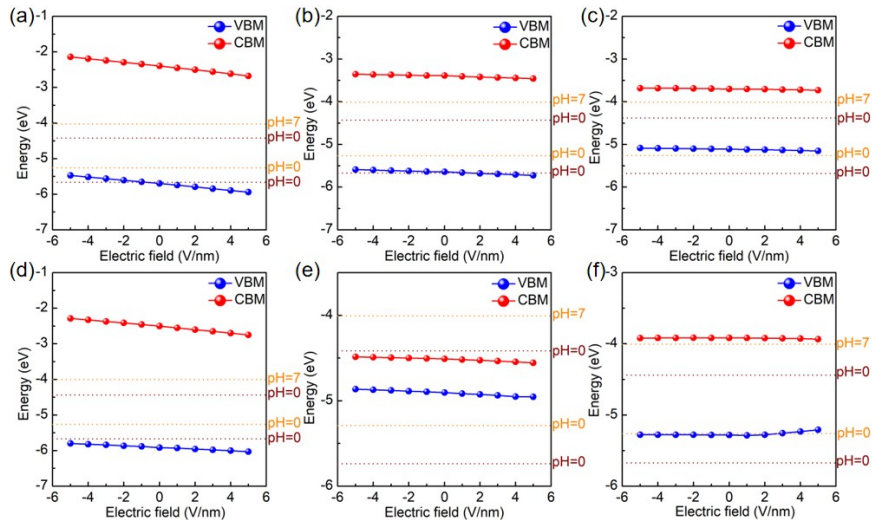


Fig S17 Band alignments of Janus (a) TeWSiN<sub>2</sub>, (b) TeWSiP<sub>2</sub>, (c) TeWSiAs<sub>2</sub>, (d) TeWGeN<sub>2</sub>, (e) TeWGeP<sub>2</sub>, and (f) TeWGeAs<sub>2</sub> under external electric field.

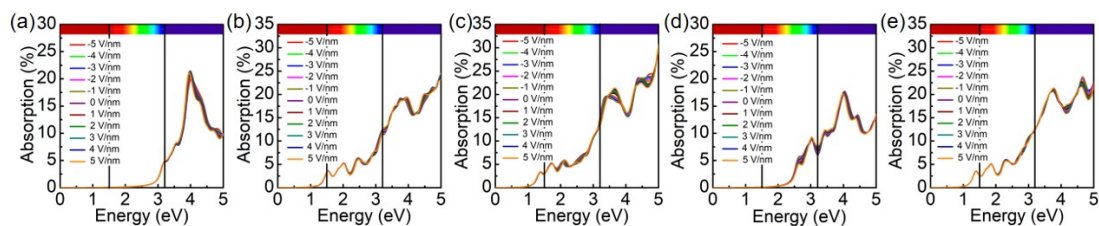


Fig S18 The light absorption of Janus (a) SWSiN<sub>2</sub>, (b) SWSiP<sub>2</sub>, (c) SWSiAs<sub>2</sub>, (d) SWGeN<sub>2</sub>, and (e) SWGeP<sub>2</sub> with external electric field.

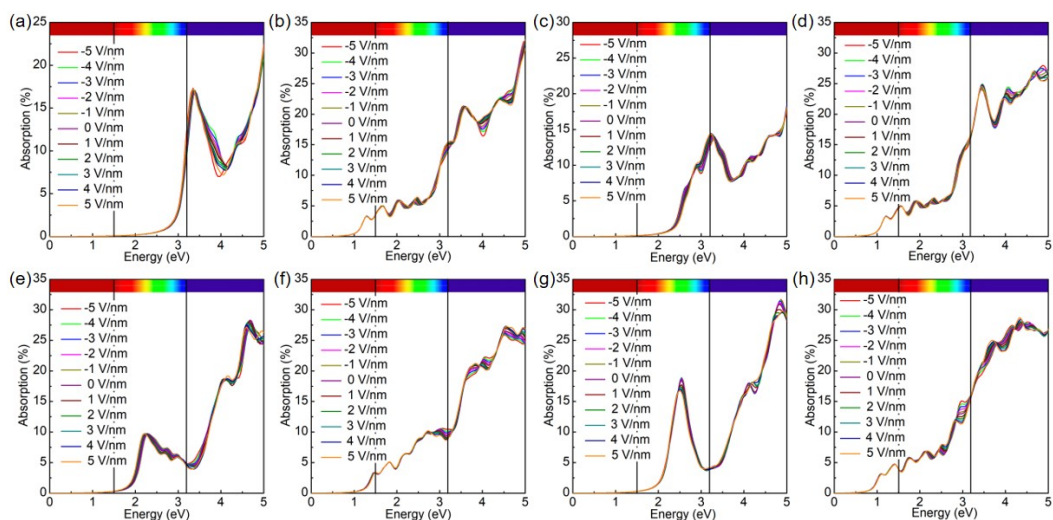


Fig S19 The light absorption of Janus (a) SeWSiN<sub>2</sub>, (b) SeWSiAs<sub>2</sub>, (c) SeWGeN<sub>2</sub>, (d) SWGeAs<sub>2</sub>, (e) TeWSiN<sub>2</sub>, (f) TeWSiP<sub>2</sub>, (g) TeWGeN<sub>2</sub>, and (h) TeWGeAs<sub>2</sub> with external electric field.