

Supporting Information

Strain and electric field induced electronic properties modifications in two-dimensional Janus SZrAZ₂ (A = Si, Ge; Z= P, As) monolayers

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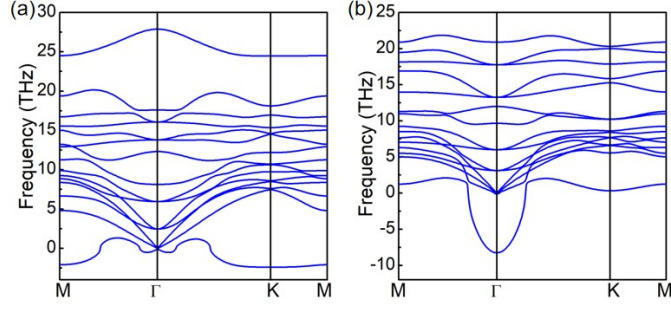


Fig S1 Phonon dispersions of the (a) SZrSiN₂ and (b) SZrGeN₂ monolayers, respectively.

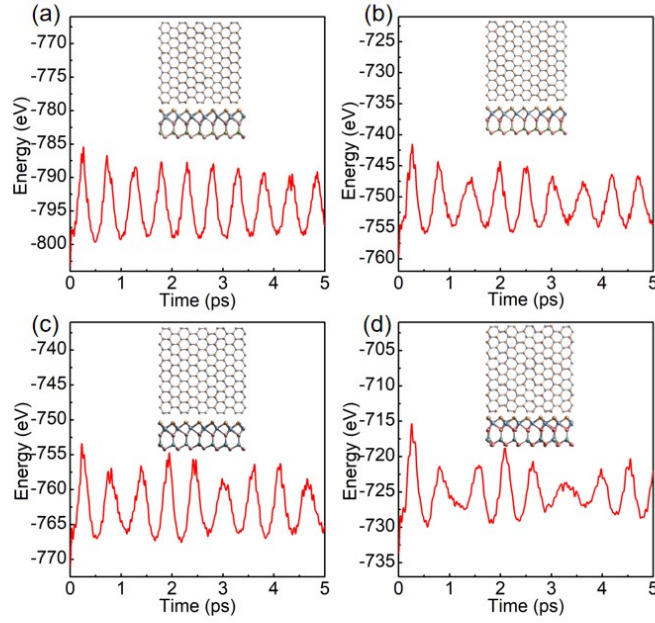


Fig S2 Variation of the energy as a function of time for the Janus (a)SZrSiP₂, (b)SZrSiAs₂, (c)SZrGeP₂, and (d)SMOGeAs₂ monolayers at 500K. The insets are the top and side views of the structure at the end of the AIMD simulation.

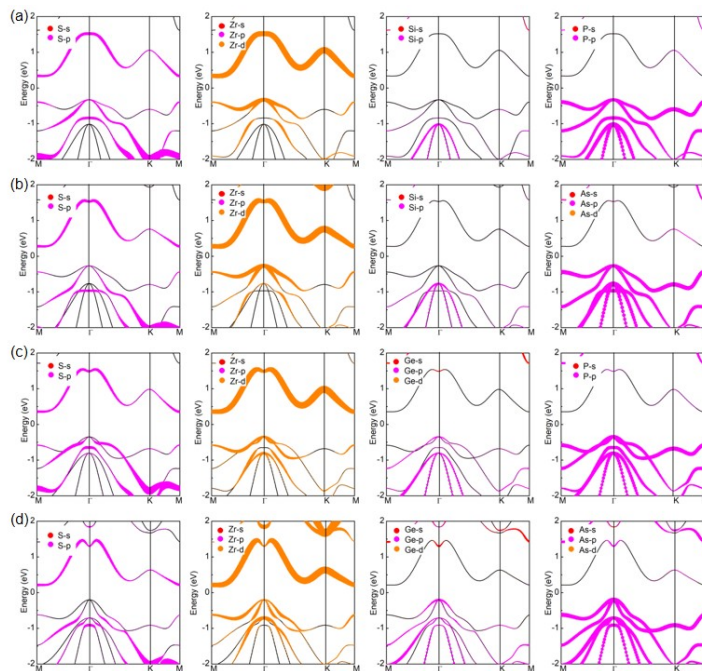


Fig S3 Projected band structure of 2D Janus (a) SZrSiP₂, (b) SZrSiAs₂, (c) SZrGeP₂ and (d) SMOGeAs₂ monolayers.

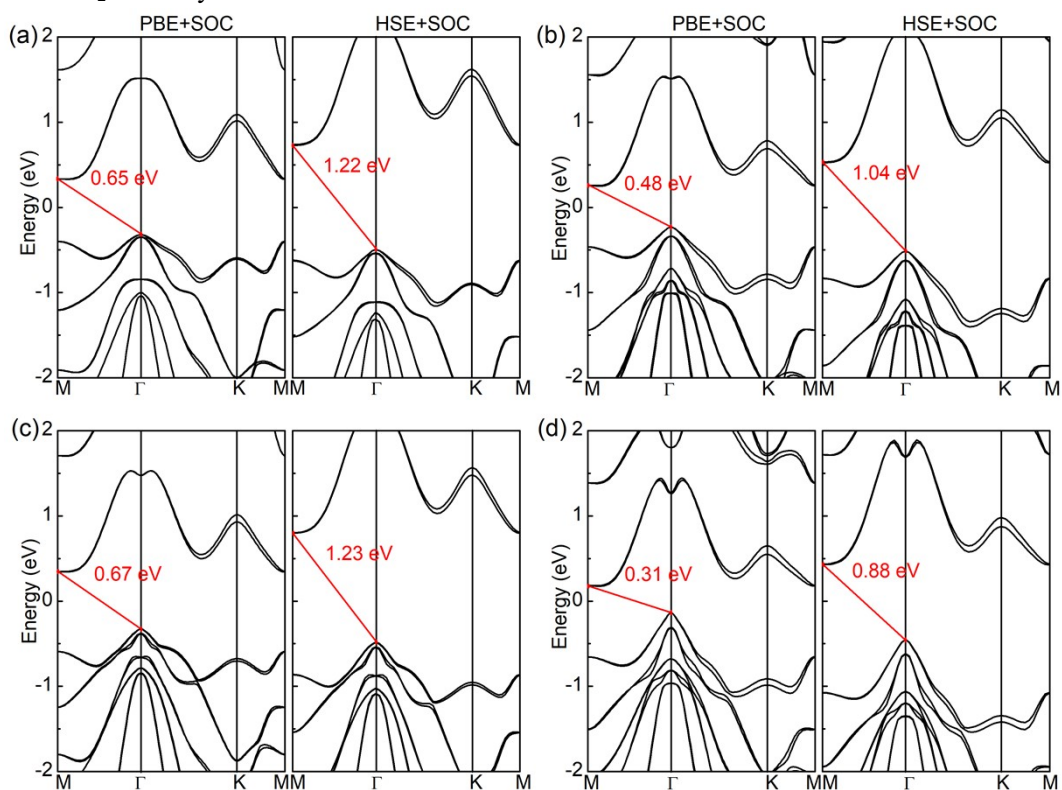


Fig. S4 Electronic band structure of 2D Janus (a) SZrSiP₂, (b) SZrSiAs₂, (c) SZrGeP₂, and (d) SZrGeAs₂ by PBE+SOC and HSE06+SOC methods.

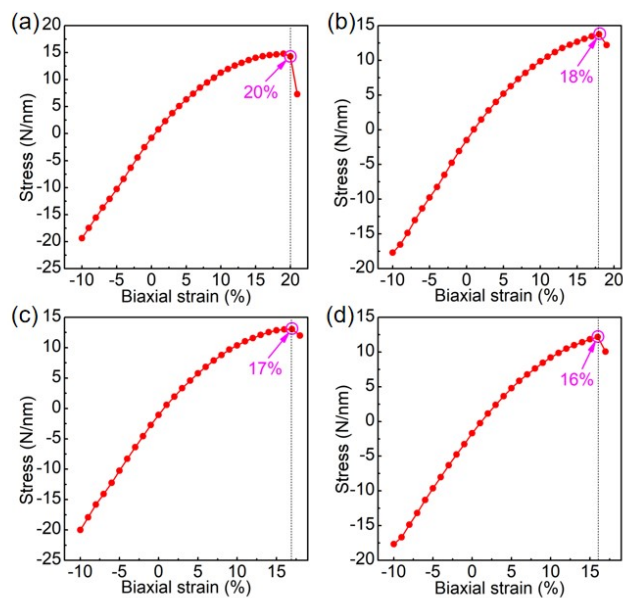


Fig S5 strain-stress curve for 2D Janus (a) SZrSiP₂, (b) SZrSiAs₂, (c) SZrGeP₂ and (d) SZrGeAs₂ monolayers.

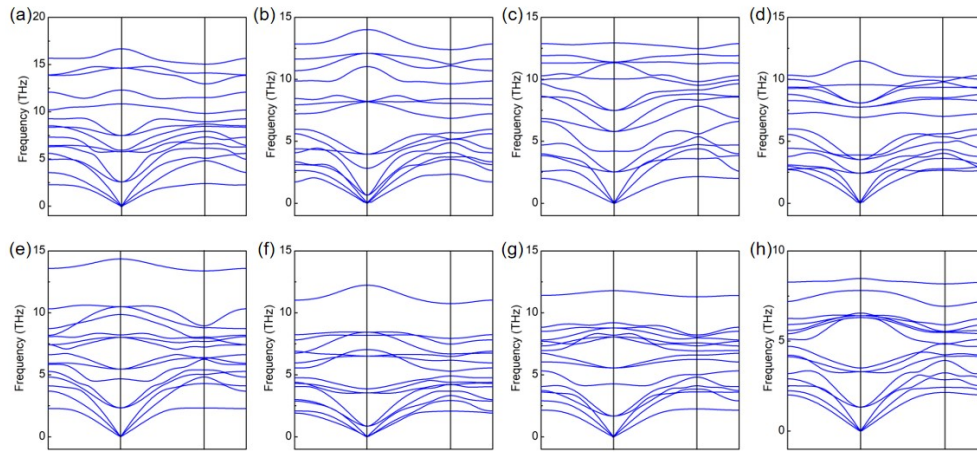


Fig S6 Phonon spectrum of SZrSiP_2 , SZrSiAs_2 , SZrGeP_2 , and SZrGeAs_2 monolayers under strain of (a-d) -10% and (e-h) +10%, respectively.

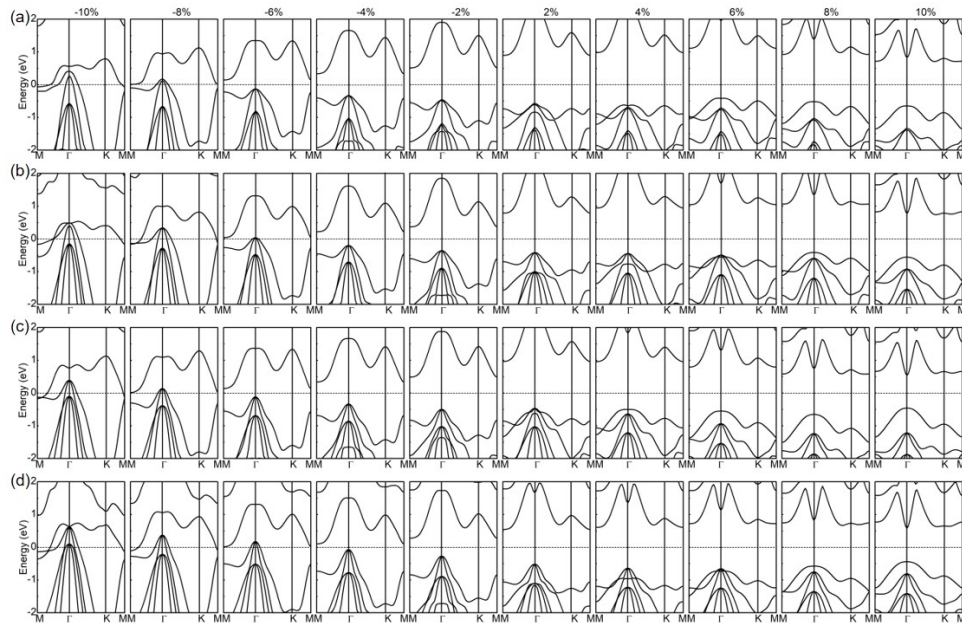


Fig S7 Electronic band structure under biaxial strain of 2D Janus (a) SZrSiP_2 , (b) SZrSiAs_2 , (c) SZrGeP_2 , and (d) SZrGeAs_2 monolayers.

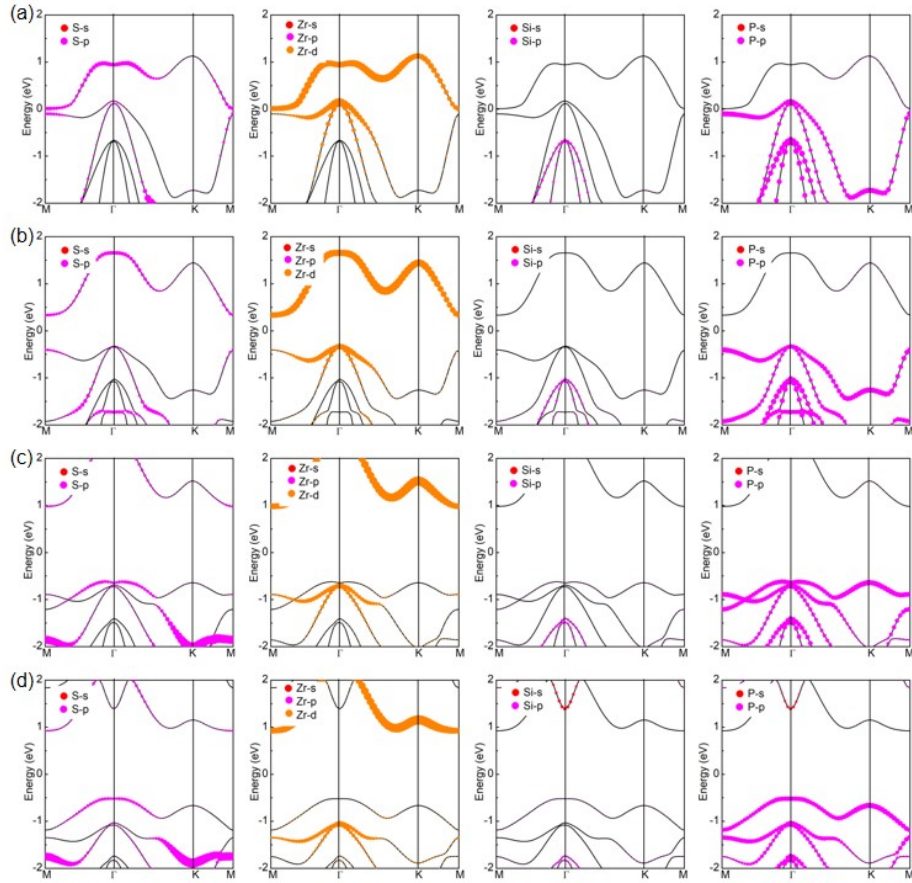


Fig S8 Orbital projected band structures for SZrSiP₂ monolayer under different strengths of different strains of (a) -8%, (b) -4%, (c) 4% and (d) 8%.

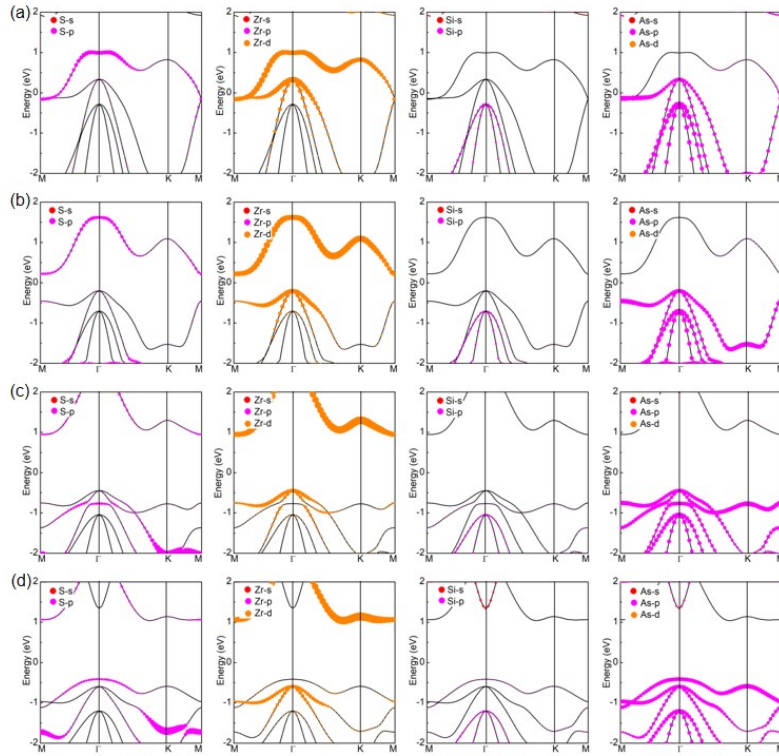


Fig S9 Orbital projected band structures for SZrSiAs₂ monolayer under different strengths of

different strains of (a) -8%, (b) -4%, (c) 4% and (d) 8%.

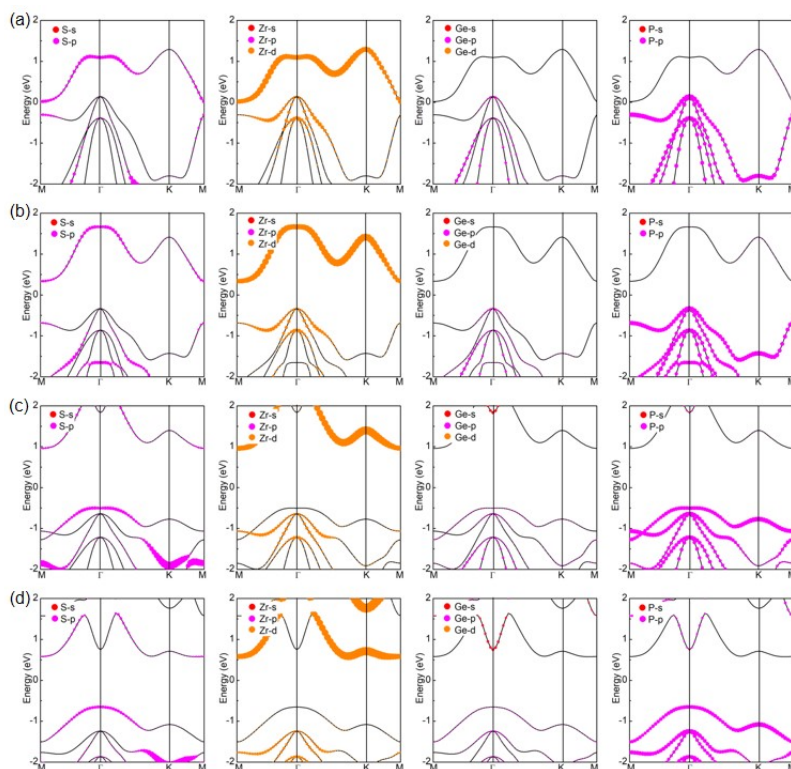


Fig S10 Orbital projected band structures for SZrGeP₂ monolayer under different strengths of different strains of (a) -8%, (b) -4%, (c) 4% and (d) 8%.

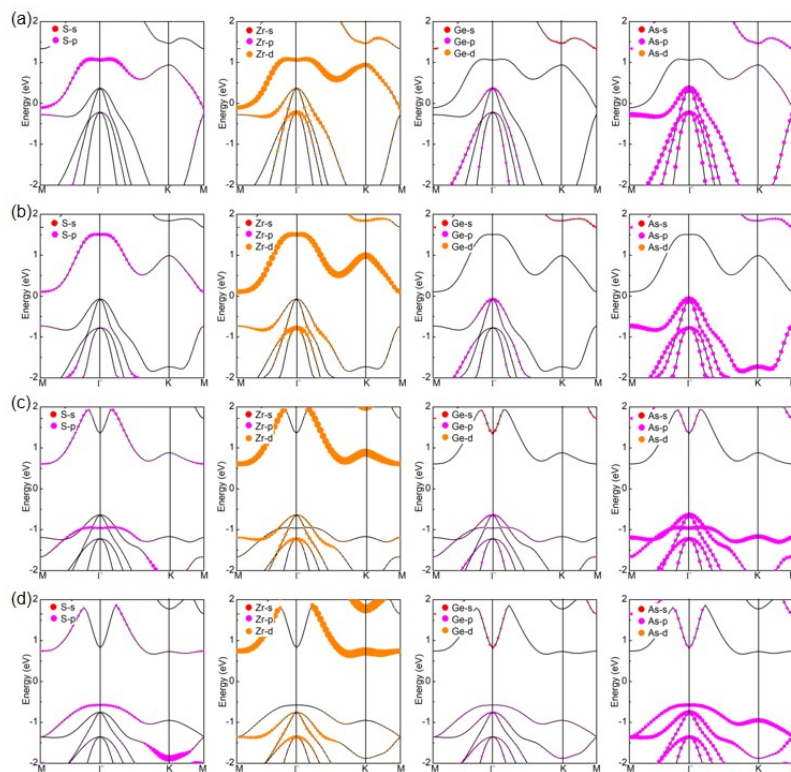


Fig S11 Orbital projected band structures for SZrGeAs₂ monolayer under different strengths of different strains of (a) -8%, (b) -4%, (c) 4% and (d) 8%.

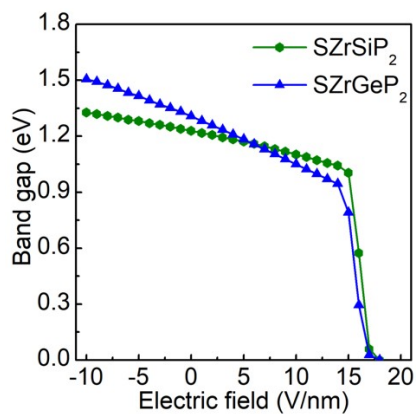


Fig S12 Band gap under external electric field of 2D SZrSiP₂ and SZrGeP₂ by HSE method.

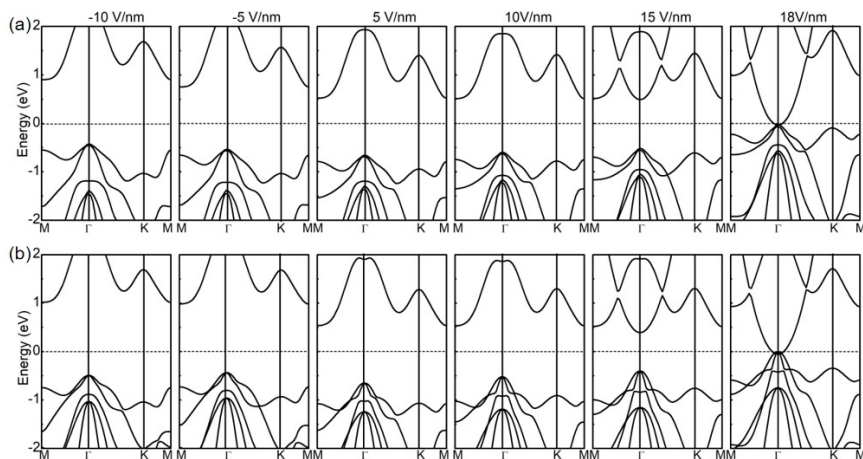


Fig S13 Electronic band structure under electric field of 2D Janus (a) SZrSiP₂, and (b) SZrGeP₂ monolayers.

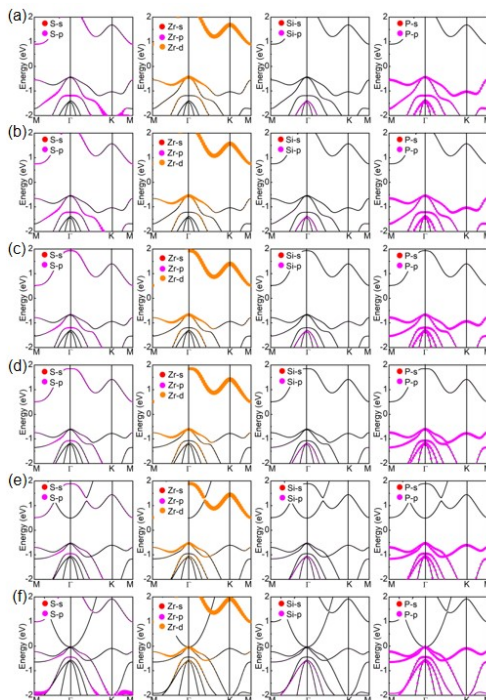


Fig S14 Orbital projected band structures for SZrSiP₂ monolayer under different strengths of different electric field of (a) -10V/nm, (b) -5V/nm, (c) +5V/nm, (d) +10V/nm, (e) +15V/nm and (f)

+18V/nm.

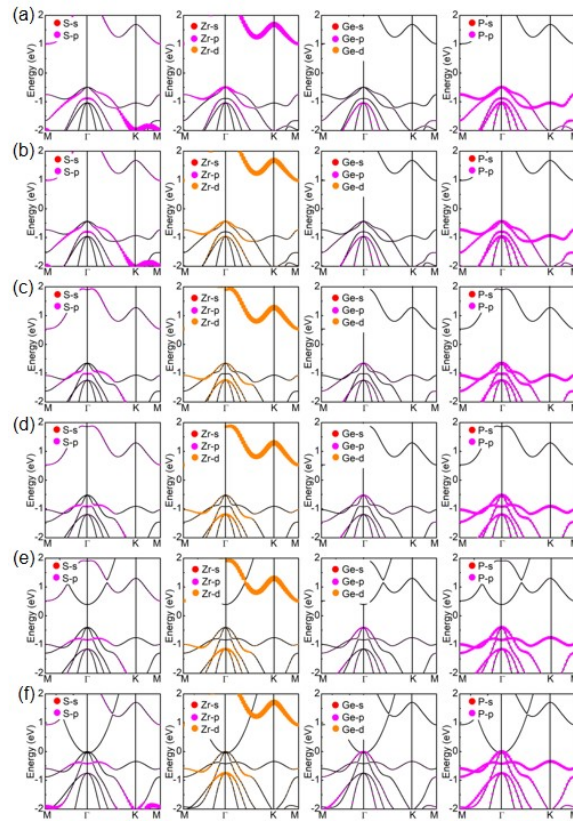


Fig S15 Orbital projected band structures for SZrGeP₂ monolayer under different strengths of different electric field of (a) -10V/nm, (b) -5V/nm, (c) +5V/nm, (d) +10V/nm, (e) +15V/nm and (f) +18V/nm.

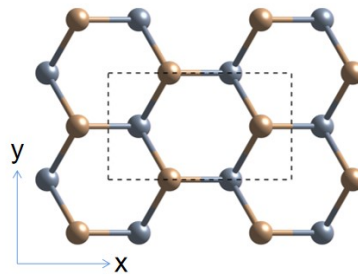


Fig S16 The calculation of carrier mobility is carried out in rectangular cell in the black dotted box, the x and y directions also been indicate.

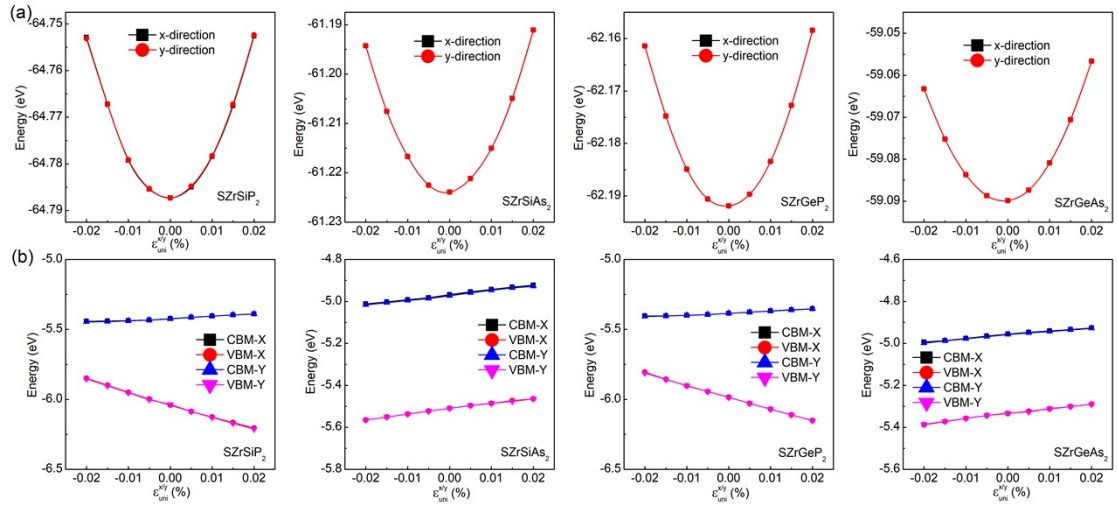


Fig S17 The uniaxial strain $\epsilon_{uni}^{x/y}$ (a) dependent energy shifting (b) CBM/VBM positions (b) of SZrAZ₂ along the two transport directions x and y. The fitting curves are presented by the solid lines.