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

Strain-engineered electronic, valley, and photocatalytic properties in Janus WSiGeZ_4 (Z = N, P, As) monolayers

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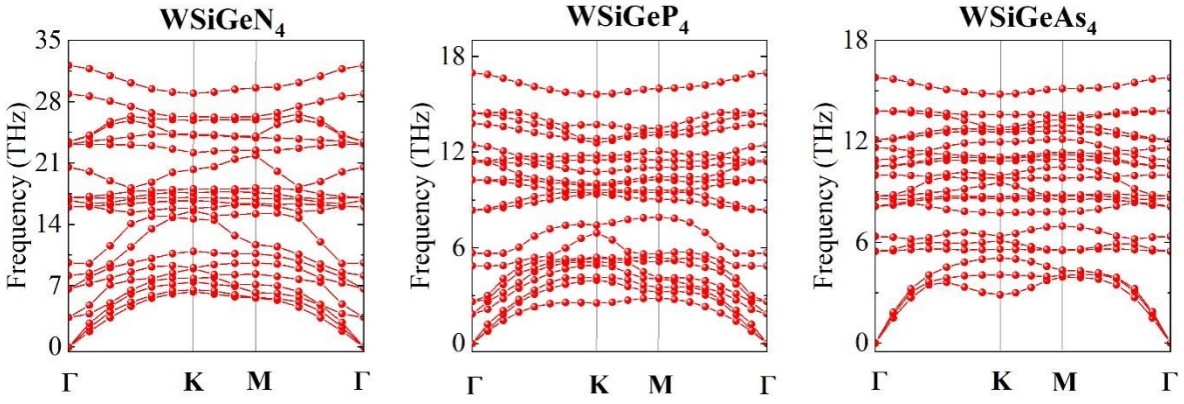

FIG. S1(a) Phonon spectrum of Janus WSiGeZ_4 monolayers.

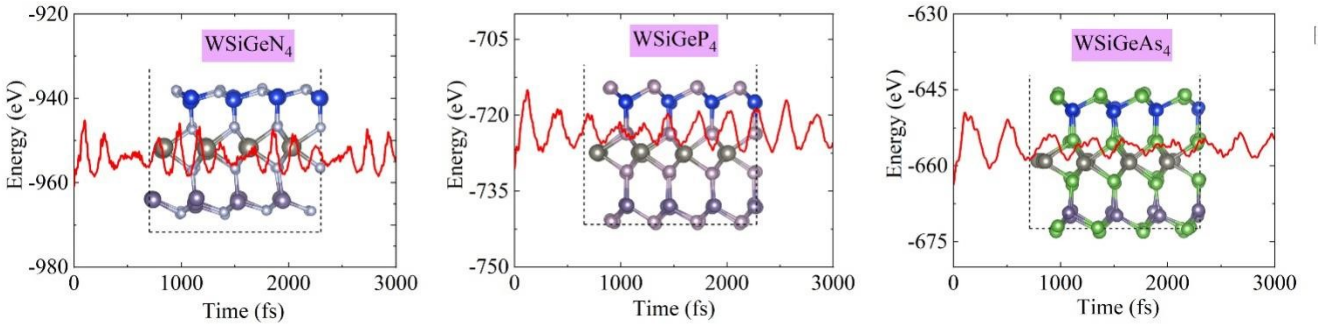

FIG. S2 Side views of Janus WSiGeZ_4 monolayers after AIMD simulations at T = 500 K.

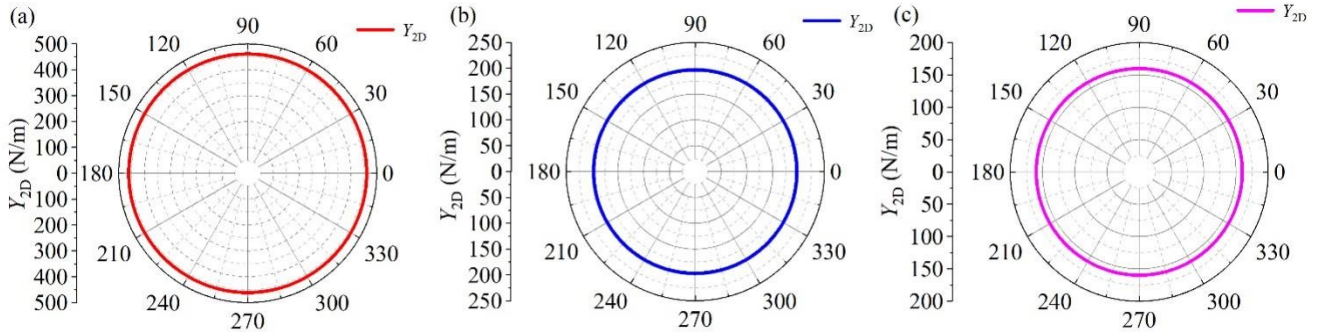

FIG. S3 The 2D Young's modulus of Janus WSiGeZ_4 monolayers.

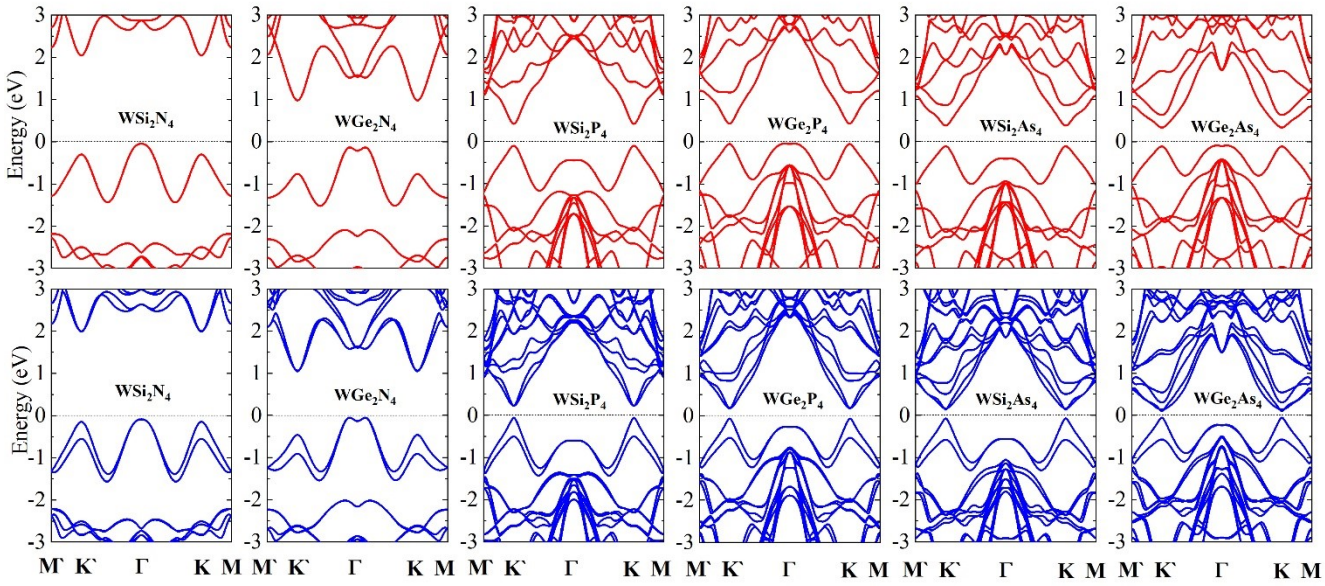

FIG. S4 The band structures of WSi_2Z_4 and WGe_2Z_4 without (red line) and with (blue line) SOC using PBE functional.

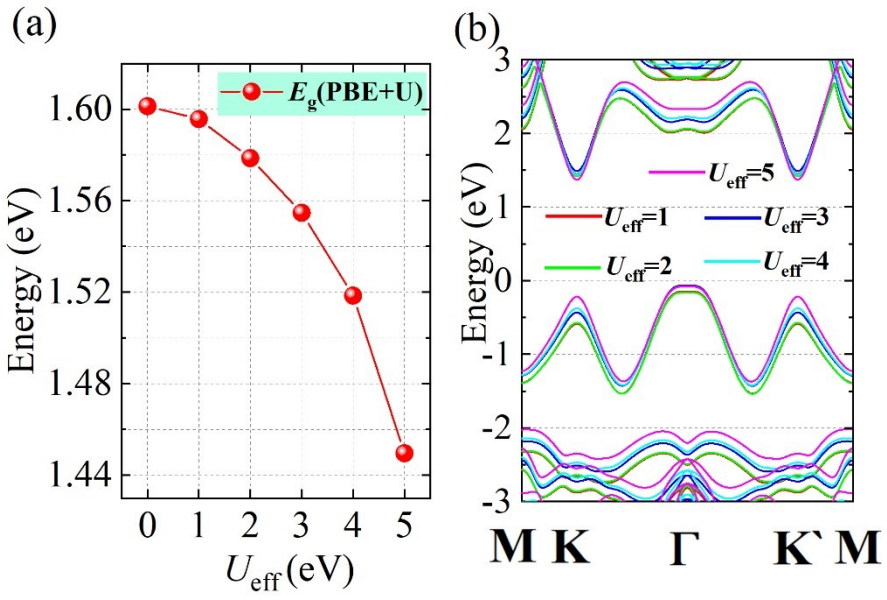

FIG. S5 The band gap (a) and (b) band structure of $WSiGeN_4$ with U_{eff}.

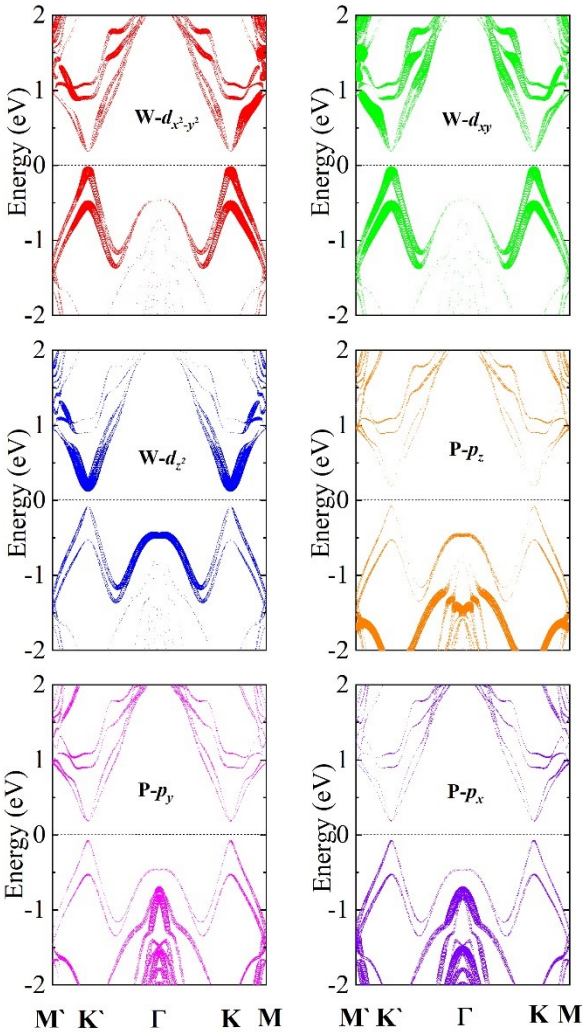

FIG. S7 The orbital projected band structure of $WSiGeP_4$ with SOC using PBE functional. The Fermi level is set at the zero energy and the size of symbol is proportional to the orbital weight.

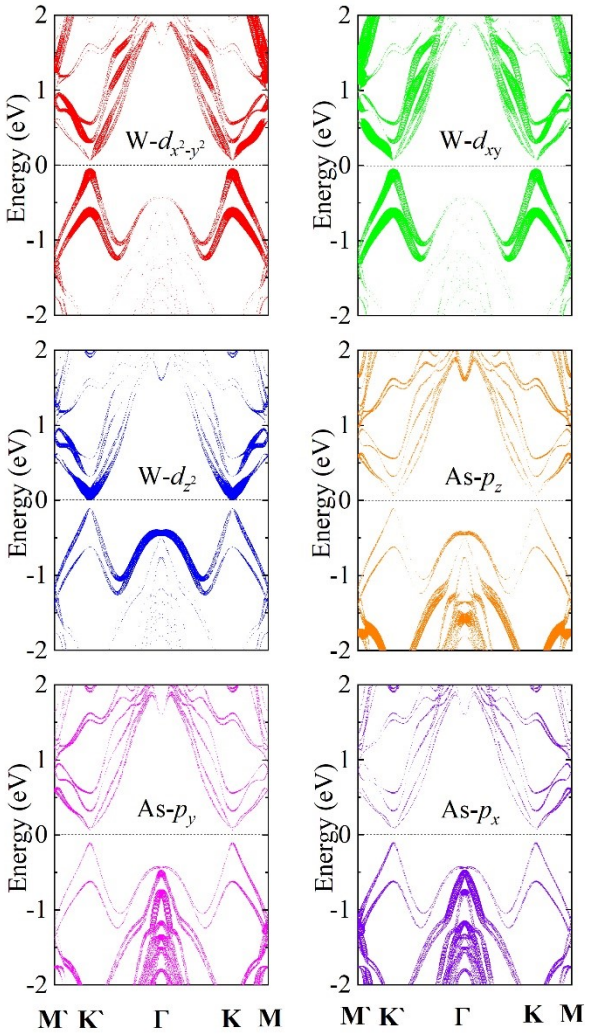

FIG. S8 The orbital projected band structure of $WSiGeAs_4$ with SOC using PBE functional. The Fermi level is set at the zero energy and the size of symbol is proportional to the orbital weight.

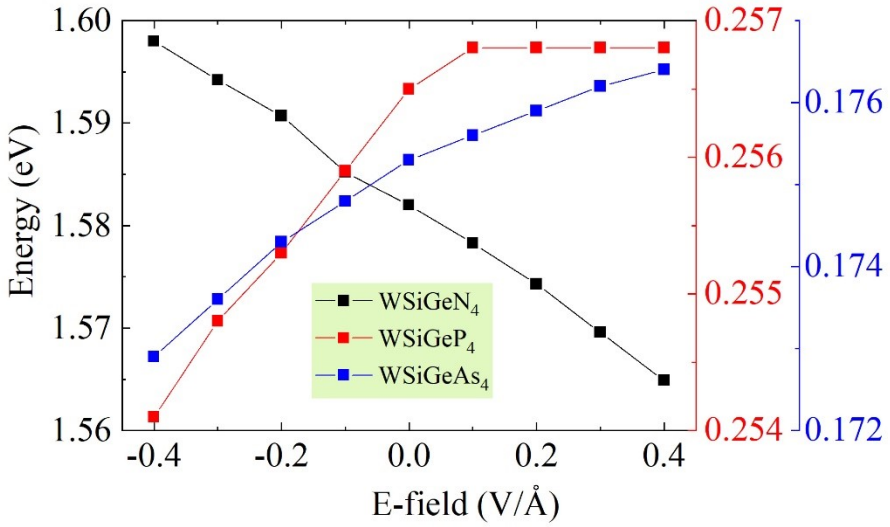

FIG. S9 The band gap of Janus $WSiGeZ_4$ monolayers with external electric field.

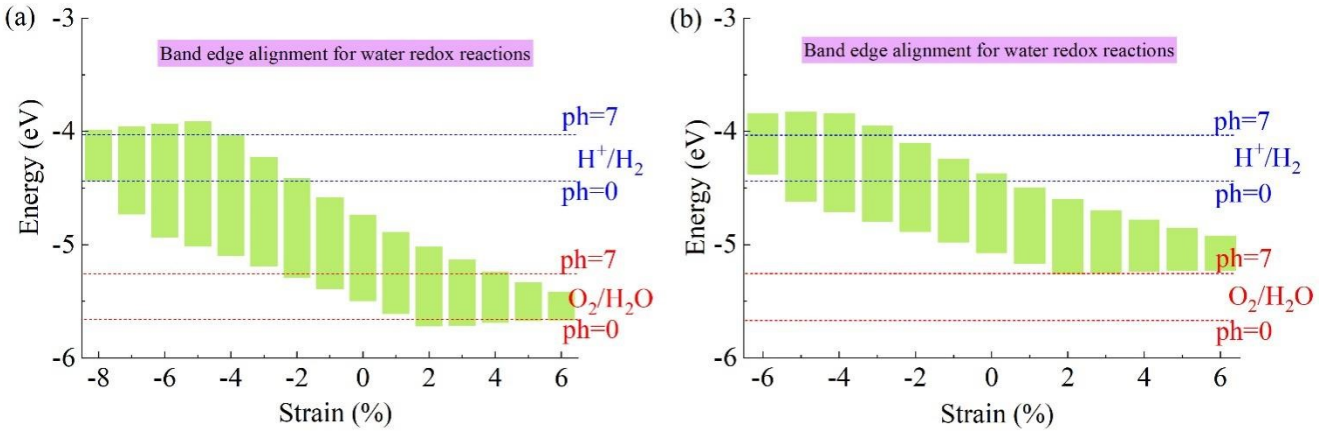

FIG. S10 Band edge alignment for water redox reactions of (a) $WSiGeP_4$ and (b) $WSiGeAs_4$ with strain at Ph=0 and 7.

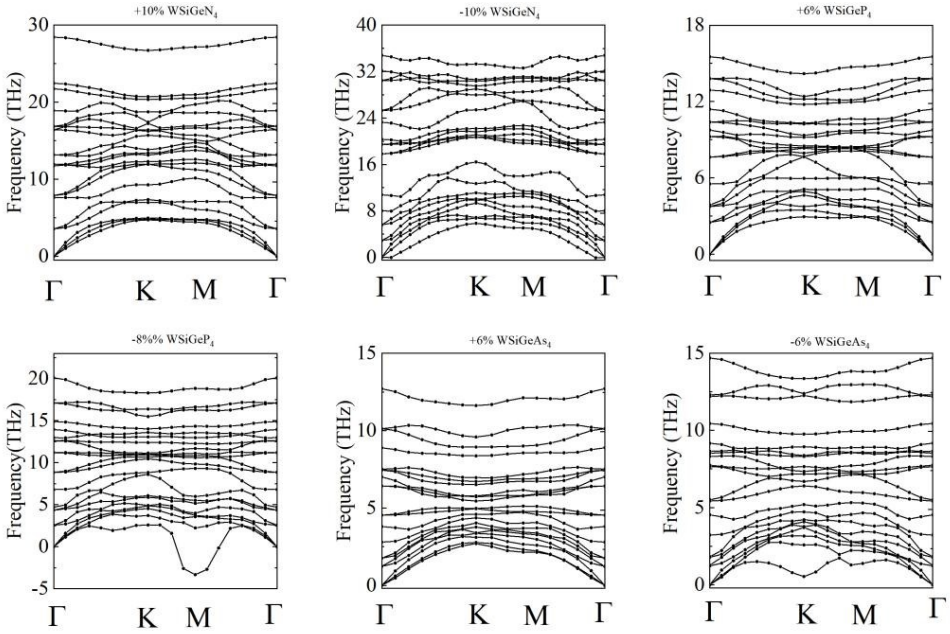

FIG. S11 Phonon spectrum of the strained Janus WSiGeZ_4 monolayers.