Supplemental Materials for "Novel valley character and tunable quasi-half-valley metal state in Janus monolayer $VSiGeP_4$"

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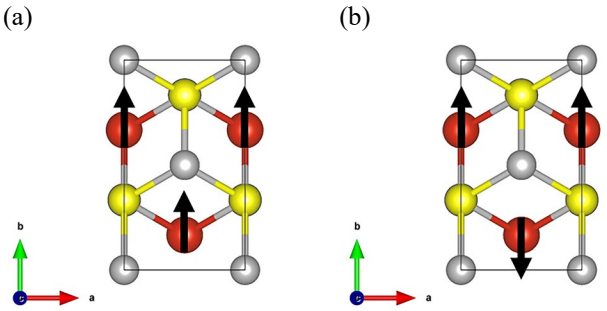


Fig. S1 The considered magnetic configurations: panel (a) and (b) are the FM and AFM configurations, respectively.

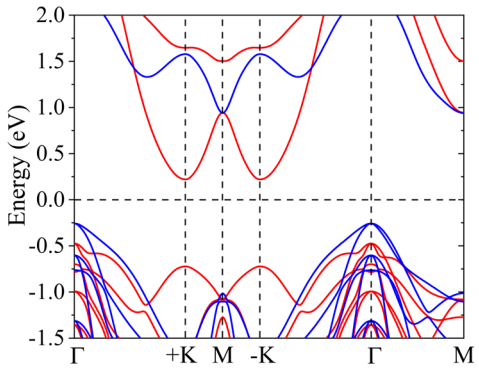
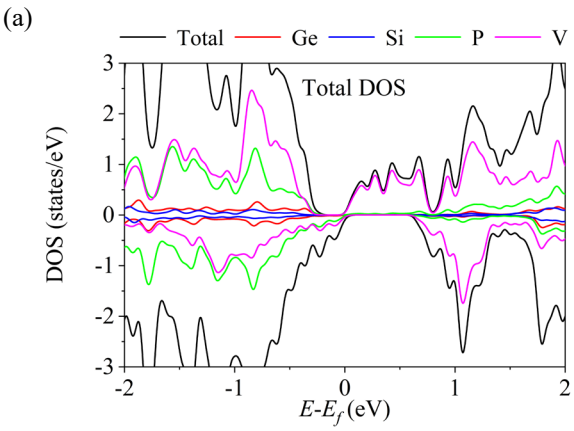
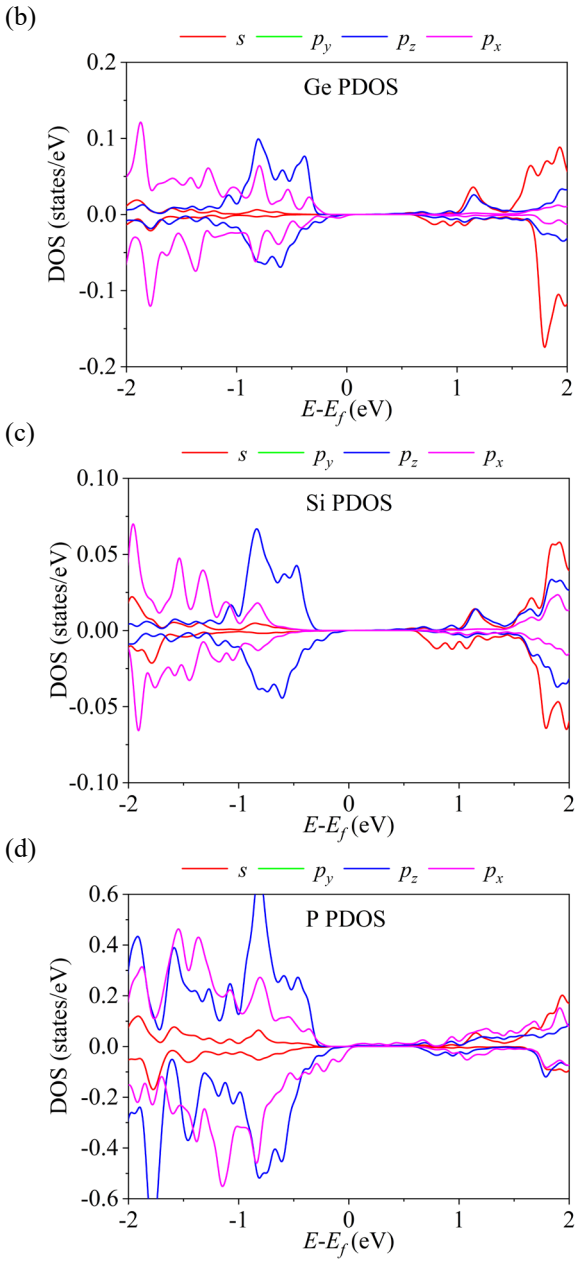


Fig. S2 The band structure at the HSE06 level for ML $VSiGeP_4$ without the involvement of the SOC effect.





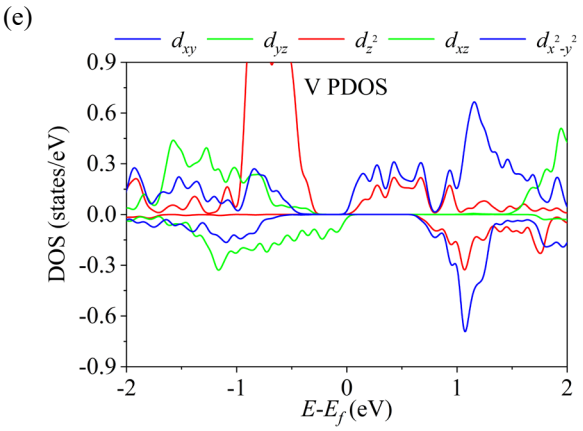
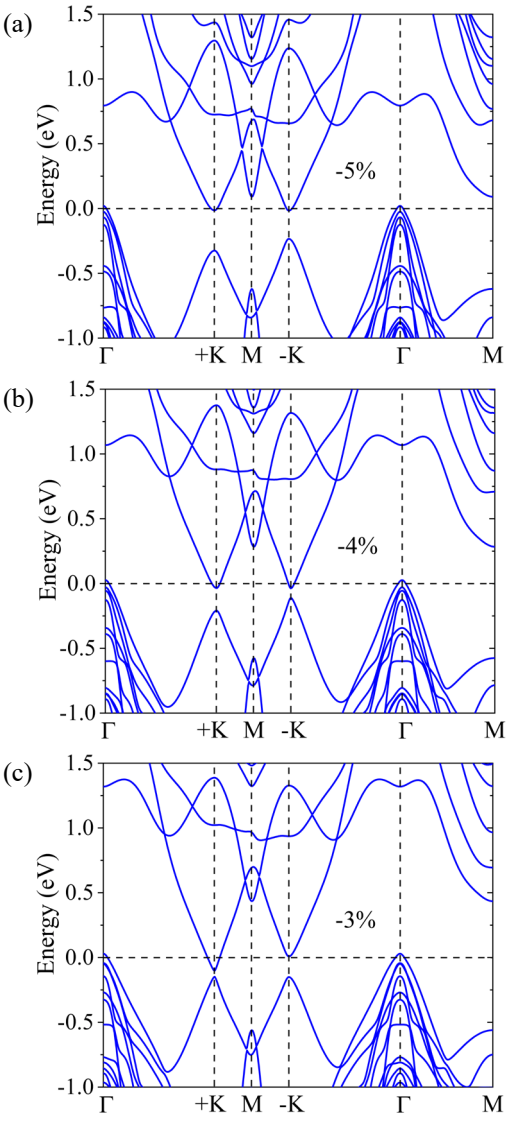
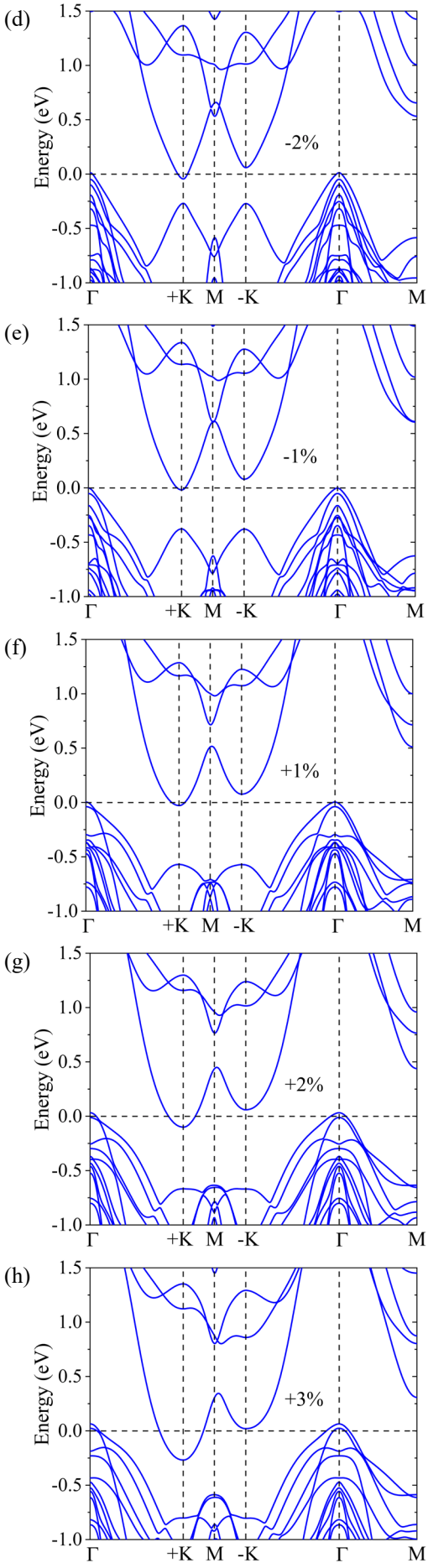


Fig. S3 (a) The total density of states (DOS) of the ML $VSiGeP_4$. (b) The partial density of states (PDOS) of Ge atoms. (c) The PDOS of Si atoms. (d) The PDOS of P atoms. (e) The PDOS of V atoms.

We calculate the total and partial density of states (DOS) of the ML $VSiGeP_4$. As drawn in Fig. S2, the CBM primarily consists of $d_{x^2-y^2}/d_{xy}$ orbitals of V, and the VBM is mainly composed of $d_{xz}+d_{yz}$ orbitals of V and minority p_x orbital of P, which is in agreement with the orbital-resolved band structure (see Fig. 3(d)).





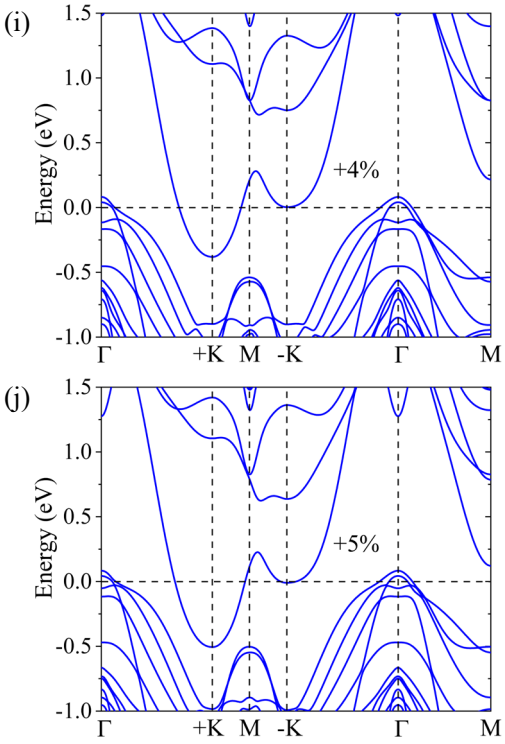


Fig. S4 The energy band structures of ML $VSiGeP_4$ by using GGA+SOC with OOP magnetization at different strains (-5% < ε < +5%).

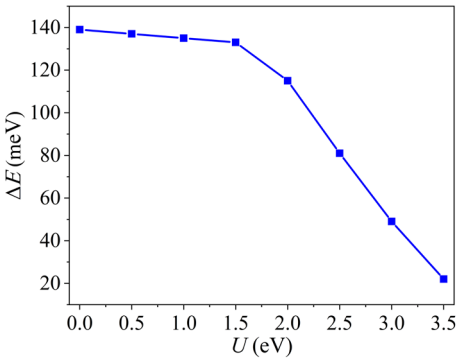
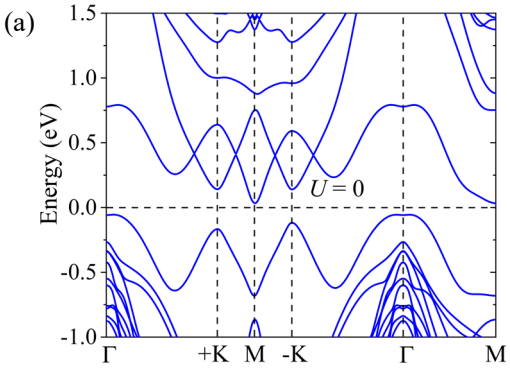
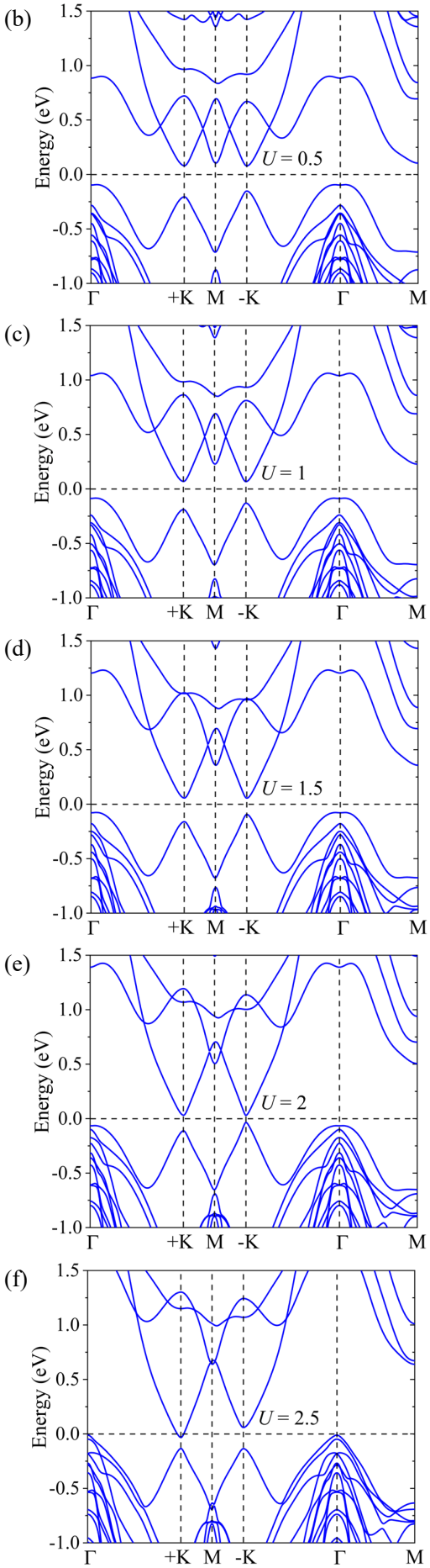


Fig. S5 The energy differences ΔE ($\Delta E = E_{AFM} - E_{FM}$) between AFM and FM states as function of U value.





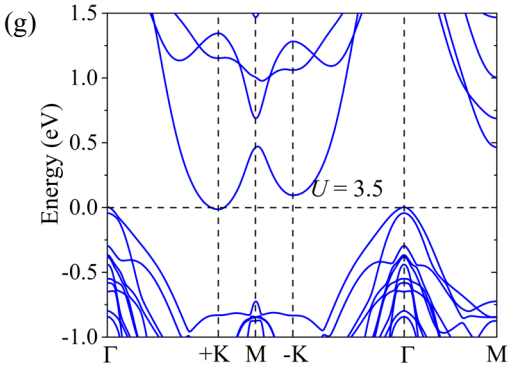


Fig. S6 The energy band structures of ML $VSiGeP_4$ by using GGA+SOC with OOP magnetization at different U values (0 eV < U < 3.5 eV).

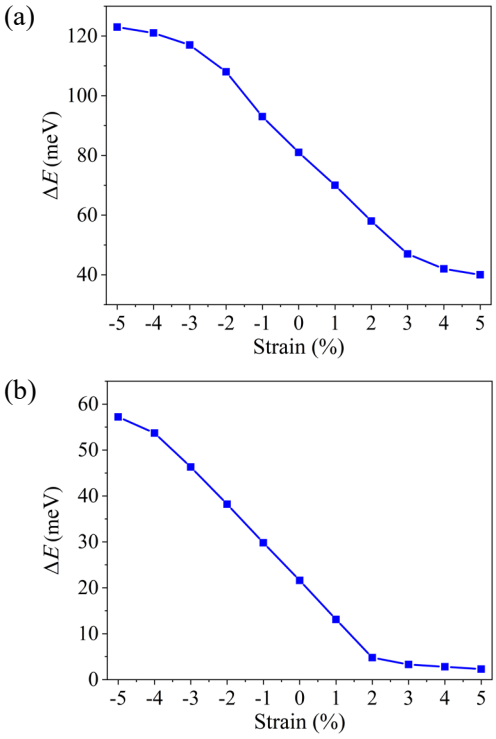
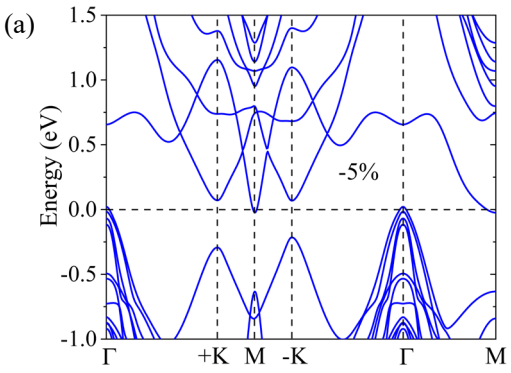
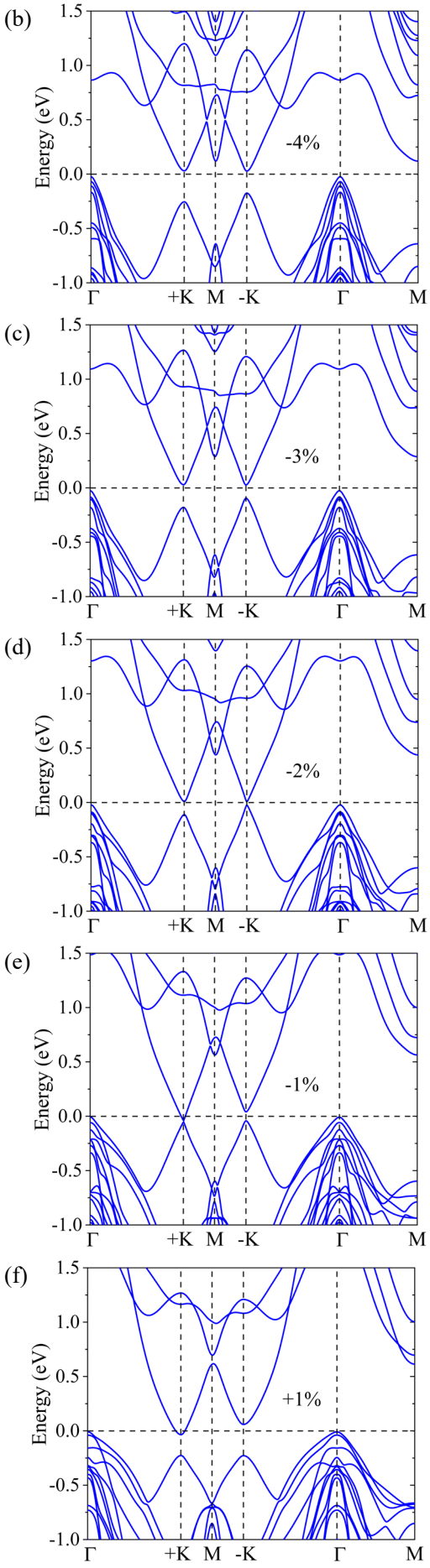


Fig. S7 For (a) U = 2.5 eV and (b) U = 3.5 eV, the energy differences ΔE ($\Delta E = E_{AFM} - E_{FM}$) between AFM and FM states as a function of strain.





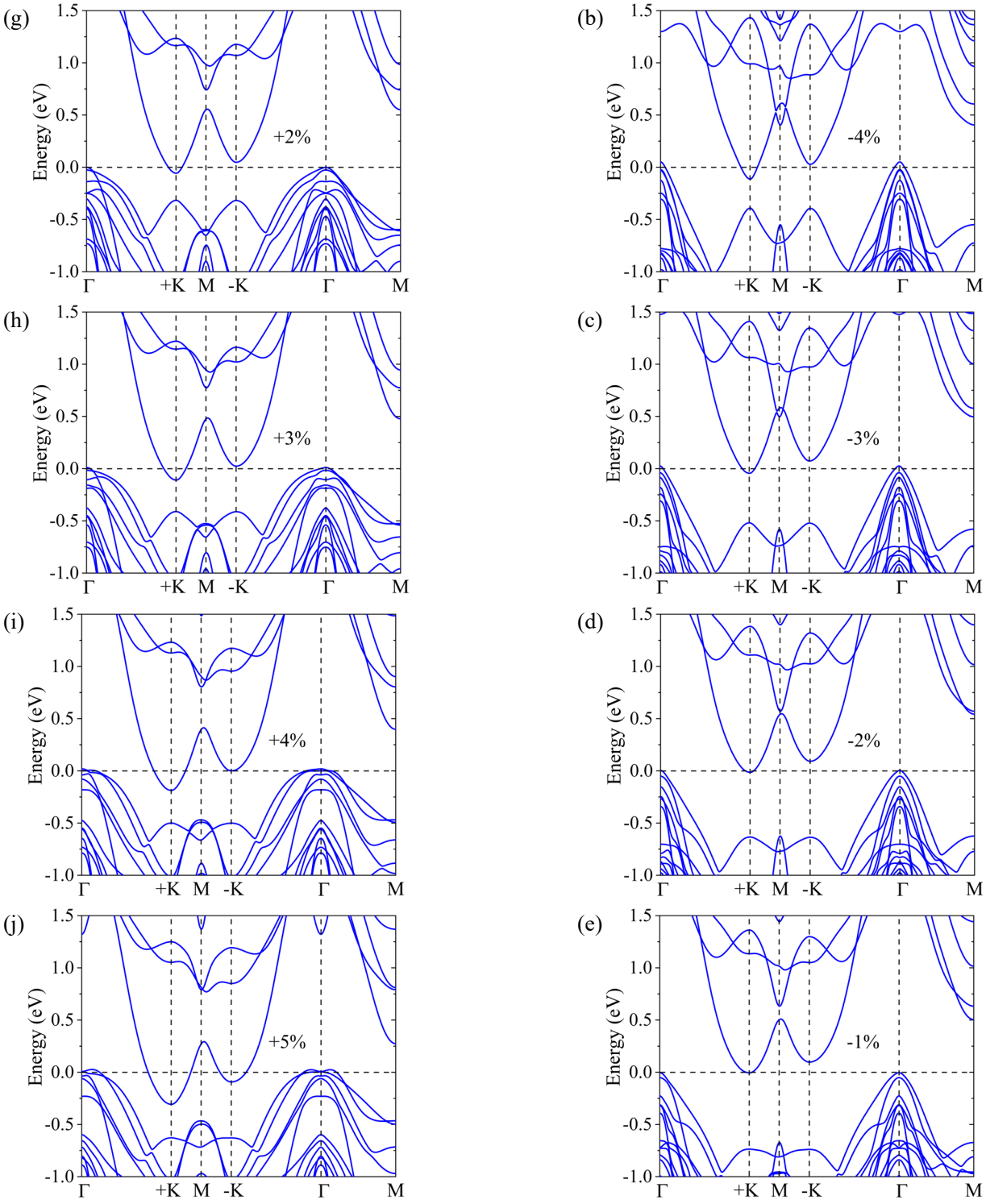
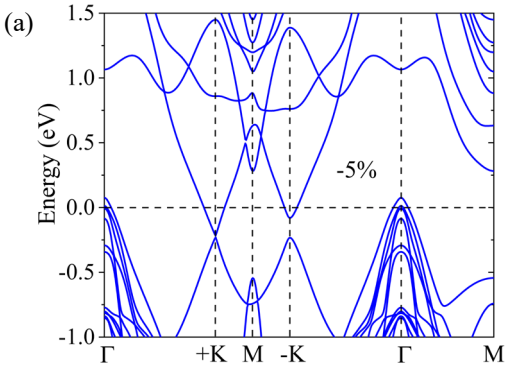


Fig. S8 For U = 2.5 eV, the energy band structures of ML $VSiGeP_4$ by using GGA+SOC with OOP magnetization at different strains (-5% < ε < +5%).



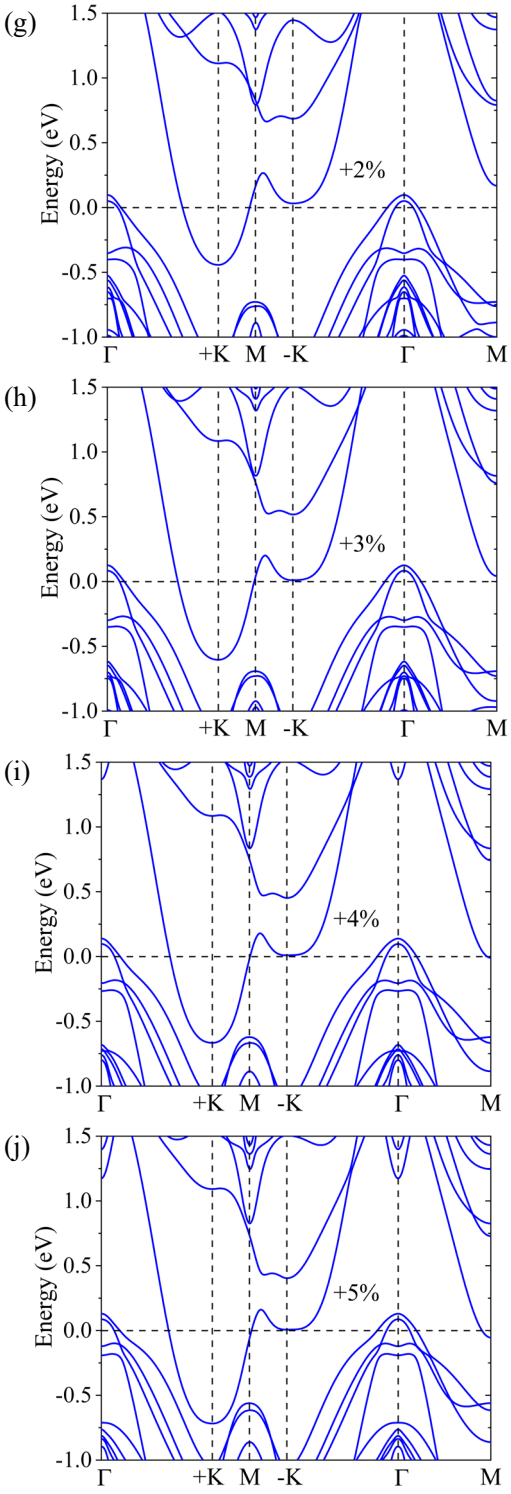
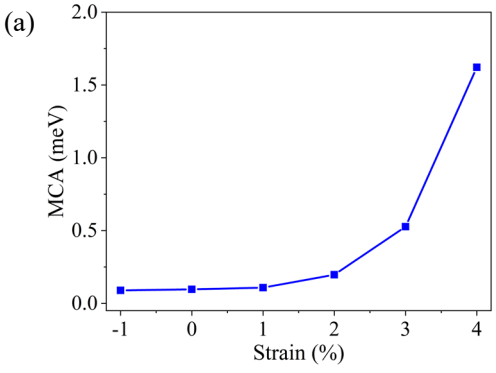


Fig. S9 For U = 3.5 eV, the energy band structures of ML $VSiGeP_4$ by using GGA+SOC with OOP magnetization at different strains (-5% < ε < +5%).



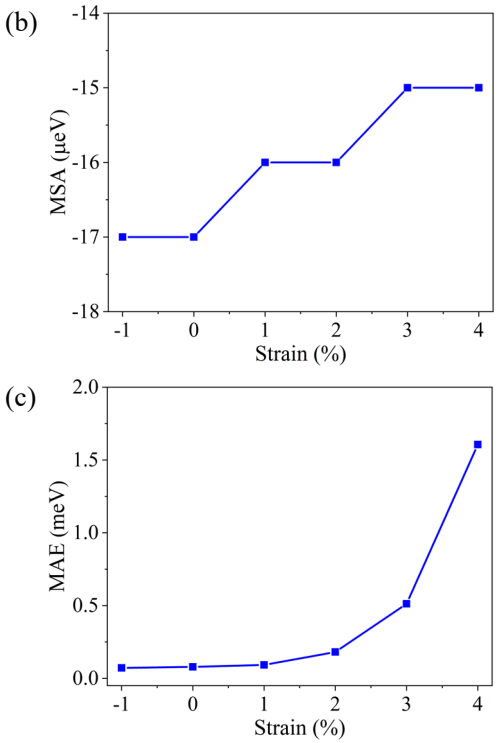


Fig. S10 For U = 2.5 eV, the MCA energy, MSA energy, and MAE as a function of strain.

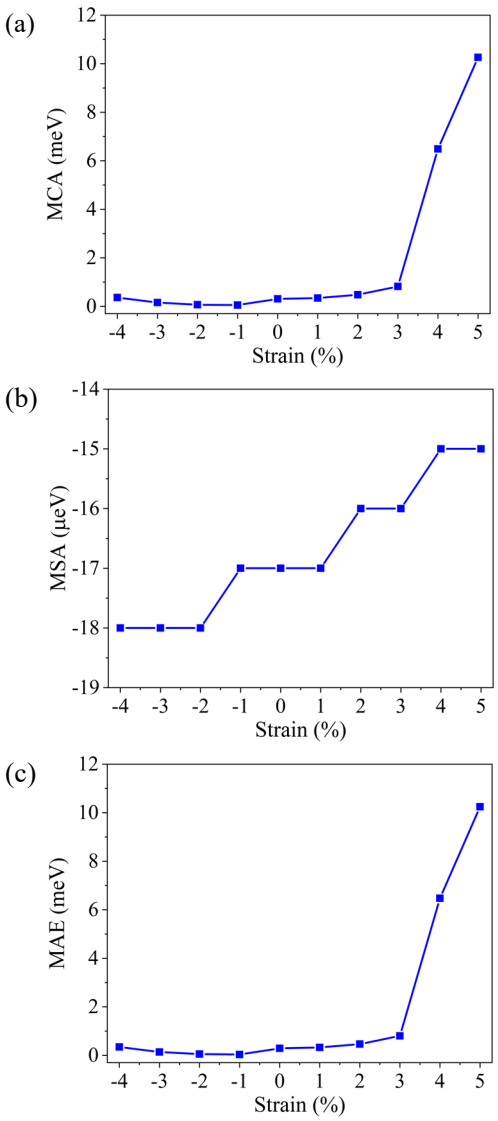


Fig. S11 For U = 3.5 eV, the MCA energy, MSA energy, and MAE as a function of strain.

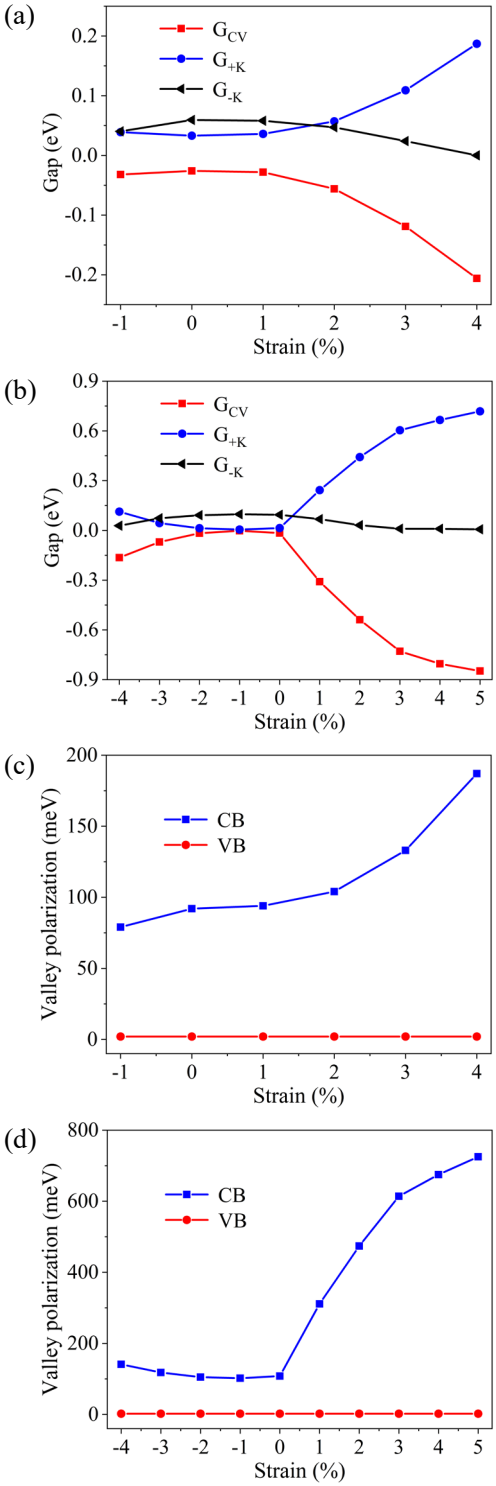


Fig. S12 For ML $VSiGeP_4$, the relevant band gap of (a) U = 2.5 eV and (b) U = 3.5 eV and the VP of (c) U = 2.5 eV and (d) U = 3.5 eV for CB and VB as a function of strain.