Supplementary Information

Influence of electronic correlation on valley and topological properties in $VSiGeP_4$ monolayer

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As shown in Fig. S1(a), for $VSiGeP_4$ monolayer at U = 0.00 eV, the projected density of states (PDOS) for V, P1, and P2 atoms overlap during -1.80 to 0.00 eV, which means the V atom is bonded with adjacent P atoms. Similarly, the Si and P1/P3 atoms and Ge and P2/P4 atoms also overlap at -1.80 to 0.00 eV, which indicates the Si and Ge atoms are bonded with the P1/P3 and P2/P4 atoms, respectively. This bonding characteristic is further demonstrated by calculating the Projected crystal orbital Hamilton population (pCOHP). As shown in Fig. S1(b), during -5.00 to 0.00 eV, the pCOHP of 3d-V and 3p-P1/P2 orbitals are positive at -5.00 to 0.00 eV, indicating the bonding state between V and P1/P2 atoms. The almost all positive pCOHP during -5.00 to 0.00 eV of 3p-Si and 3p-P1/P3 orbitals and 4p-Ge and 3p-P2/P4 orbitals also indicates the bonding state between Si and P1/P3 and Ge and P2/P4 atoms. As shown in Fig. S1(c), during this bonding progress, the V, Si, and Ge atoms lose electrons, while the P atoms accept electrons. Similarly, for $VSiGeP_4$ monolayer at U = 3.00 eV, all V, Si, and Ge atoms also bonded with the adjacent P atoms. During this combing progress, the electrons are transformed from V, Si, and Ge atoms to P atoms because the P atoms have larger electronegativity than V, Si, and Ge atoms.

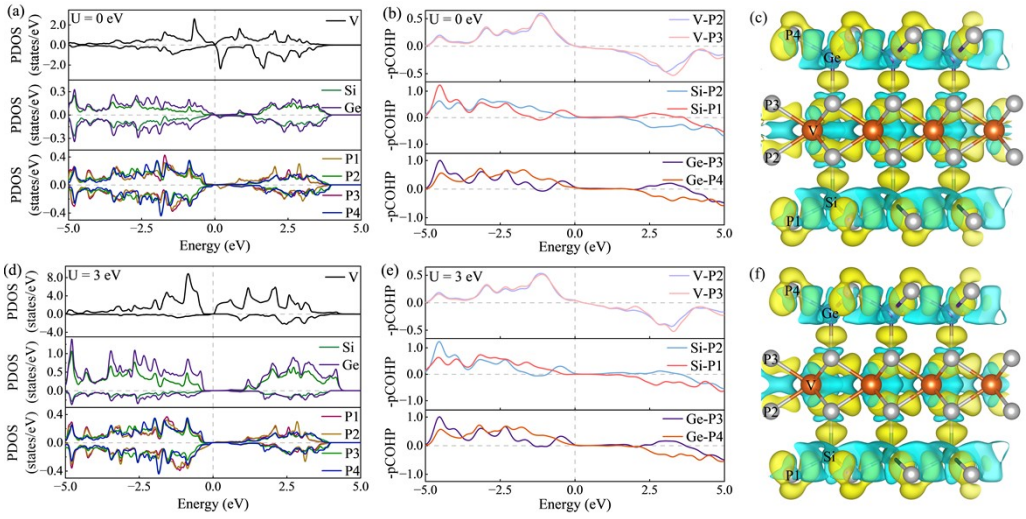

Fig. S1. (a) Projected density of states (PDOS) for V, Si, Ge, and P atoms in $VSiGeP_4$ monolayer at U = 0.00 eV. (b) Projected crystal orbital Hamilton population (pCOHP) of V-3d and P1/P2-3p orbitals, Si-3p and P1-3p orbitals, Ge-4p and P-3p orbitals for $VSiGeP_4$ monolayer wat U = 0.00 eV. (c) Charge density difference of $VSiGeP_4$ monolayer at U = 0.00 eV. (d) Projected density of states (PDOS) for V, Si, Ge, and P atoms in $VSiGeP_4$ monolayer at U = 3.00 eV. (e) Projected crystal orbital Hamilton

population (pCOHP) of V-3d and P1/P2-3p orbitals, Si-3p and P1-3p orbitals, Ge-4p and P-3p orbitals for $VSiGeP_4$ monolayer wat U = 3.00 eV. (f) Charge density difference of $VSiGeP_4$ monolayer at U = 3.00 eV.

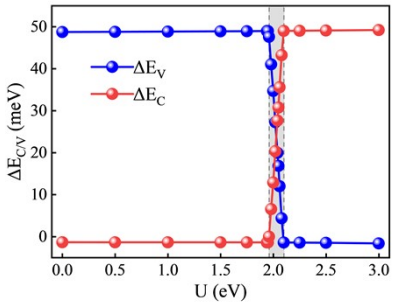

Fig. S2. The ΔE_C (red line) and ΔE_V (blue line) of $VSiGeP_4$ monolayer at different U values.

Fig. S2 shows the energy difference between K and K' points of $VSiGeP_4$ monolayer as a function of U value. As the U is smaller than 1.96 eV, the energy difference (ΔE_V) is mainly contributed by the electrons of valence band. In the range of 1.96 ~ 2.10 eV, ΔE_V reduces sharply and ΔE_C rapidly increases. When the U exceeds 2.10 eV, ΔE_C is dominant by the electrons of conduction band. ΔE_V and ΔE_C correspond to the valence and conduction bands, respectively.

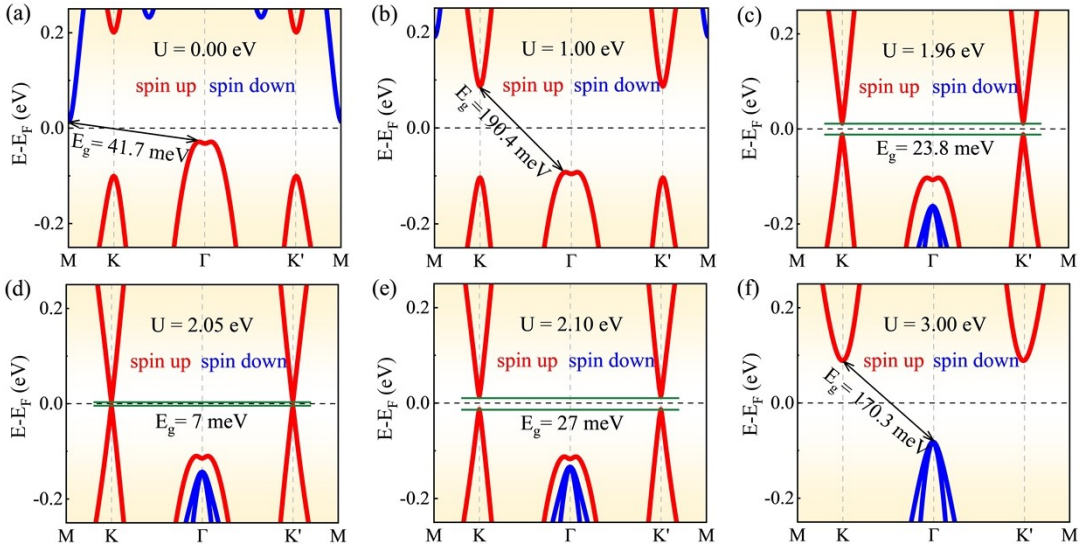

Fig. S3. Spin-resolved energy band structures without considering SOC effect for $VSiGeP_4$ monolayer at different U values.

Fig. S3 shows the spin-resolved band structures of $VSiGeP_4$ monolayer at different U values without considering SOC effect. When the U is set to 0 eV, $VSiGeP_4$ monolayer behaves as an indirect band gap BMS with a band gap of 41.7 meV, as shown in Fig. S3(a). As the U = 1.00 eV, $VSiGeP_4$ monolayer keeps the semiconductor characteristic with a band gap of 109.4 meV, as shown in Fig. S3(b). As U set to 1.96, 2.05, and 2.10 eV, $VSiGeP_4$ monolayer becomes a direct band gap semiconductor with a band gap of 23.8, 7.0, and 27.0 meV, respectively, as shown in Fig. S3(c), S3(d), and S3(e). At U = 3.00 eV, $VSiGeP_4$ monolayer becomes the indirect band gap BMS with a band gap of 170.3 meV. Notably, due to the absence of SOC effect, the energies of K and K' points are degenerate for all the above cases.

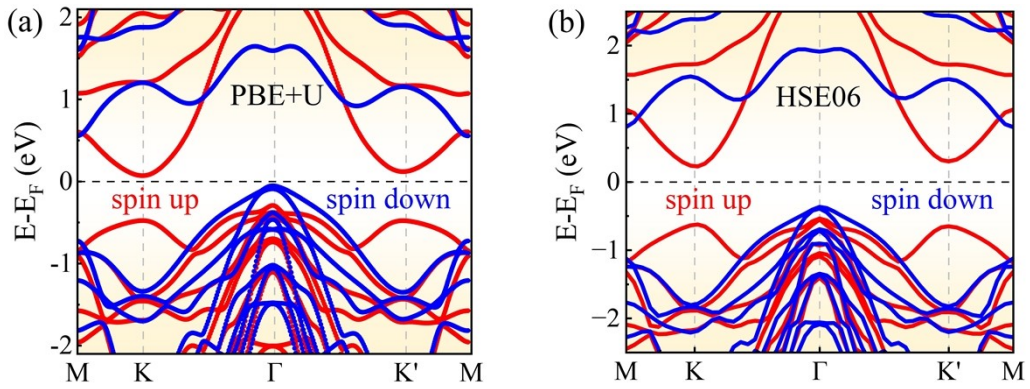

Figure S4. Spin-resolved energy band structures with (a) PBE+U (U = 3.0 eV) and (b) HSE06 method.

As shown in Fig. S4, spin-resolved energy band structures of $VSiGeP_4$ monolayer are calculated by PBE+U (U = 3.0 eV) and HSE06 methods. The electronic features near the Fermi level are nearly same.

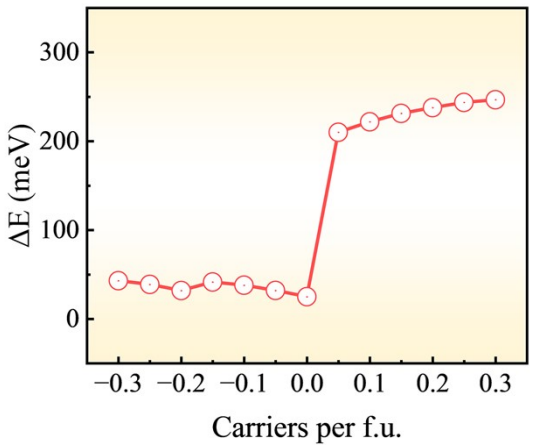

Fig. S5. The energy differences of $VSiGeP_4$ monolayer between AFM and FM ordering ($\Delta E = E_{AFM} - E_{FM}$) with various doping concentrations.

With the change of doping concentration, ΔE of $VSiGeP_4$ monolayer remains positive, showing the FM ground state for $VSiGeP_4$ monolayer, as shown in Fig. S5.

As shown in Figure S6(a), with doping 0.05 holes per f.u, the energy band of $VSiGeP_4$ monolayer from the spin-down channel at Γ point crosses the Fermi level, resulting in a half metal state. It means that 100% spin-down carriers will be excited at the Γ point, which is very important for spintronics. Similarly, $VSiGeP_4$ monolayer also presents a half metal characteristic with doping 0.10 ~ 0.20 holes per f.u., as drawn in Fig. S6(b)-S6(d). As doping concentration of holes exceeds 0.20 holes per f.u., both the energy bands of spin-up and spin-down channels cross the Fermi level, resulting in a metal state, as indicated in Fig. S6(e) and S6(f). As shown in Fig. 6(g), with doping 0.05 electrons per f.u., the energy band of $VSiGeP_4$ monolayer from the spin-up channel at K point crosses the Fermi level. In this case, 100% spin-up carriers will be excited at the K point. As doping concentration exceeds 0.05 electrons per f.u., both the energy bands of K and K' points from spin-up channel cross the Fermi level, as shown in Fig. S4(h)-S4(l).

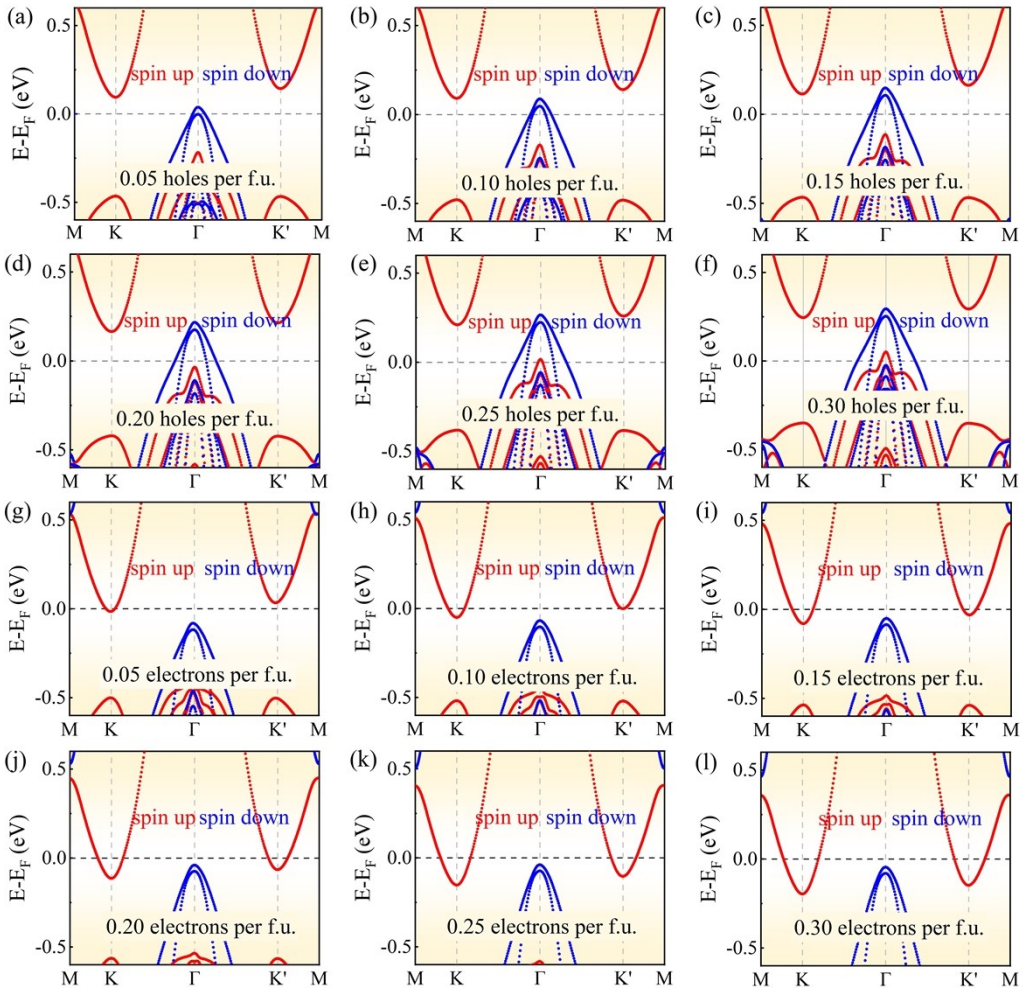

Fig. S6. The energy band structures of $VSiGeP_4$ monolayer with various carrier doping concentrations at U = 3.00 eV.