Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplemental Materials for "Strain-engineering induced topological phase transitions and multiple valley states in Janus monolayer $VCSiN_4$"

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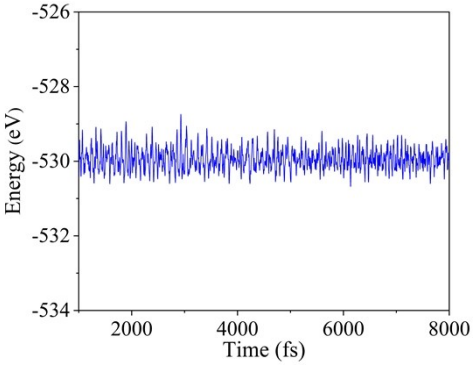


Fig. S1 The AIMD simulation of $VCSiN_4$ at 300 K.

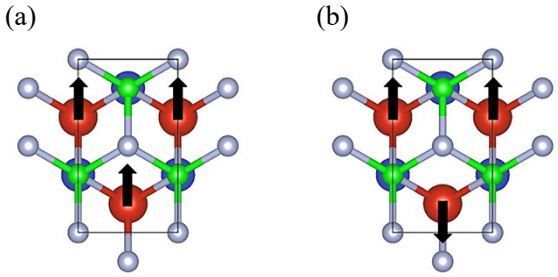
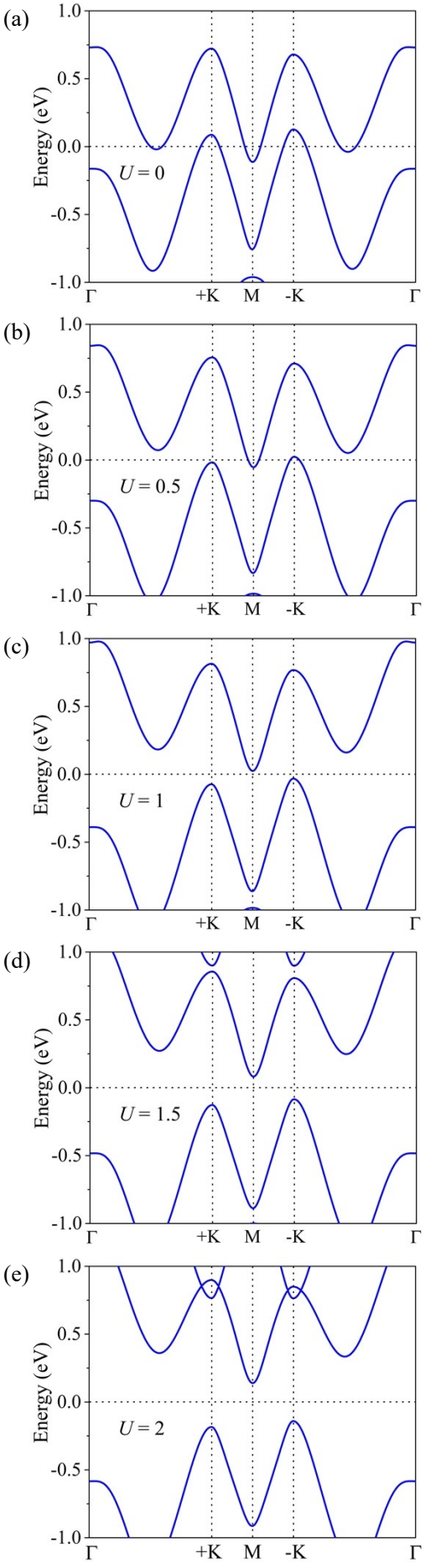


Fig. S2 The considered magnetic configurations: panel (a) is for the FM configuration, and panel (b) is for the AFM configuration.

Table S1 The equilibrium lattice constants (*a*), space group, crystal symmetry, magnetic ground state, and formation energy of monolayers VC_2N_4, $VCSiN_4$, and VSi_2N_4.

	VC_2N_4	$VCSiN_4$	VSi_2N_4
a (Å)	2.57	2.77	2.89
space group	*P*6*m*2	*P*3*m*1	*P*6*m*2
crystal symmetry	D_{3h}	C_{3v}	D_{3h}
magnetic ground state	FM	FM	FM
formation energy (eV)	2.63	3.10	3.81



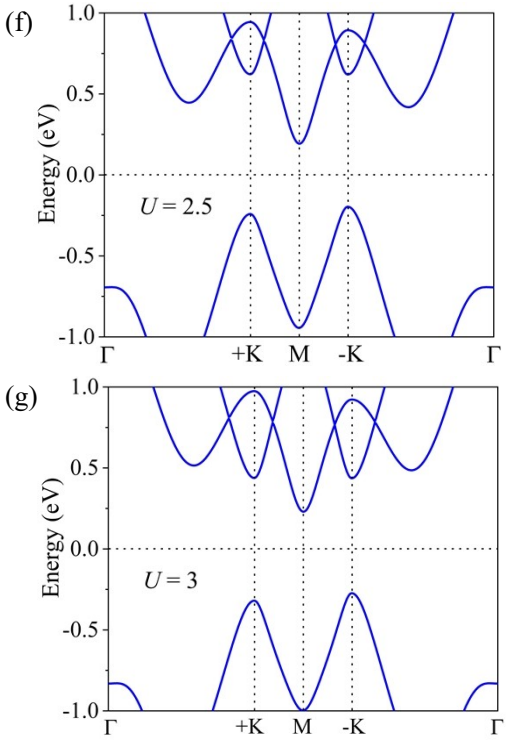


Fig. S3 The electronic band structures by using GGA+*U* method with OOP magnetic anisotropy (*U* values vary from 0 to 3 eV).

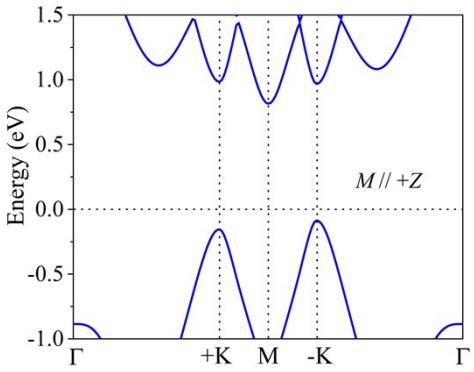
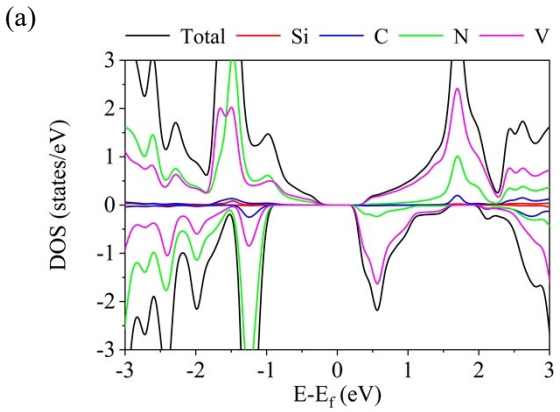


Fig. S4 The electronic band structures by using HSE06+SOC with OOP magnetic anisotropy.



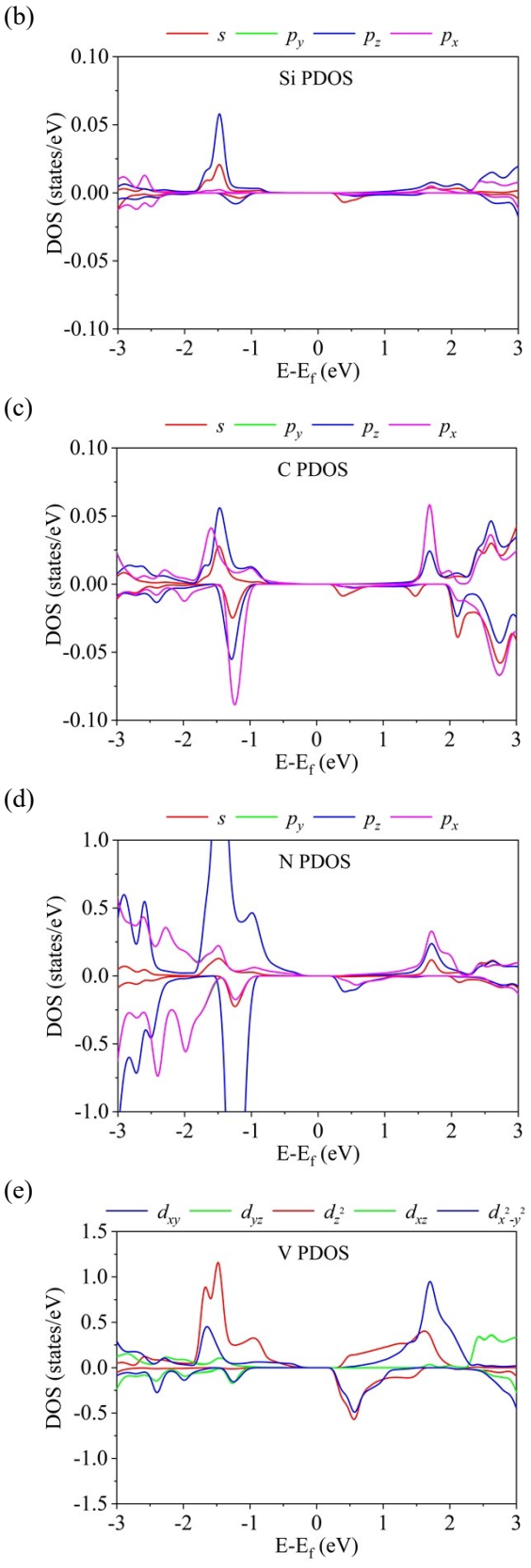
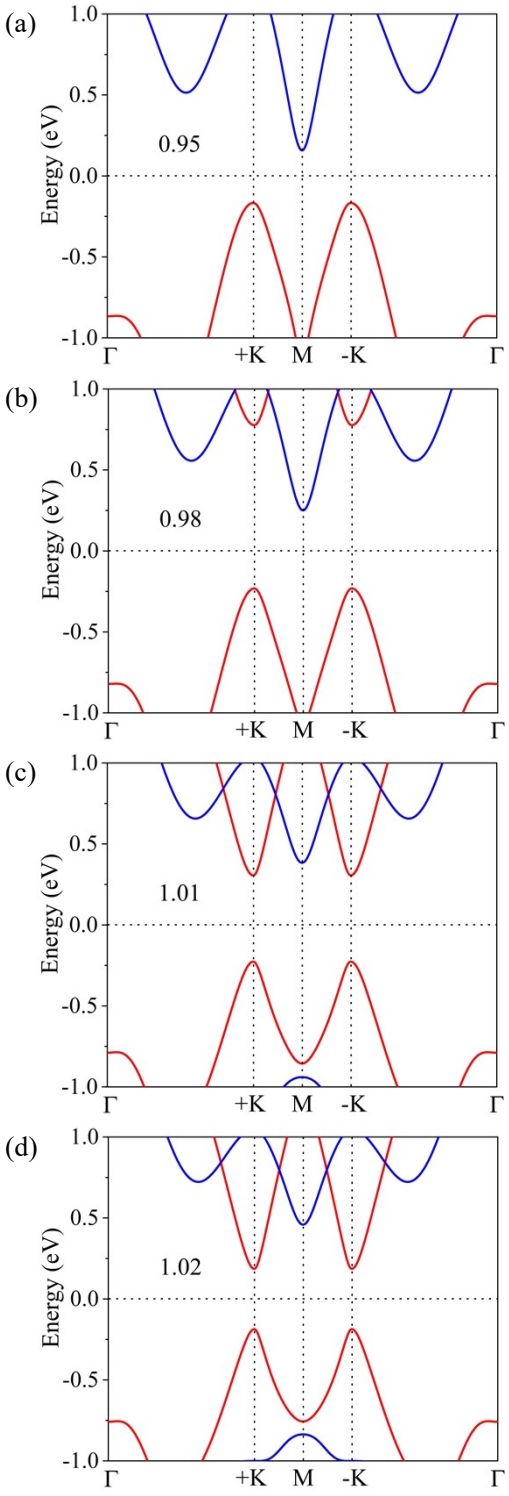


Fig. S5 (a) The total density of states (DOS) of the $VCSiN_4$. (b) The partial density of states (PDOS) of Si atoms. (c) The PDOS of C atoms. (d) The PDOS of N atoms. (e) The PDOS of V atoms.

The total and partial density of states (DOS) of the $VCSiN_4$ are calculated. As is exhibited in Fig. S5, we can observe that both CBM and VBM are mainly composed of $d_{x^2-y^2}/d_{xy}$ orbitals of V atoms and minority p_x/p_z orbitals of N atoms, which is consistent with that of orbital-resolved electronic band structure (see Fig. 3).



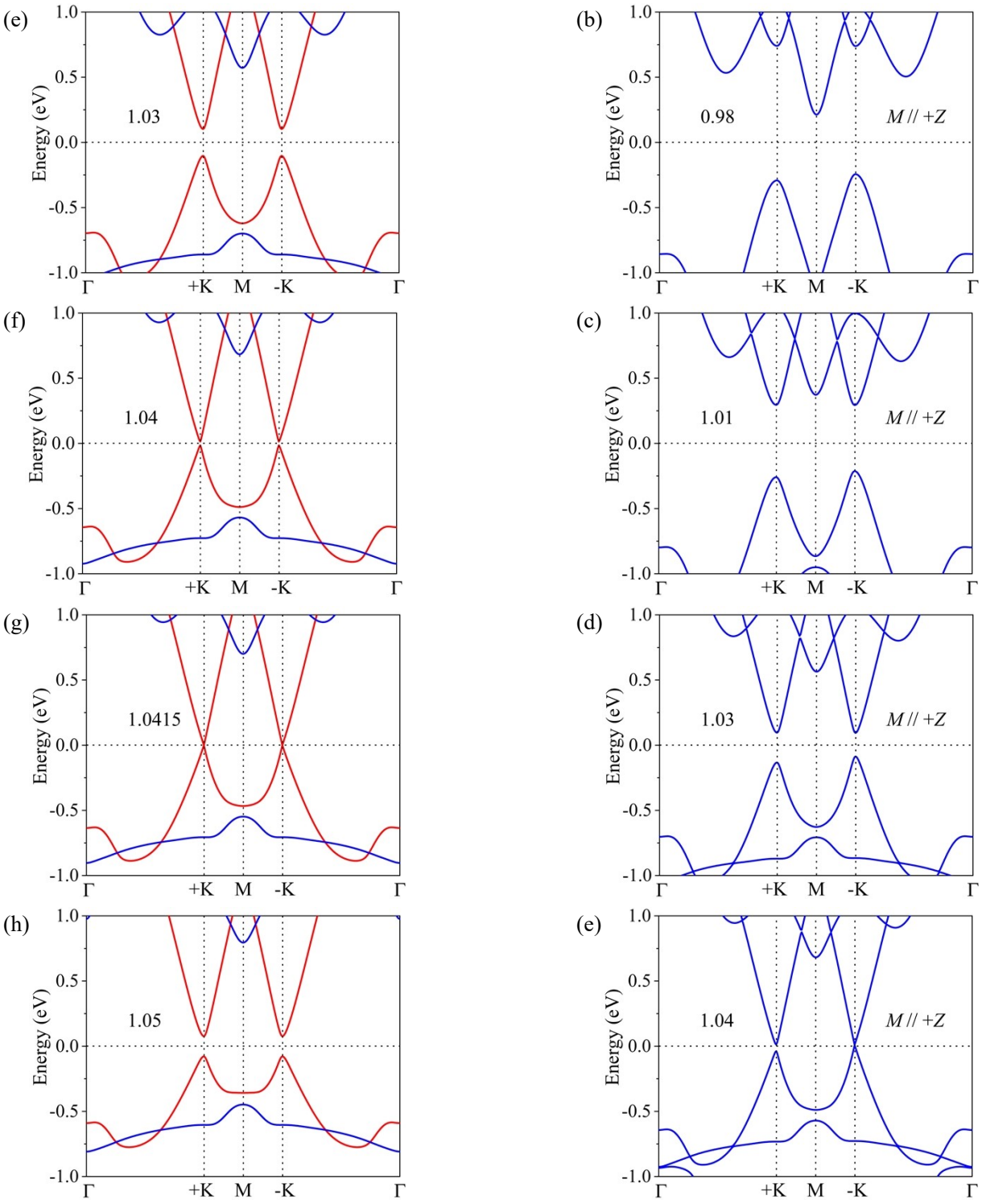


Fig. S6 The electronic band structures by using GGA at eight different a/a_0 values.

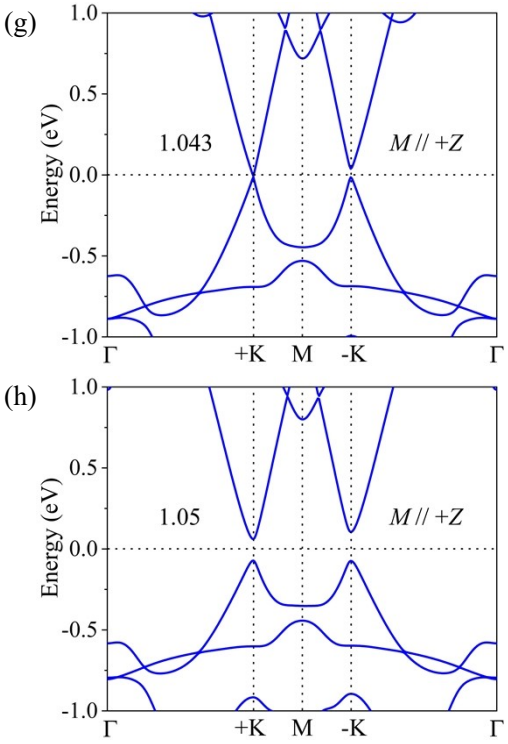
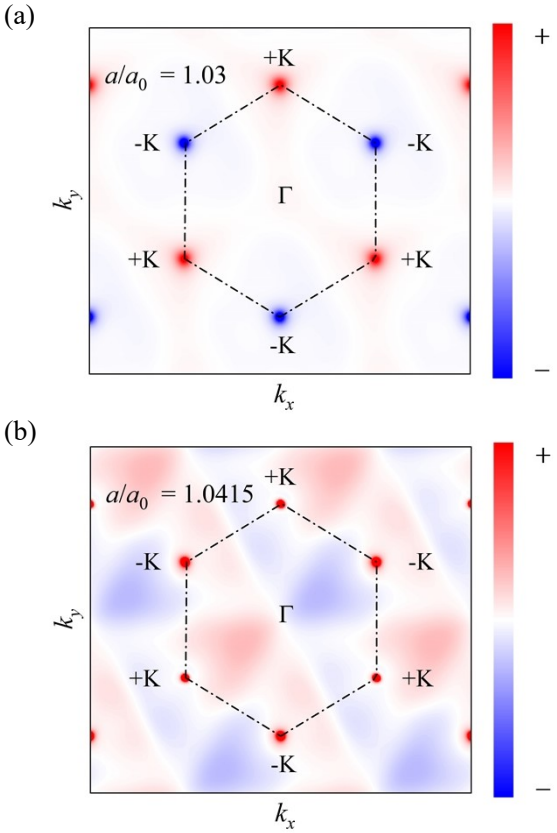


Fig. S7 The electronic band structures by using GGA+SOC with OOP magnetic anisotropy at eight different a/a_0 values.



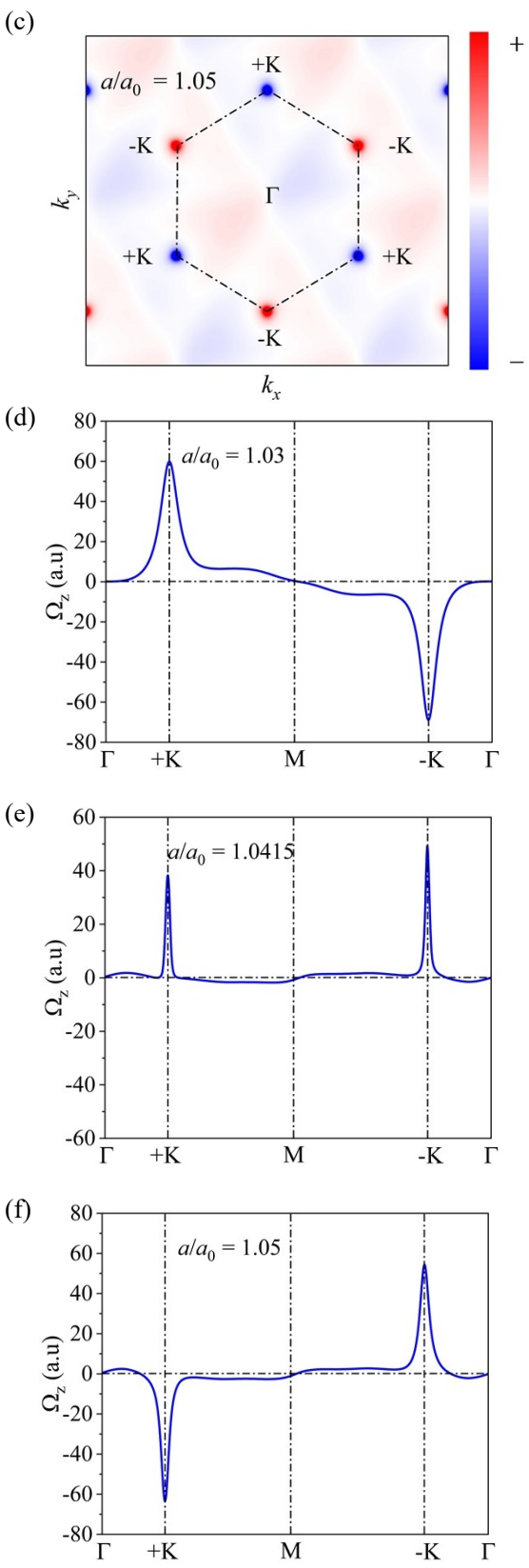


Fig. S8 The Berry curvature in the 2D BZ with (a) $a/a_0 = 1.03$, (b) $a/a_0 = 1.0415$, and (c) $a/a_0 = 1.05$. The Berry curvature along the high symmetry points with (d) $a/a_0 = 1.03$, (e) $a/a_0 = 1.0415$, and (f) $a/a_0 = 1.05$.

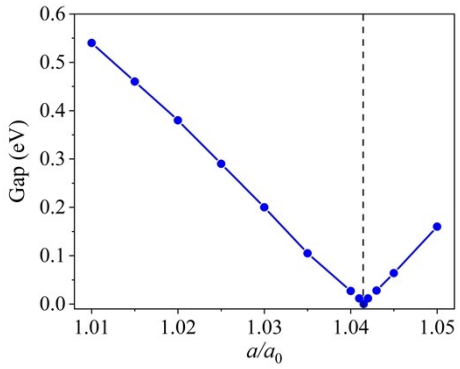
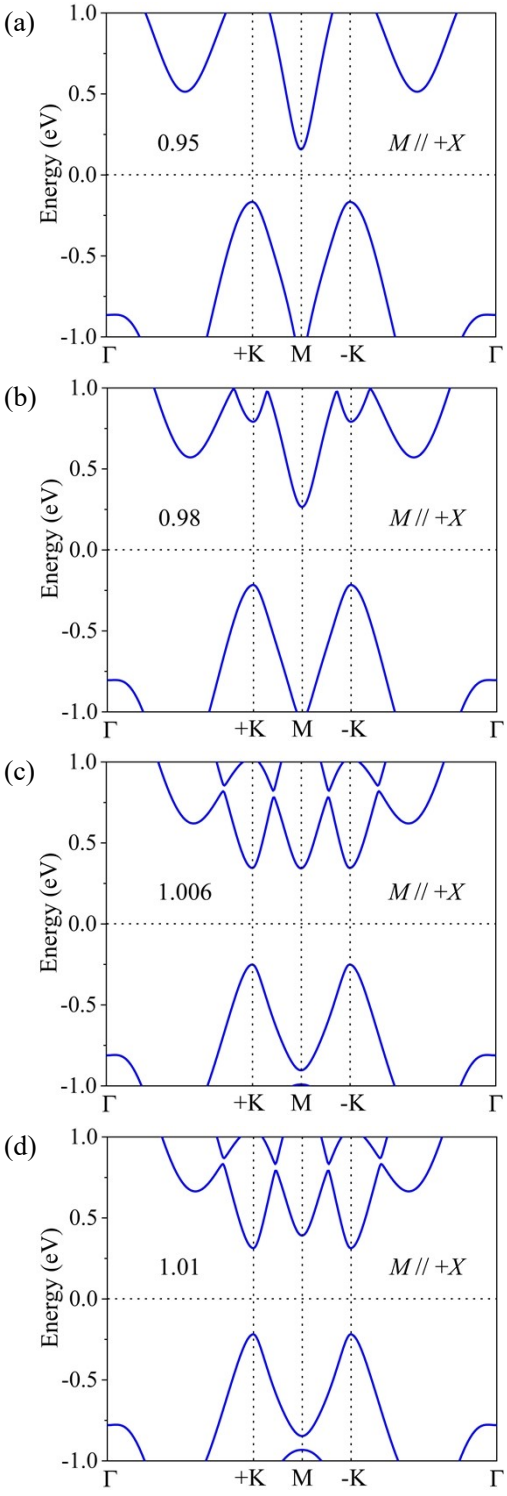


Fig. S9 The global band gaps with SOC (IP magnetic anisotropy) as a function of a/a_0.



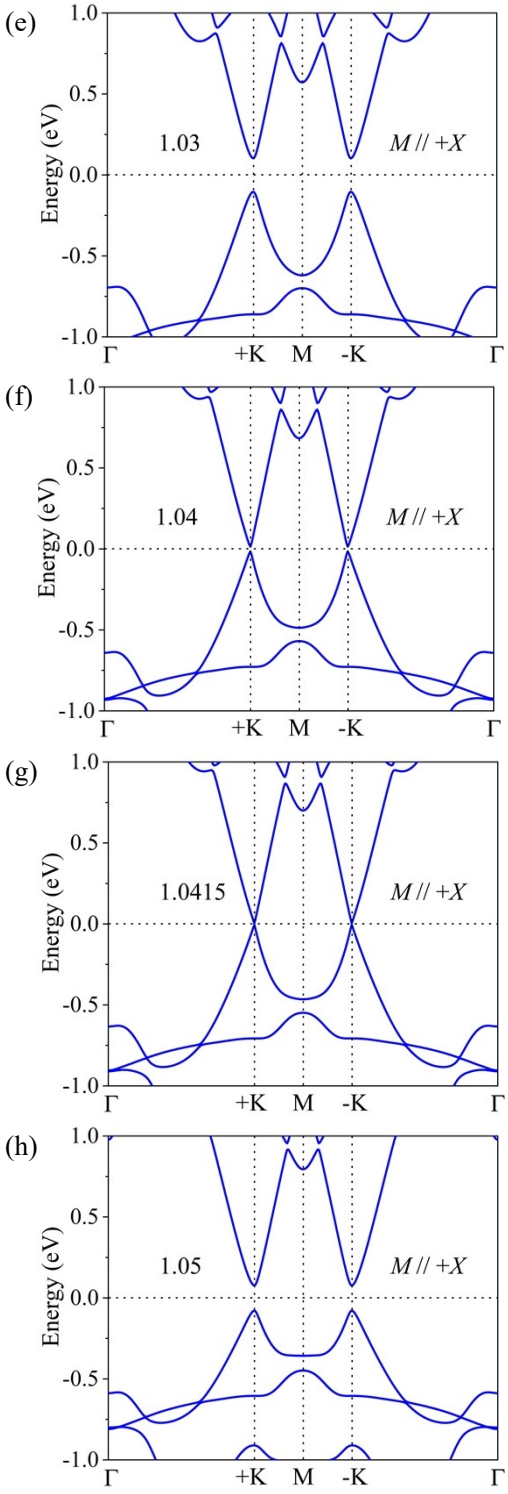


Fig. S10 The electronic band structures by using GGA+SOC with IP magnetic anisotropy at eight different a/a_0 values.