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Supporting Information for

Two-dimensional transitional metal dihydrides crystals with anisotropic and spin-polarized Fermi Dirac cone

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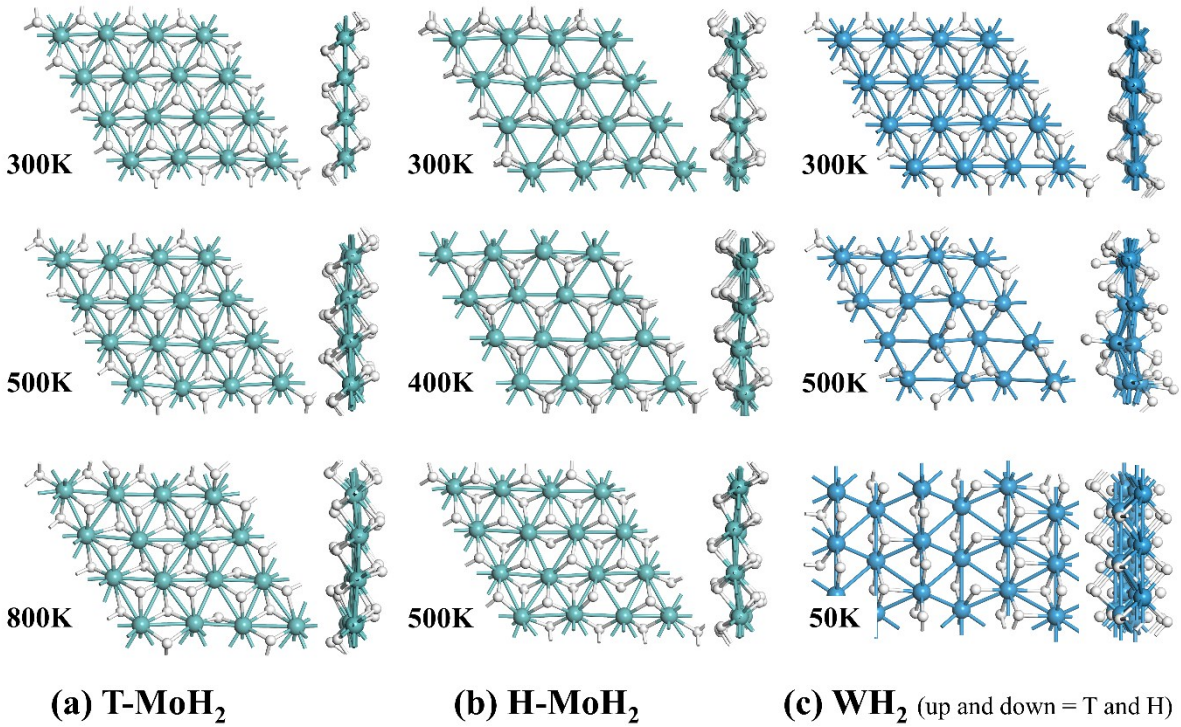

Figure S1. The structural snapshots of Born-Oppenheimer Molecular Dynamic simulations for (a) T-MoH_2, (b) H-MoH_2, (c) WH_2 (up and down = T and H) nanosheets, respectively.

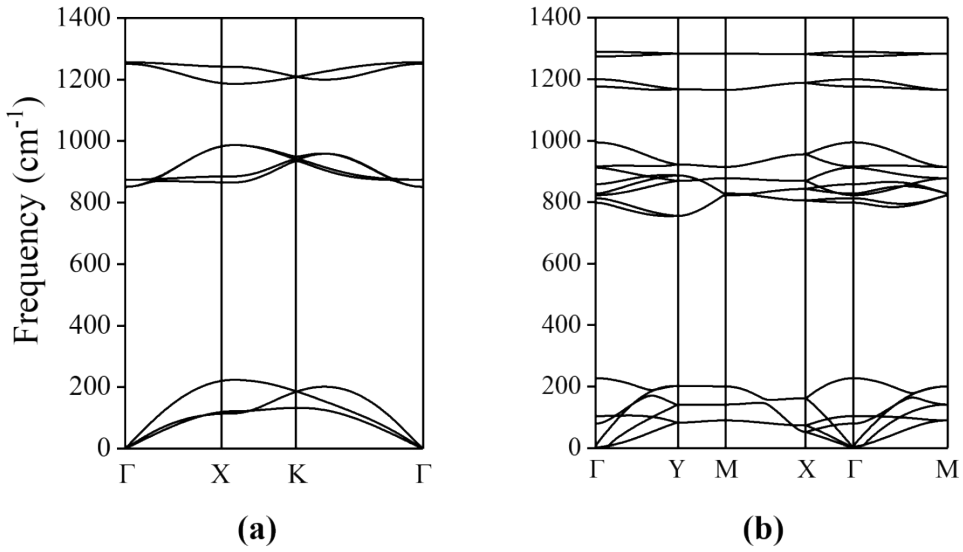

Figure S2. The phonon dispersion spectra of 2D (a)T-WH_2 and (b)H-WH_2.

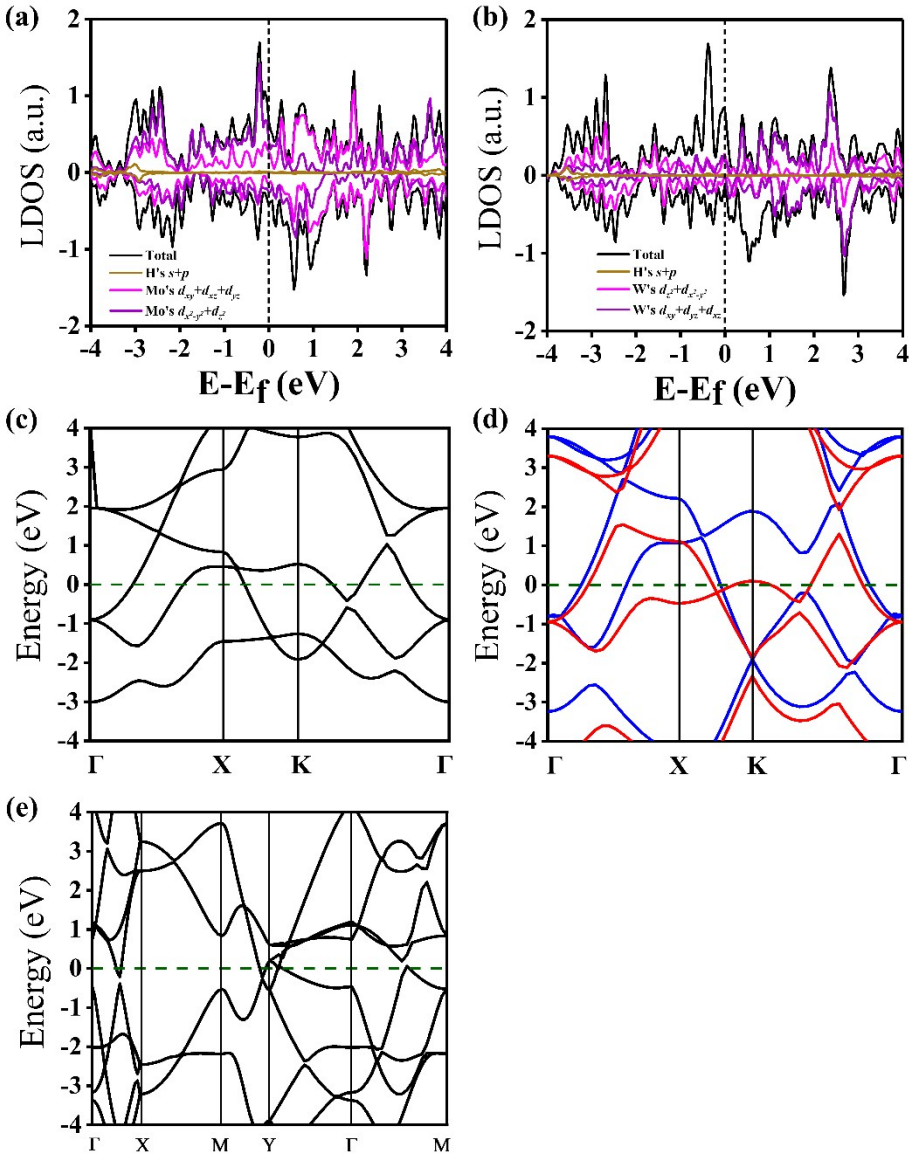

Figure S3. The partial DOS projected on atomic orbitals of 2D (a) T-MoH_2, (b) T-WH_2, band structure of (c) H-MoH_2, (d) T-WH_2 and (e) H-WH_2. The fermi level is set as 0 eV.

Table S1. The energy difference between unit-cell of T-MH_2 and H-MH_2 in ground state in eV per unit cell.

system	T-MoH_2	H-MoH_2	T-WH_2	H-WH_2
ΔE	0.000	0.455	0.000	0.364

Table S2. The calculated metal-hydrogen (M-H) bond strength of 2D MH_2 in eV per M-H bond.

system	T-MoH_2	H-MoH_2	T-WH_2	H-WH_2
E_{BS}	1.800	1.691	1.600	1.521

Table S3. The energy difference between FM, NM and AFM states of unit-cell of 2D MH_2 monolayers in ground state in eV per metal atom.

system		E_{FM}	E_{AFM}	E_{NM}
MoH_2	T	0.000	0.038	0.248
	H	/	/	/
WH_2	T	0.000	0.114	0.201
	H	0.110	0.000	0.247