**Electronic Supporting Information**

# Controlled 2H/1T Phase Transition in $MoS_2$ Monolayer by Strong Interface with $M_2C$ MXene: A Computational Study

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**Table S1.** The computed lattice parameters (Å) and bond lengths (Å) of various $M_2C$-typed MXenes, 1T-$MoS_2$, and 2H-$MoS_2$ monolayers.

| | lattice parameters | bond length |
|---|---|---|
| $Ti_2C$ | 3.04 | 2.10 |
| $V_2C$ | 2.88 | 1.99 |
| $Cr_2C$ | 2.80 | 1.93 |
| $Zr_2C$ | 3.27 | 2.27 |
| $Nb_2C$ | 3.11 | 2.16 |
| $Mo_2C$ | 2.98 | 2.09 |
| $Hf_2C$ | 3.20 | 2.24 |
| $Ta_2C$ | 3.07 | 2.15 |
| $W_2C$ | 2.96 | 2.09 |
| 1T-$MoS_2$ | 3.13 | 2.43 |
| 2H-$MoS_2$ | 3.17 | 2.40 |

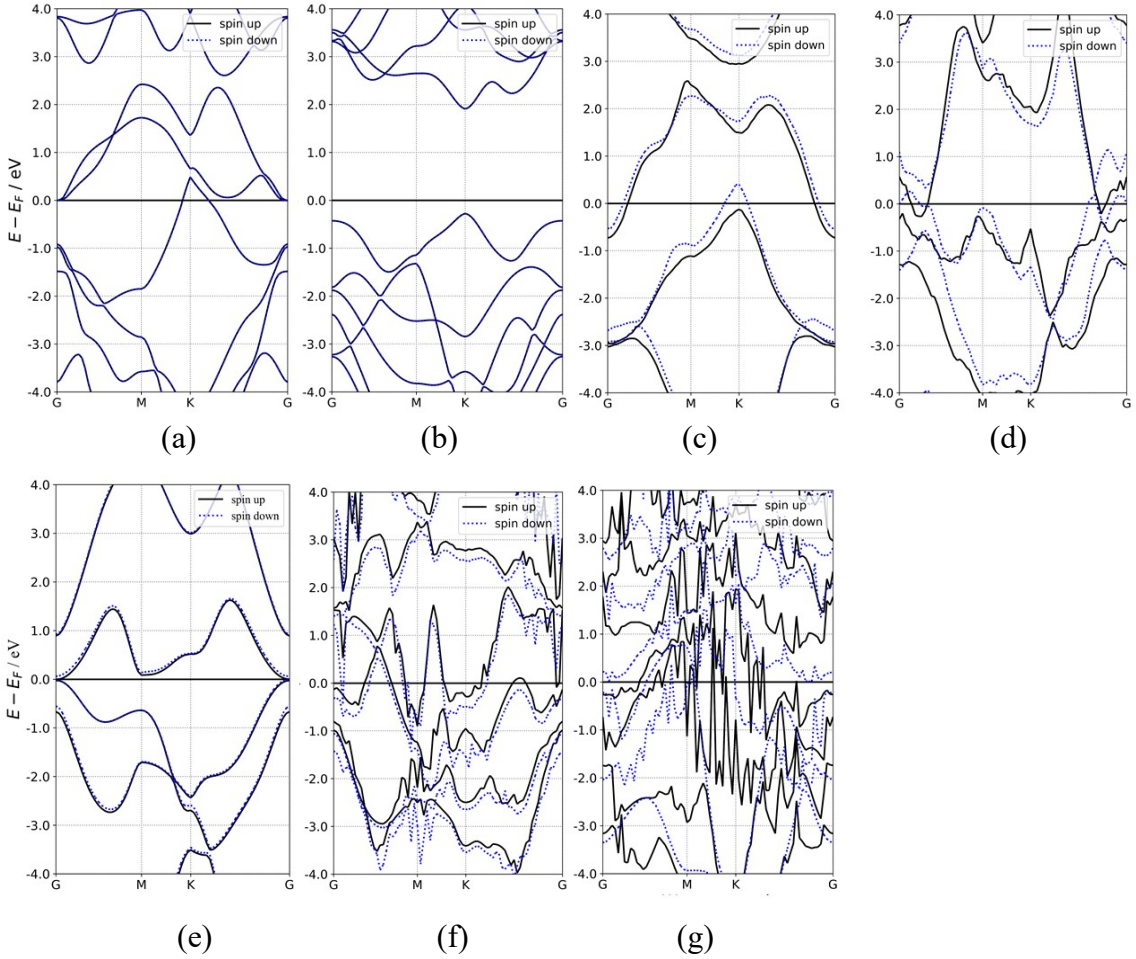



**Fig. S1**. The computed band structures of pristine (a) 1T-$MoS_2$, (b) 2H-$MoS_2$, (c) $Ti_2C$, (d) $Zr_2C$, (e) $Hf_2C$, (f) $Nb_2C$, and (g) $Ta_2C$ nanosheets. The Fermi level was set to zero.

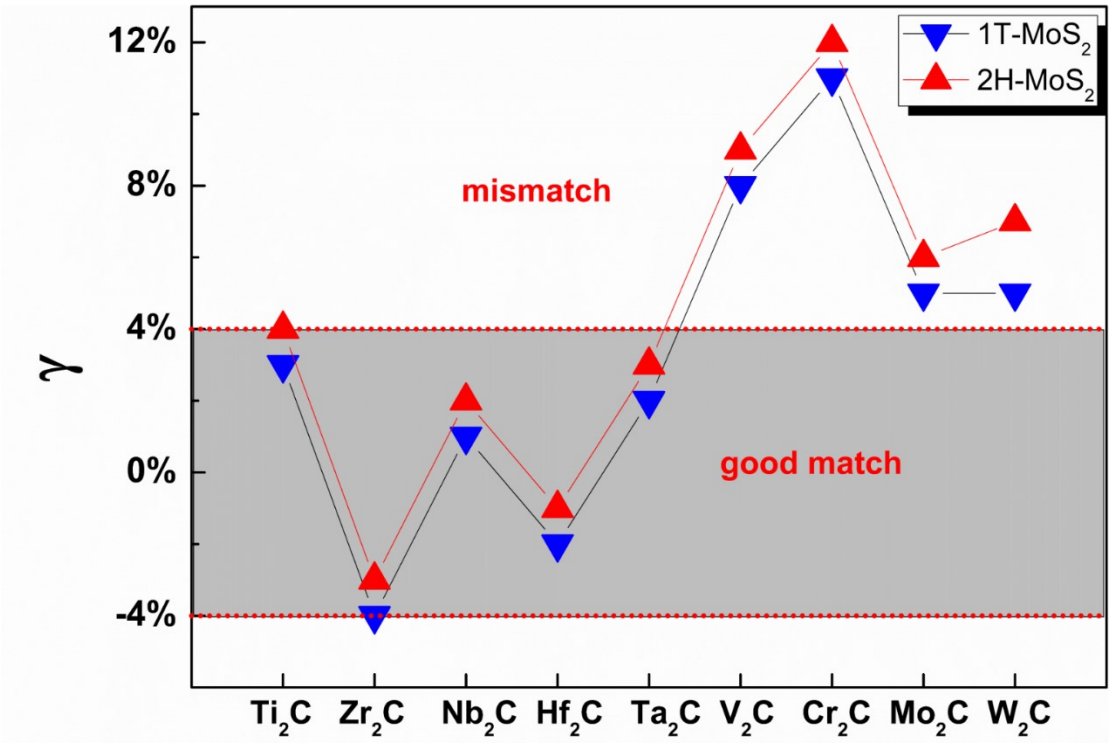



**Fig. S2**. The computed lattice mismatch (γ) between 1T- or 2H-$MoS_2$ monolayers and $M_2C$-type MXene nanosheets.

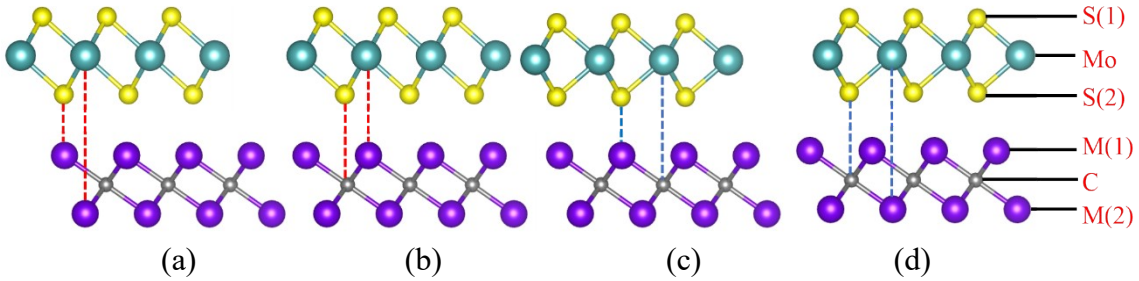



**Fig. S3**. The considered initial configrations for (a) and (b) 1T-$MoS_2$, (c) and (d) 2H-$MoS_2$ monolayer on $M_2C$-MXenes.

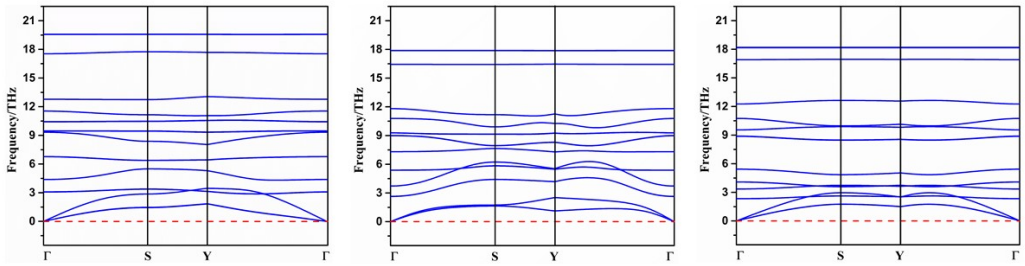
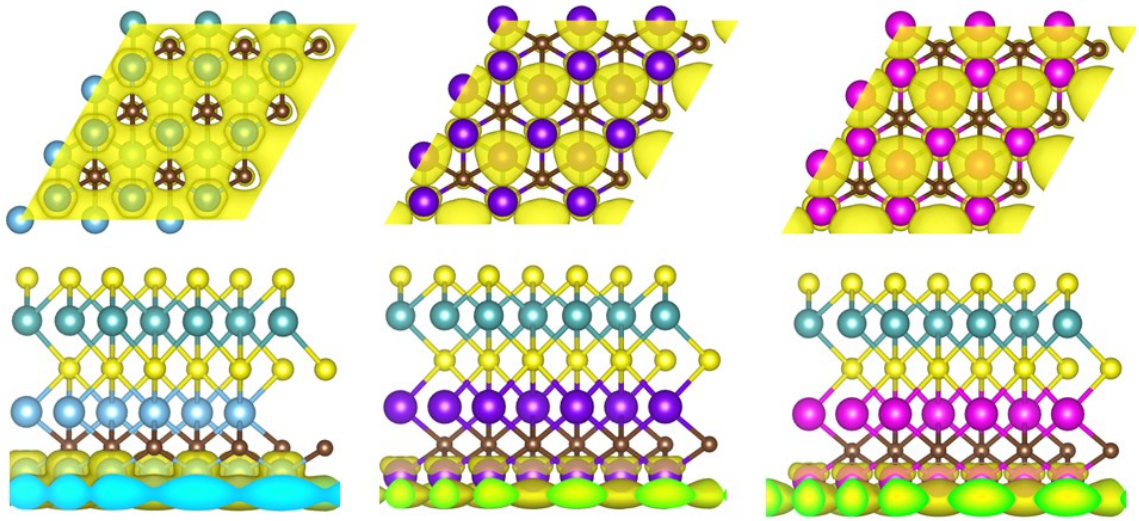



**Fig. S4.** The computed phonon dispersions of 1T-$MoS_2$/$M_2C$ heterostructures, where M represents (a) Ti, (b) Zr and (c) Hf, respectively.



(a) (b) (c)

**Fig. S5.** The iso-surface of the spin-resolved density pictures of (a) 1T-$MoS_2$/$Ti_2C$, (b) 1T-$MoS_2$/$Zr_2C$, and (c) 1T-$MoS_2$/$Hf_2C$ heterostructures. The iso-value is set to be 0.005 e$Å^{-2}$.

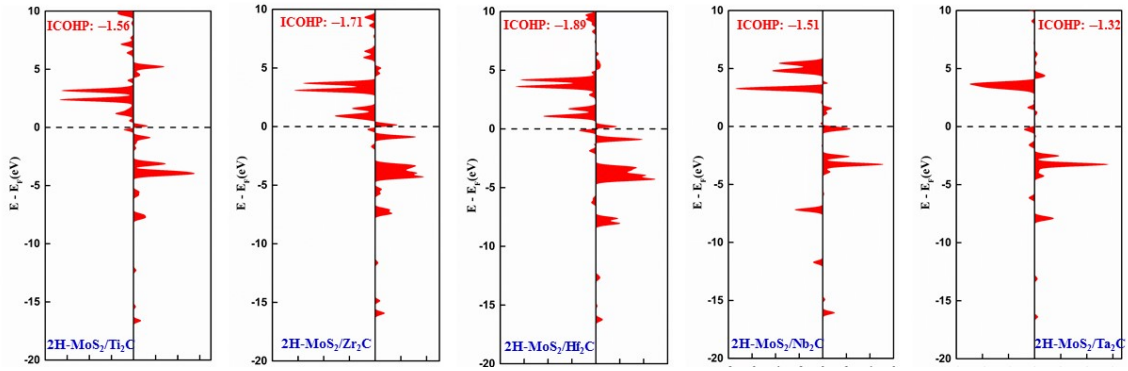
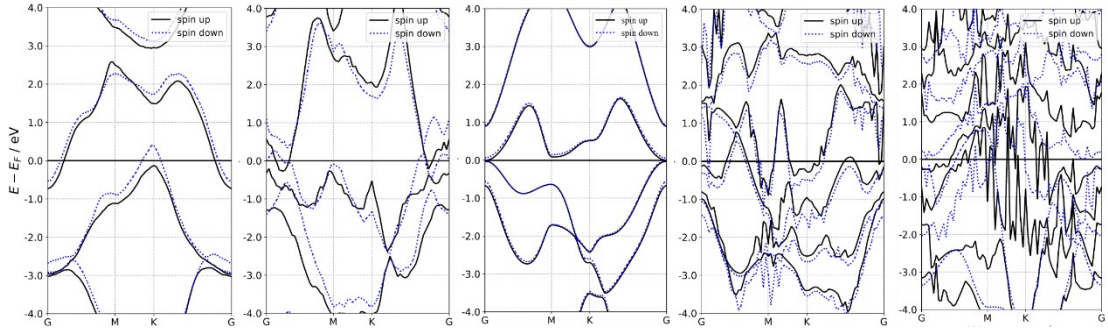



**Fig. S6.** The crystal orbital Hamilton population (COHP) between the S and metal atoms in 2H-$MoS_2$/$M_2C$ heterostructures.




(a) (b) (c) (d) (e)

**Fig. S7.** The computed band structures of 2H-$MoS_2$/$M_2C$ heterostructures, where M represents (a) Ti, (b) Zr, (c) Hf, (d) Nb, and (e) Ta, respectively. The Fermi level was set to zero.