Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Modulating Schottky Barrier of MXenes/2D SiC contacts via functional groups and biaxial strain: A First-Principles Study

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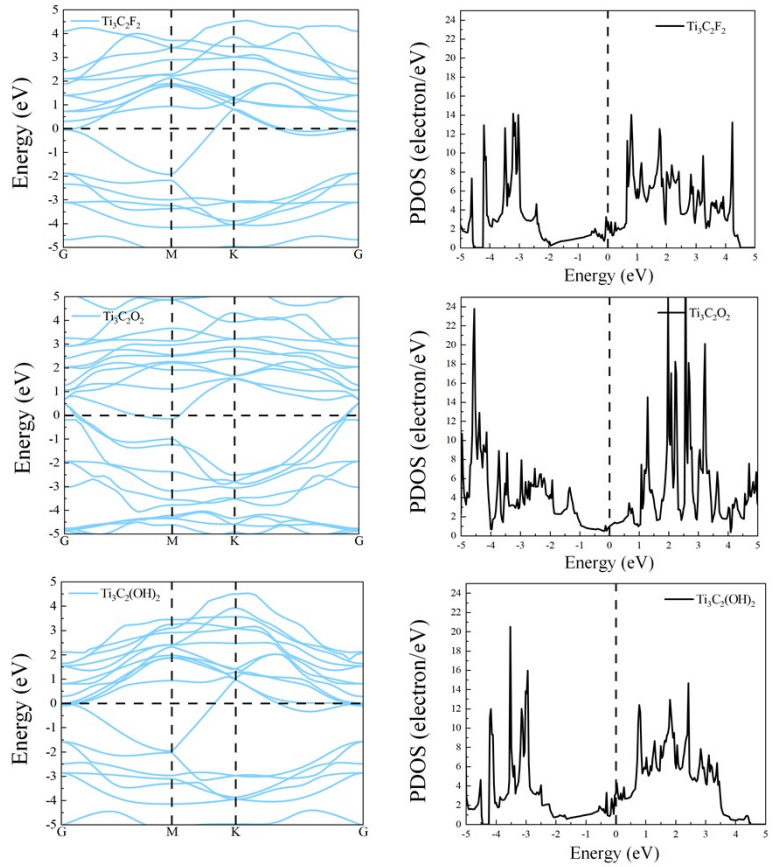

Figure S1. The band structures and PDOS of $Ti_3C_2T_2$. (The E_F is set to zero)

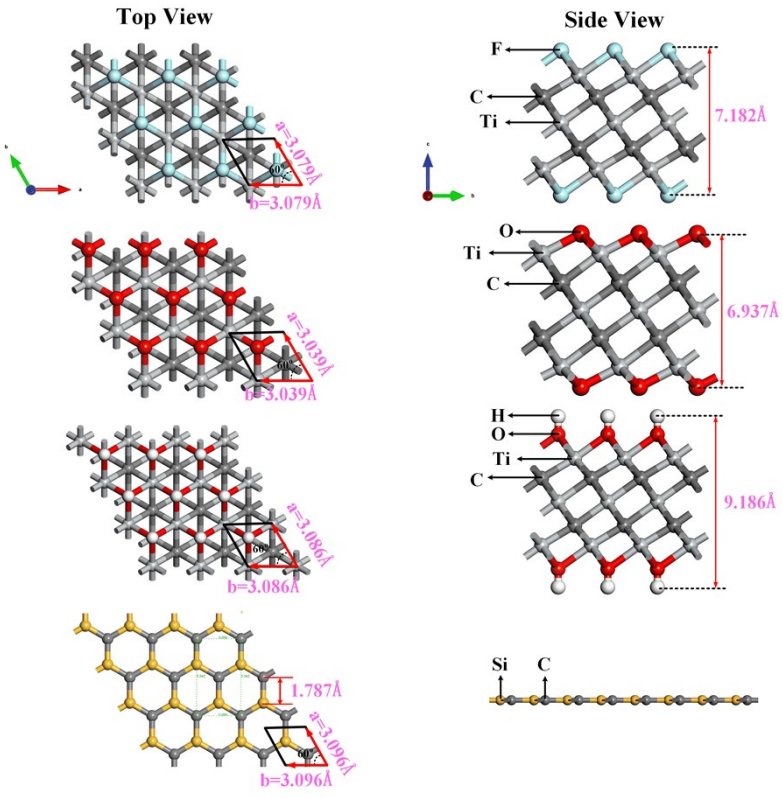

Figure S2. Top and Side views of crystal structures of $Ti_3C_2T_2$ and SiC.

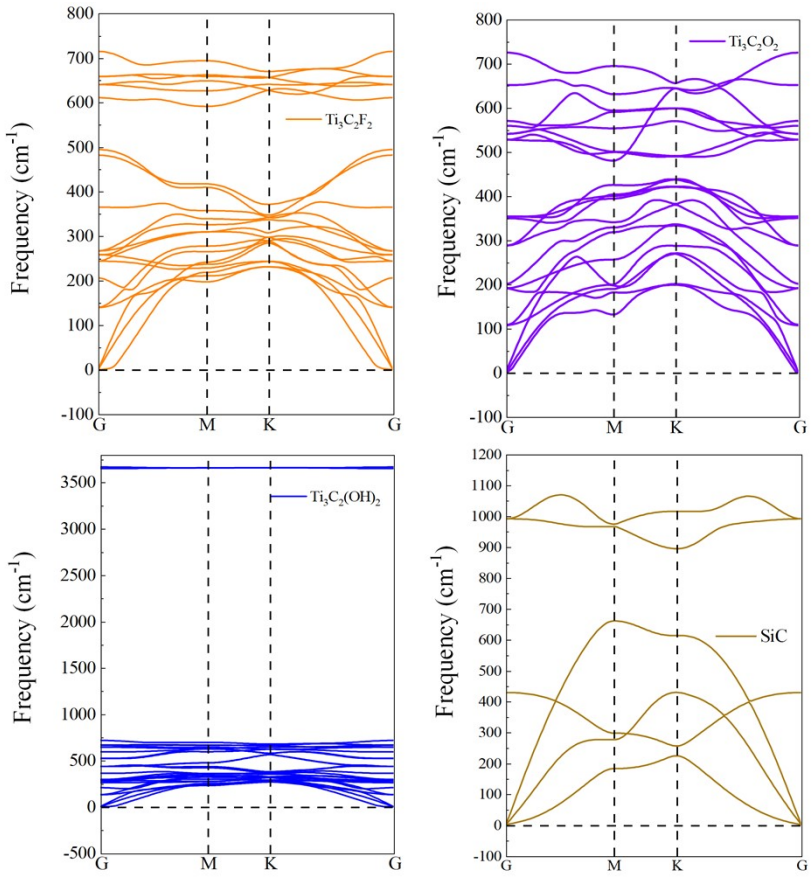

Figure S3. The phonon dispersion spectra of $Ti_3C_2T_2$ and SiC.

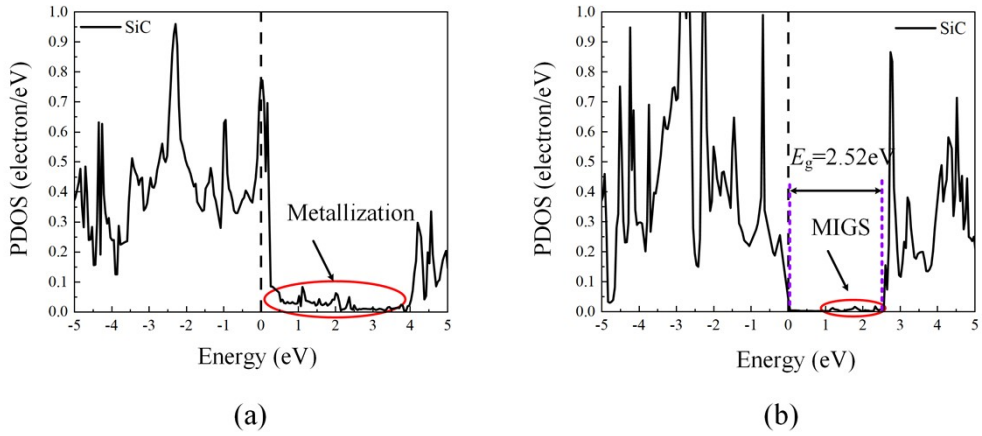

Figure S4. PDOS of SiC in (a) $Ti_3C_2O_2$/SiC(A) contact, (b) $Ti_3C_2O_2$/SiC(B) contact (The E_F is set to zero).

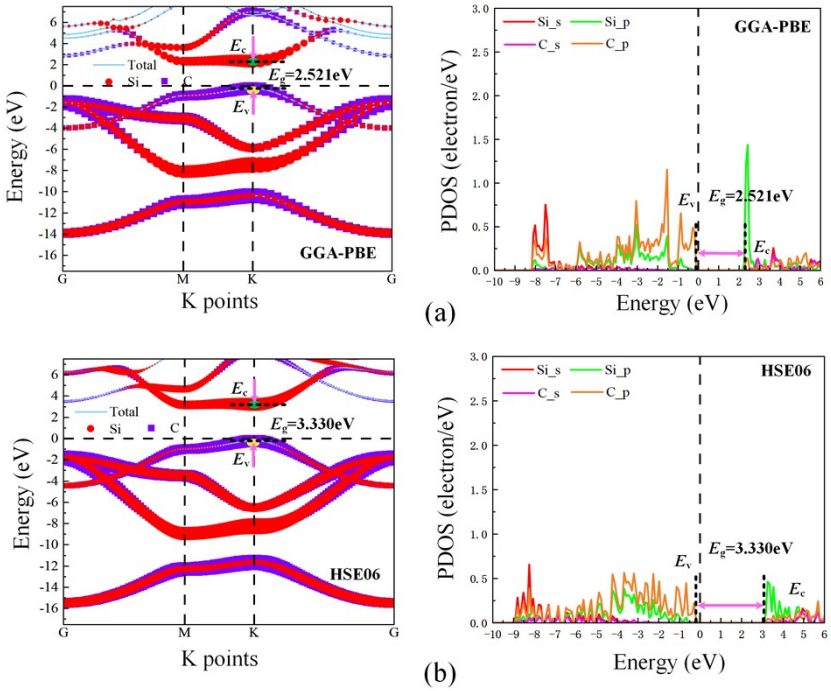

Figure S5. Band structures and PDOS of SiC calculated from (a) PBE and (b) HSE06 functional, respectively. (The E_F is set to zero).