Supporting information

Tight-binding model for the electronic structure of MXene monolayers

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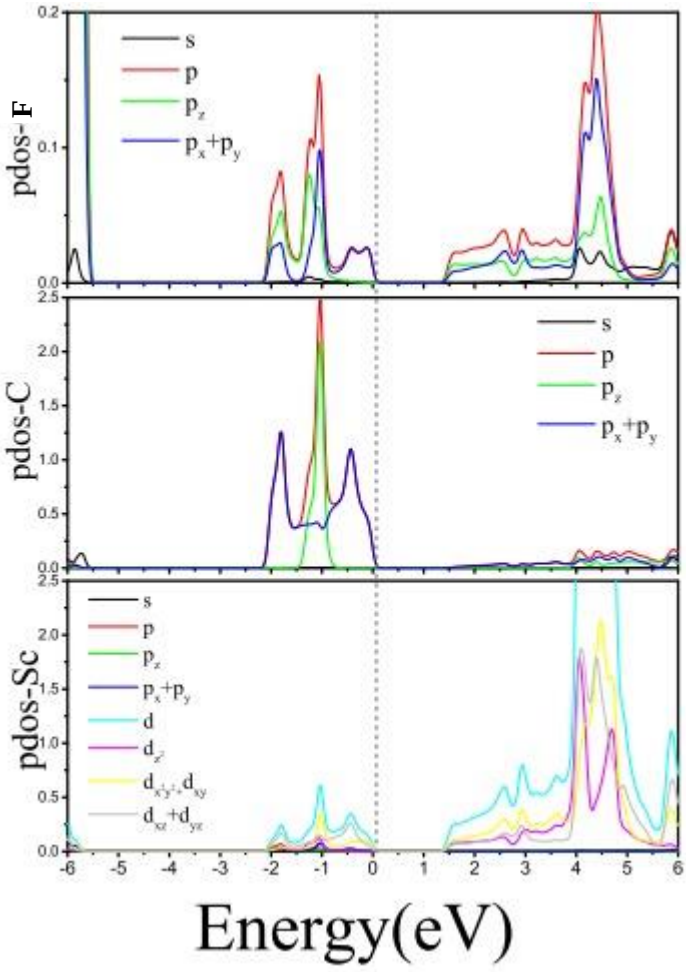

Fig. SI1: The projected density of states (PDOS) on atomic orbitals of Sc, F, and C atoms of Sc_2CF_2, respectively. Fermi energy is located at zero.

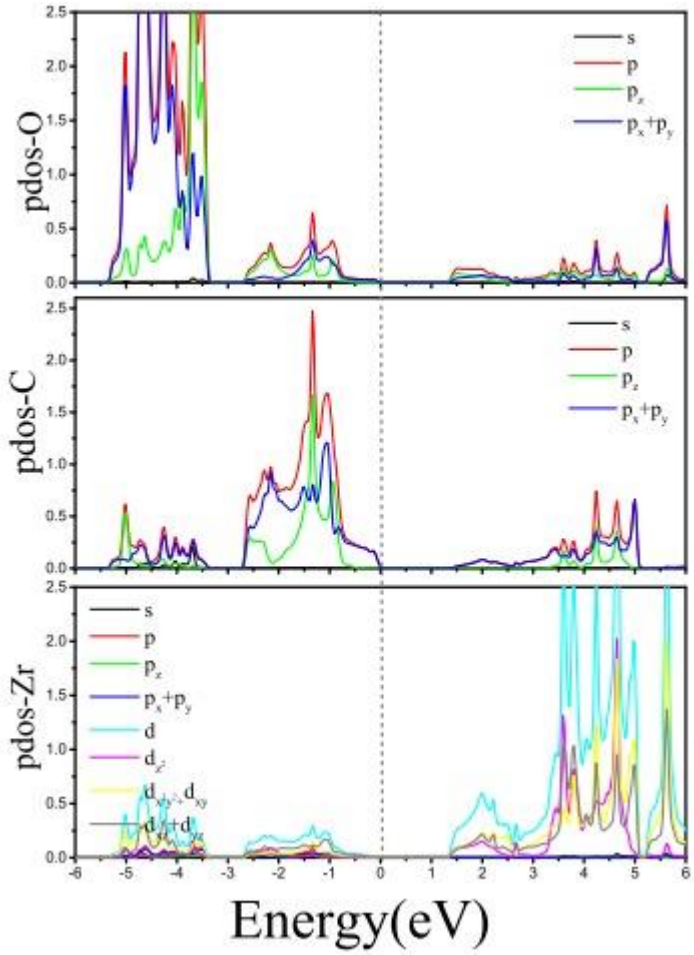

Fig. SI2: The projected density of states (PDOS) on atomic orbitals of Zr, O, and C atoms of Zr2CO2, respectively. Fermi energy is located at zero.

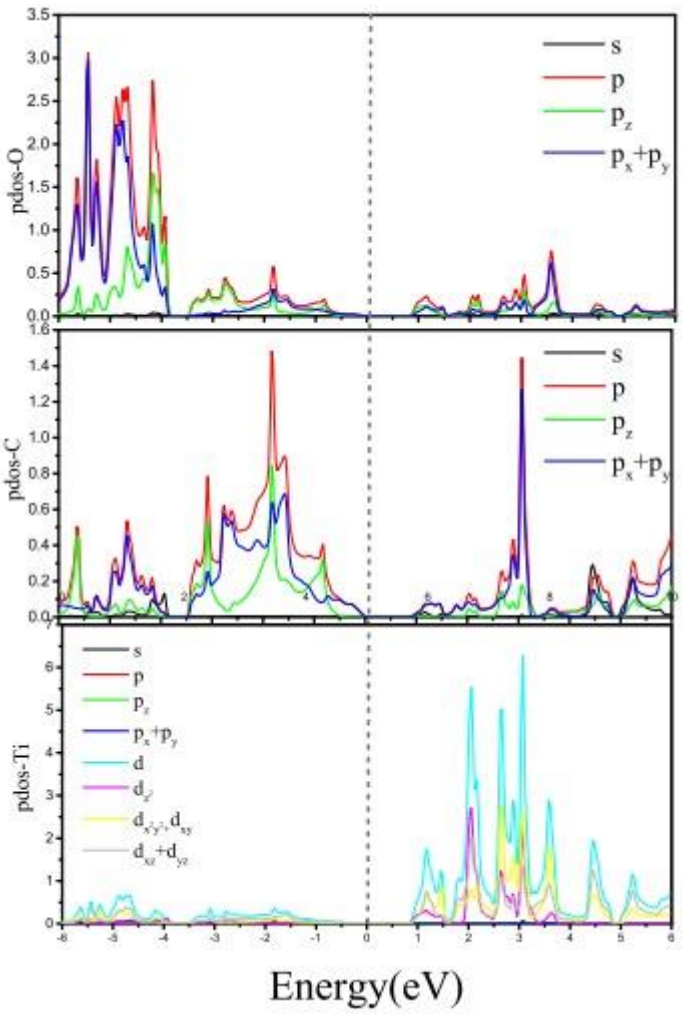

Fig. SI3: The projected density of states (PDOS) on atomic orbitals of Ti, O, and C atoms of Ti_2CO_2, respectively. Fermi energy is located at zero.