

Adsorption of Toxic Gases by Transition Metal Doped Ti_2CO_2 MXene: A DFT study

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†Electronic supplementary information (ESI) available:

Fig. S1 presents the band structures of pristine Ti_2CO_2 and vacancy-defective Ti_2O_2 after the adsorption of four gas molecules: (a) CO, (b) NO, (c) SO_2 , and (d) HF.

Fig. S2 shows the adsorption configurations of four gas molecules on the Fe-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF, including both top and side views.

Fig. S3 shows the density of states (PDOS) of the Fe-doped adsorption systems: (a) CO, (b) NO, (c) SO_2 , (d) HF.

Fig. S4 shows the charge density difference (CDD) diagrams of the Fe-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF.

Fig. S5 shows the adsorption configurations of four gas molecules on the Co-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF, including both top and side views.

Fig. S6 shows the band structure diagrams of the Co-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF.

Fig. S7 shows the density of states (PDOS) of the Co-doped adsorption systems: (a) CO, (b) NO, (c) SO_2 , (d) HF.

Fig. S8 shows the charge density difference (CDD) diagrams of the Co-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF.

Fig. S9 shows the adsorption configurations of four gas molecules on the Ni-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF, including both top and side views.

Fig. S10 shows the band structure diagrams of the Ni-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF.

Fig. S11 shows the charge density difference (CDD) diagrams of the Ni-doped system: (a) CO, (b) NO, (c) SO_2 , and (d) HF.

Fig. S12 shows the density of states (PDOS) of the Ni-doped adsorption systems: (a) CO, (b) NO, (c) SO_2 , (d) HF.

Table S1 Abbreviations and Corresponding terminology.

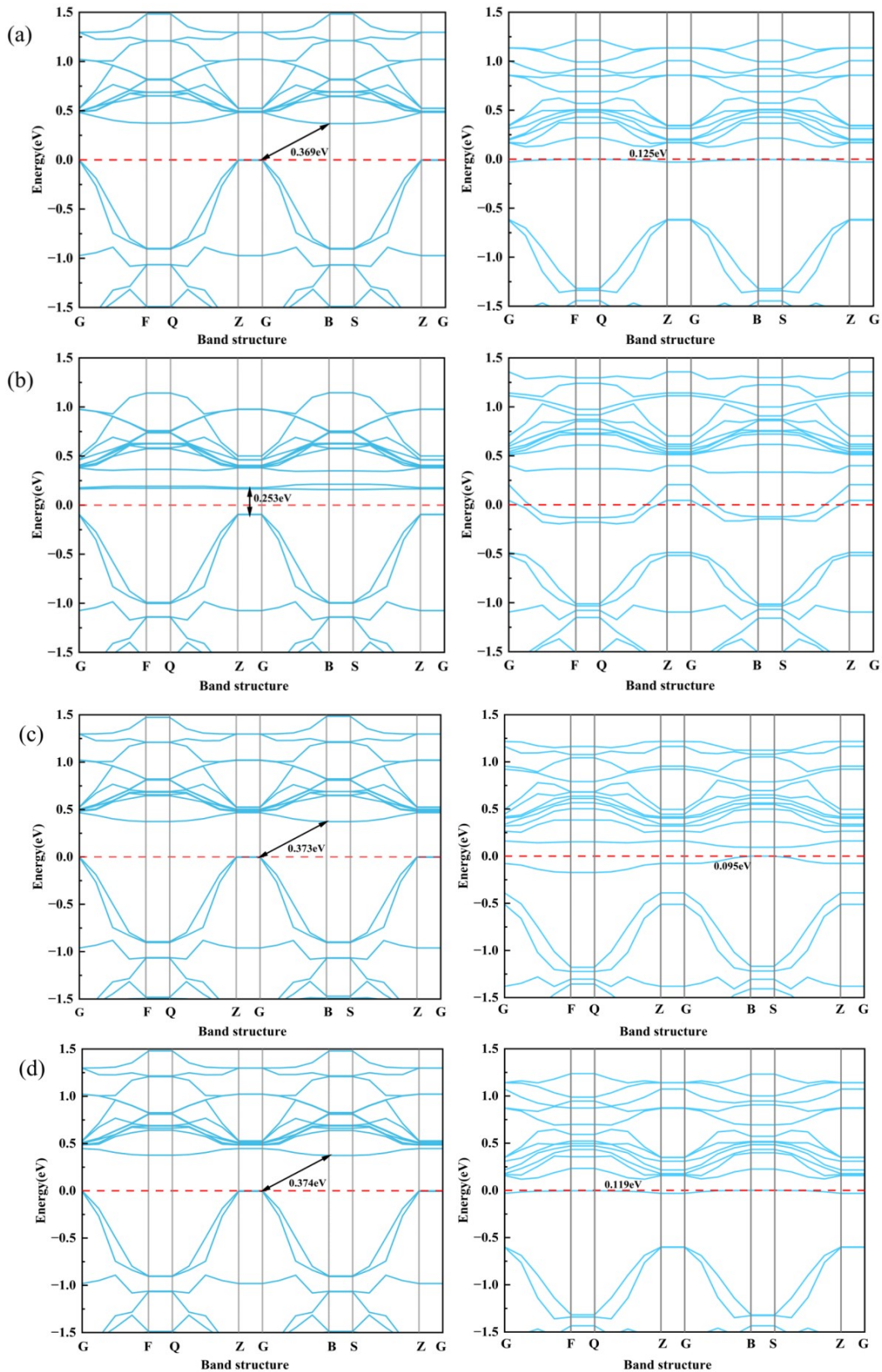


Fig. S1 shows the band structure diagrams of pristine Ti_2CO_2 and $\text{V-Ti}_2\text{CO}_2$ after the adsorption of CO, NO, SO_2 and HF: (a) $\text{Ti}_2\text{CO}_2\text{-CO}$, $\text{VTi}_2\text{CO}_2\text{-CO}$; (b) $\text{Ti}_2\text{CO}_2\text{-NO}$, $\text{VTi}_2\text{CO}_2\text{-NO}$; (c) $\text{Ti}_2\text{CO}_2\text{-SO}_2$, $\text{V-Ti}_2\text{CO}_2\text{-SO}_2$; (d) $\text{Ti}_2\text{CO}_2\text{-HF}$, $\text{VTi}_2\text{CO}_2\text{-HF}$

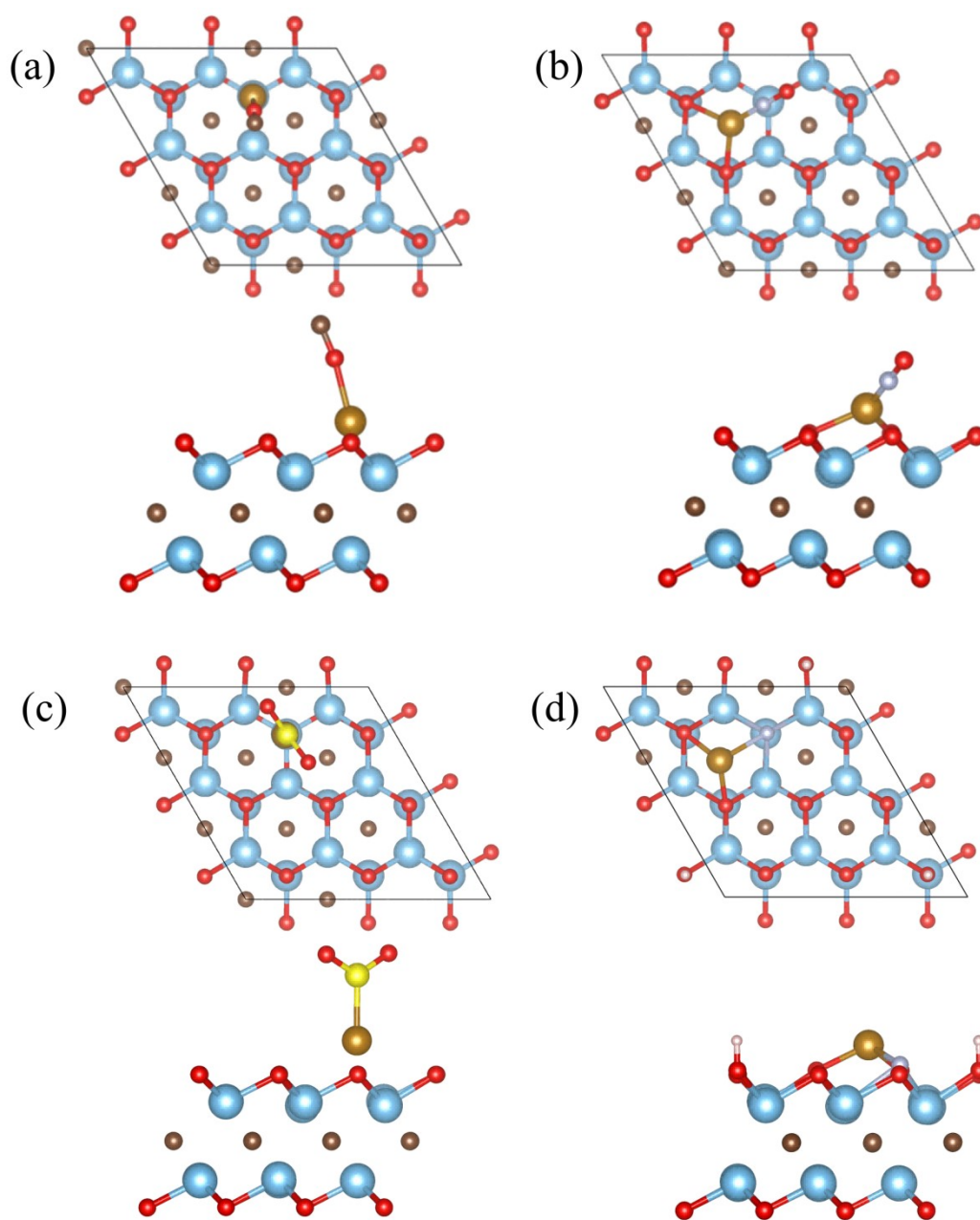


Fig. S2 shows the optimized structures of (a) CO/Fe-Ti₂CO₂, (b) NO/Fe-Ti₂CO₂, (c) SO₂/Fe-Ti₂CO₂ and (d) HF/Fe-Ti₂CO₂

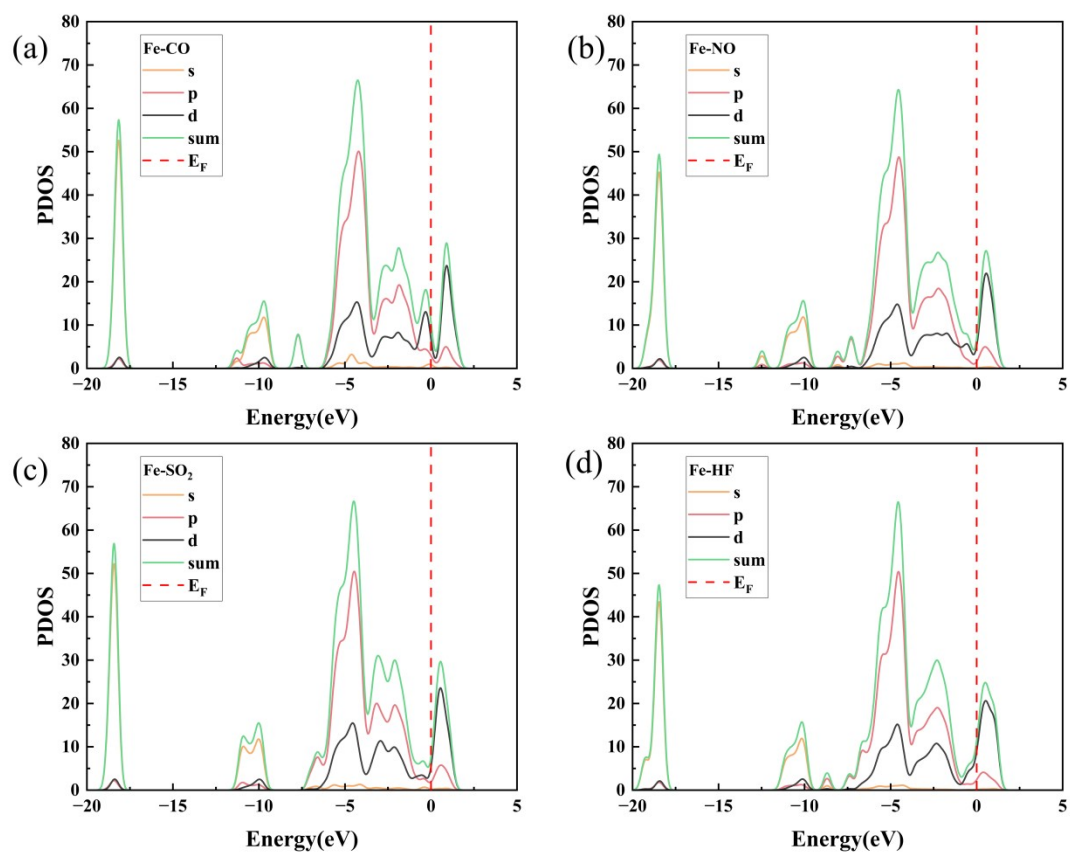


Fig. S3 shows the density of states (PDOS) of the Fe-doped adsorption systems: (a) CO/Fe-Ti₂CO₂, (b) NO/Fe-Ti₂CO₂, (c) SO₂/Fe-Ti₂CO₂, (d) HF/Fe-Ti₂CO₂

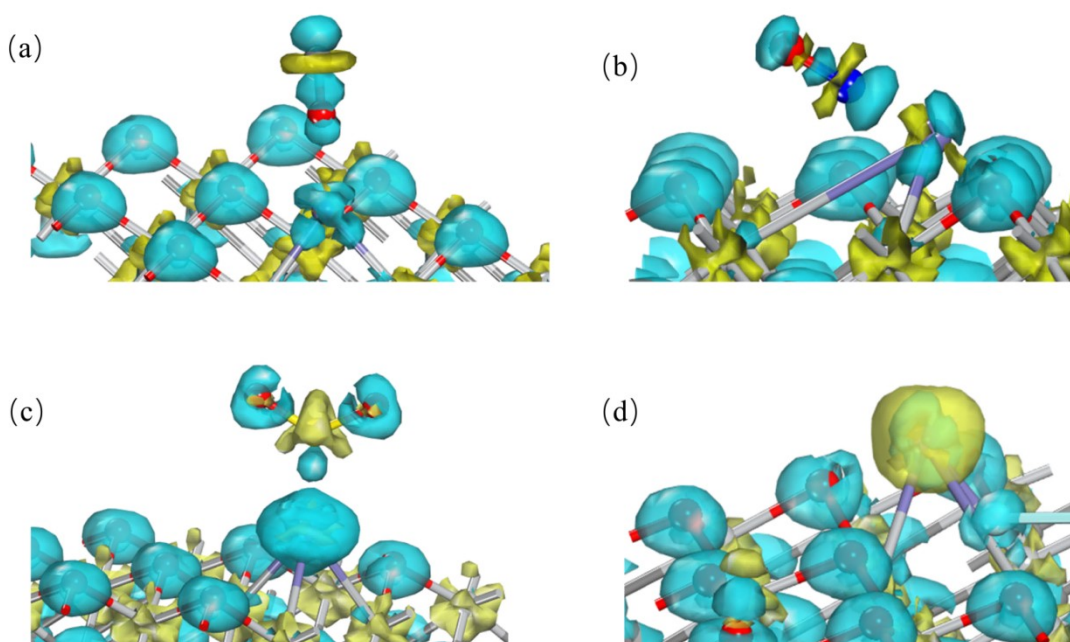


Fig. S4 shows the charge density difference (CDD) of the Fe-doped system: (a) CO/Fe-Ti₂CO₂, (b) NO/Fe-Ti₂CO₂, (c)SO₂/Fe-Ti₂CO₂, (d)HF/Fe-Ti₂CO₂

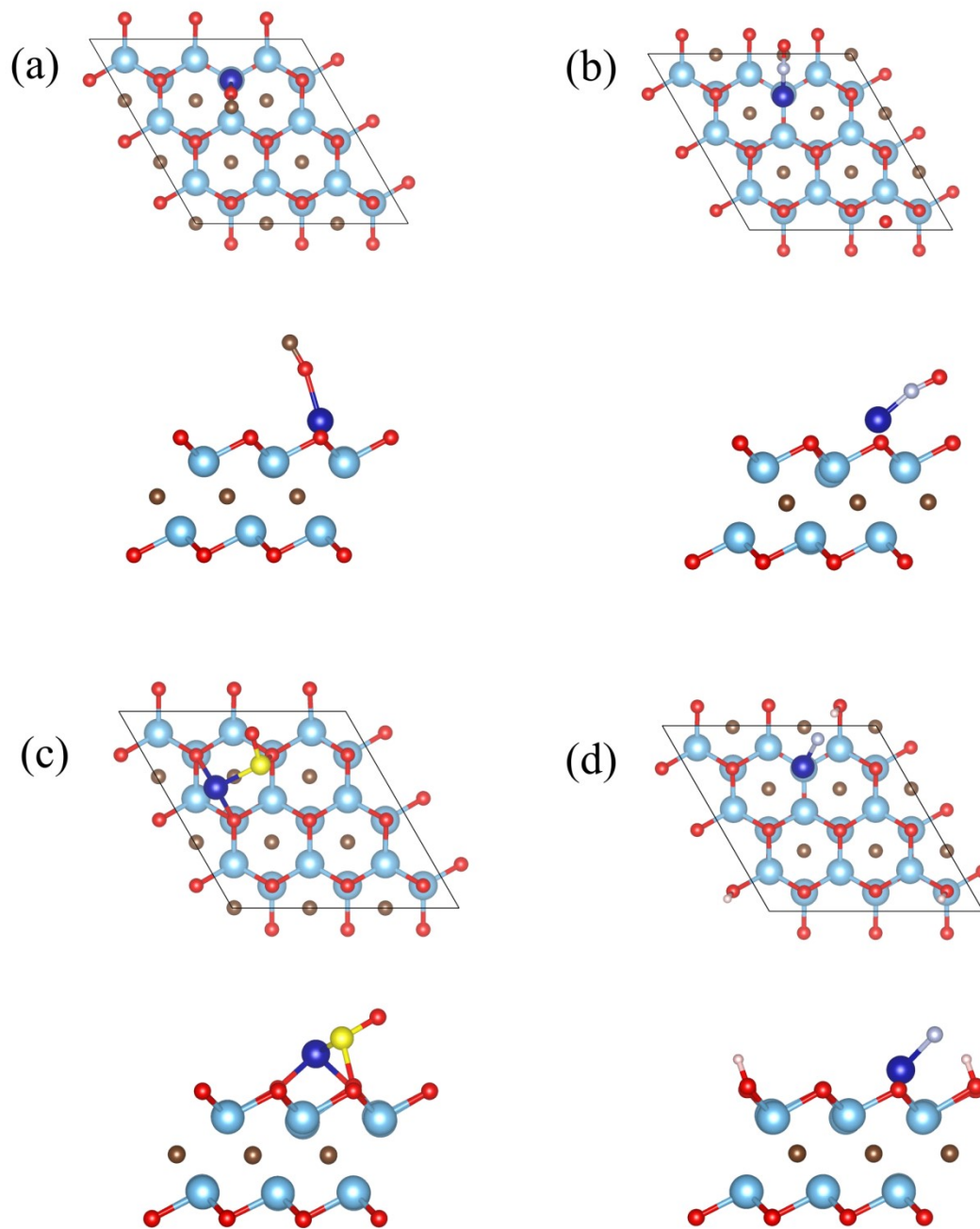


Fig. S5 shows the optimized structures of (a) CO/Co-Ti₂CO₂, (b) NO/Co-Ti₂CO₂, (c) SO₂/Co-Ti₂CO₂ and (d) HF/Co-Ti₂CO₂.

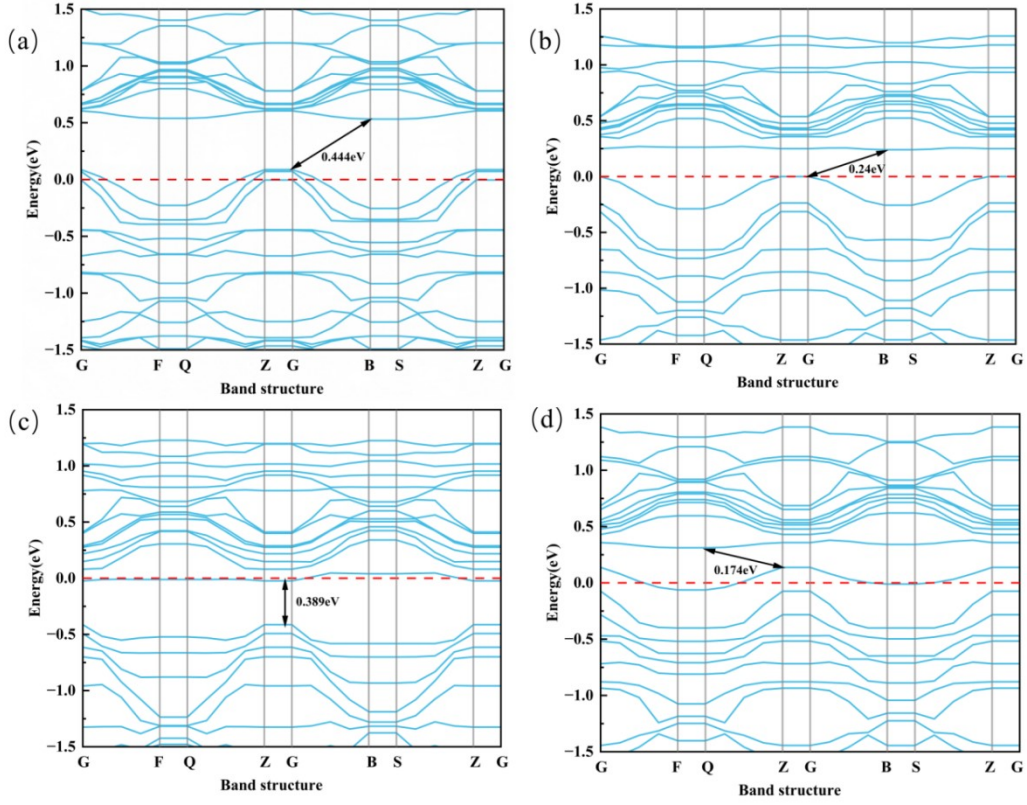


Fig. S6 shows the band structure diagrams of the Co-doped system: (a) CO/Co-Ti₂CO₂, (b) NO/Co-Ti₂CO₂, (c) SO₂/Co-Ti₂CO₂ and (d) HF/Co-Ti₂CO₂.

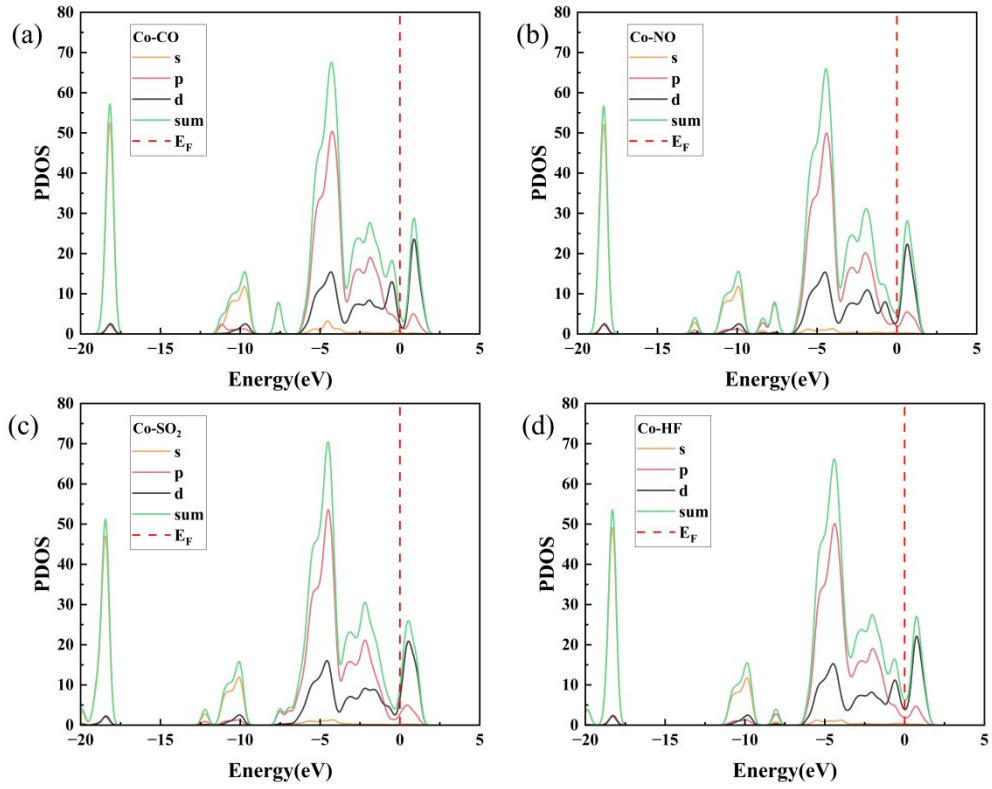


Fig. S7 shows the density of states (PDOS) of the Co-doped adsorption systems: (a) CO/Co-Ti₂CO₂, (b) NO/Co-Ti₂CO₂, (c) SO₂/Co-Ti₂CO₂, (d) HF/Co-Ti₂CO₂

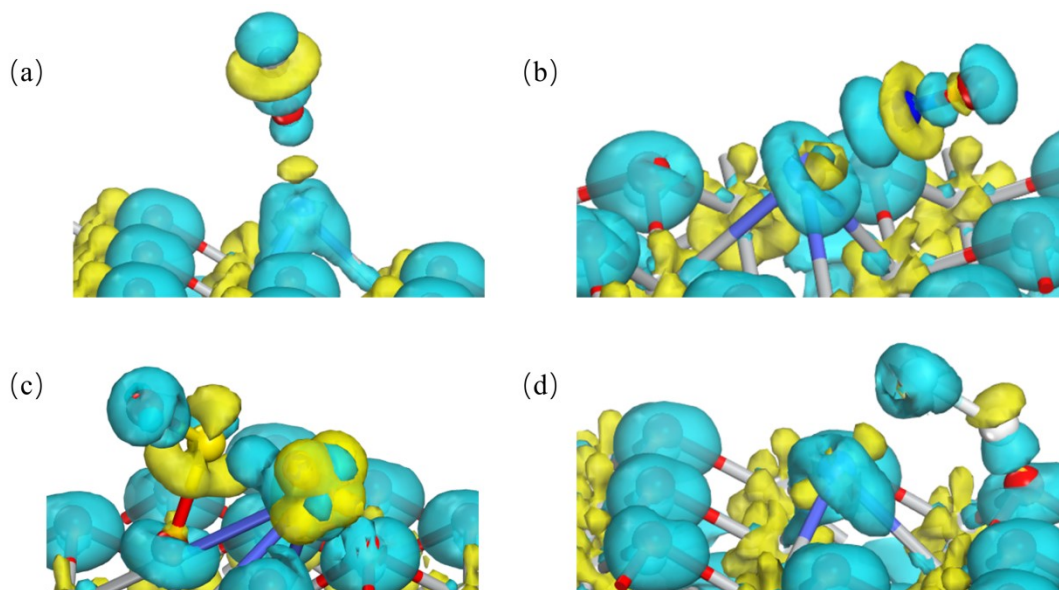


Fig. S8 shows the charge density difference (CDD) diagrams of the Co-doped system: (a) CO/Co-Ti₂CO₂, (b) NO/Co-Ti₂CO₂, (c) SO₂/Co-Ti₂CO₂ and (d) HF/Co-Ti₂CO₂.

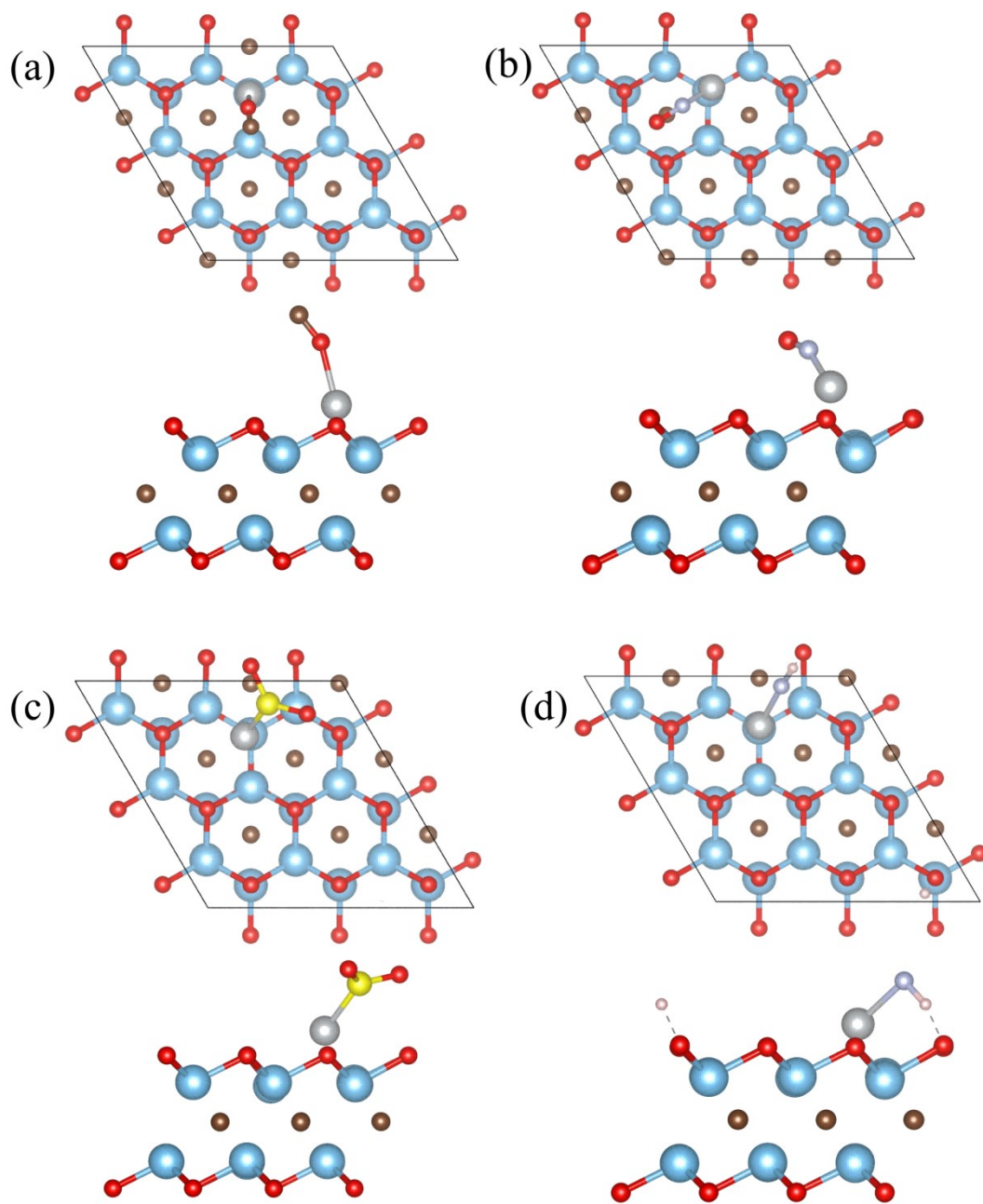


Fig. S9 shows the optimized structures of (a) CO/Ni-Ti₂CO₂, (b) NO/Ni-Ti₂CO₂, (c) SO₂/Ni-Ti₂CO₂ and (d) HF/Ni-Ti₂CO₂.

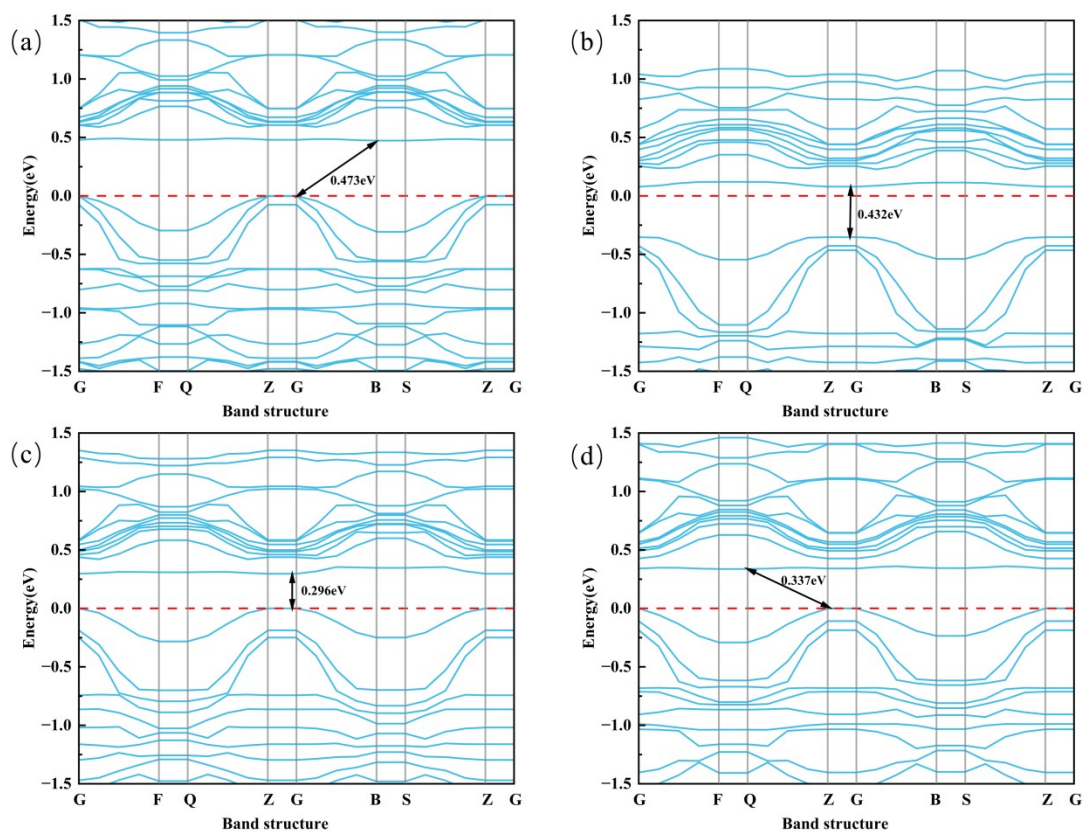


Fig. S10 shows the band structure diagrams of the Ni-doped system: (a) CO/Ni-Ti₂CO₂, (b) NO/Ni-Ti₂CO₂, (c) SO₂/Ni-Ti₂CO₂ and (d) HF/Ni-Ti₂CO₂.

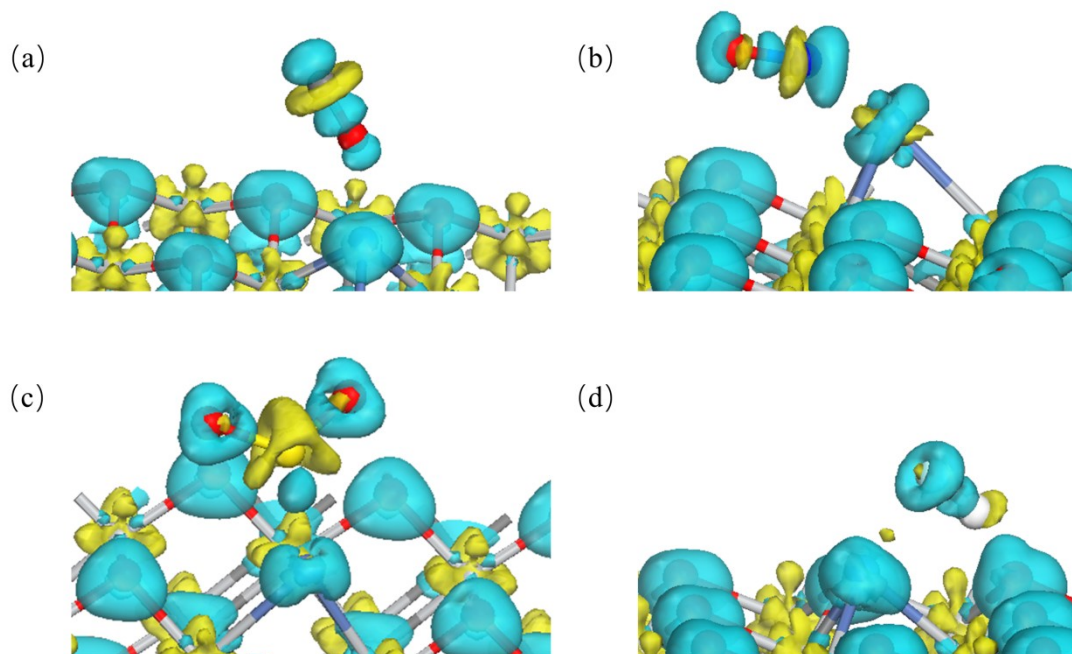


Fig. S11 shows the charge density difference (CDD) diagrams of the Ni-doped system: (a) CO/Ni-Ti₂CO₂, (b) NO/Ni-Ti₂CO₂, (c) SO₂/Ni-Ti₂CO₂ and (d) HF/Ni-Ti₂CO₂.

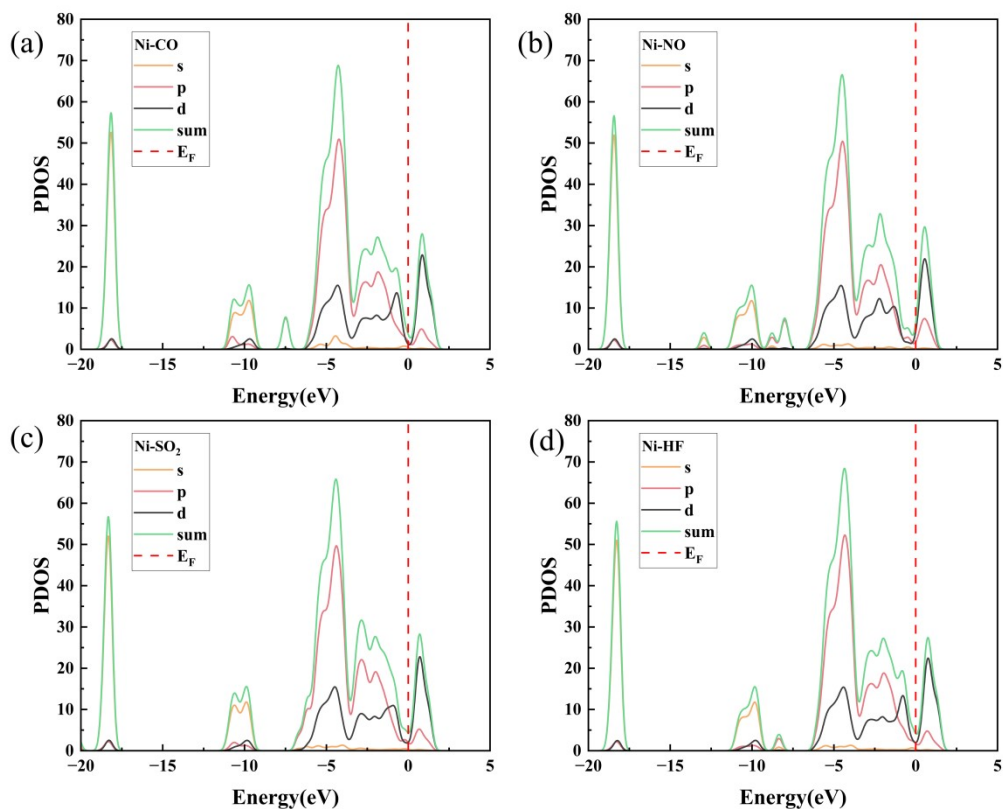


Fig. S12 shows the density of states (PDOS) of the Ni-doped adsorption systems: (a) CO/Ni-Ti₂CO₂, (b) NO/Ni-Ti₂CO₂, (c) SO₂/Ni-Ti₂CO₂, (d) HF/Ni-Ti₂CO₂.

Table S1 Abbreviations and Corresponding terminology

Abbreviations	Corresponding terminology
Ti ₂ CO ₂	Oxygen-terminated titanium carbide MXene
TM-Ti ₂ CO ₂	Transition metal-doped Ti ₂ CO ₂
Fe-Ti ₂ CO ₂	Fe-doped Ti ₂ CO ₂
Co-Ti ₂ CO ₂	Co-doped Ti ₂ CO ₂
Ni-Ti ₂ CO ₂	Ni-doped Ti ₂ CO ₂
VTi ₂ CO ₂	O-vacancy structures
CO	Carbon monoxide
NO	Nitric oxide
SO ₂	Sulfur dioxide
HF	Hydrogen fluoride
2D	Two-dimensional
PDOS	Partial density of states
TDOS	Total density of states
CDD	Charge differential density

CBM	Conduction band minimum
VBM	Valence band maximum
DFT	Density functional theory
GGA	Generalized gradient approximation
PBE	Perdew-Burke-Ernzerhof
DNP	Polarized double numerica
BSSE	Basis Set Superposition Error
SCF	Self-consistent field