



## Supporting Information

# A Theoretical Study of Fe Adsorbed on Pure and Nonmetal (N, F, P, S, Cl)-Doped $\text{Ti}_3\text{C}_2\text{O}_2$ for Electrocatalytic Nitrogen Reduction

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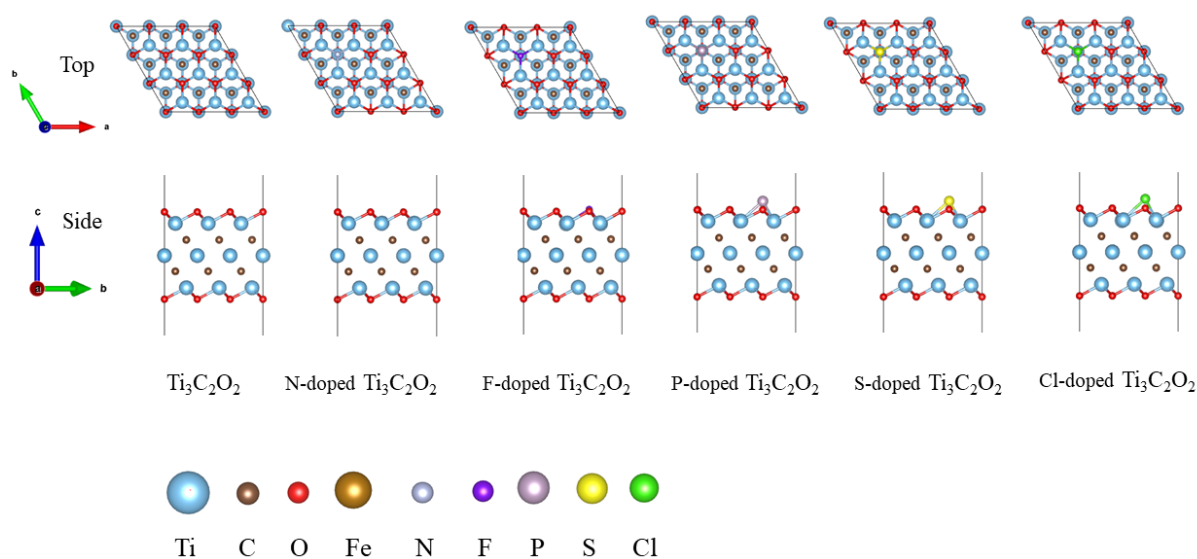
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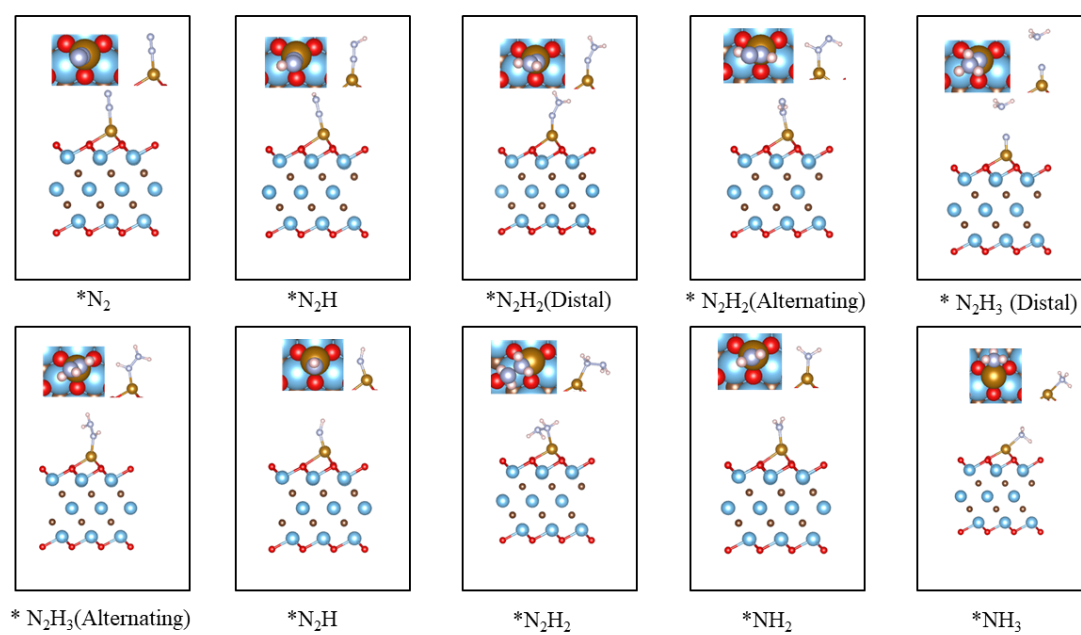
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**Figure S1.** Top and side views of  $\text{Ti}_3\text{C}_2\text{O}_2$  and its nonmetal doped structure.



**Figure S2.** Optimized structures of all the possible elementary steps in NRR, taking Ti<sub>3</sub>C<sub>2</sub>O<sub>2</sub> as an example. Other nonmetal-doped Ti<sub>3</sub>C<sub>2</sub>O<sub>2</sub> show similar geometric structures.