

SUPPORTING INFORMATION

*CO adsorption, oxidation and carbonate formation mechanisms on  $Fe_3O_4$  surfaces*

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Figure S1. Configurations of least stable CO adsorption and oxidation on Fe<sub>tet1</sub> termination

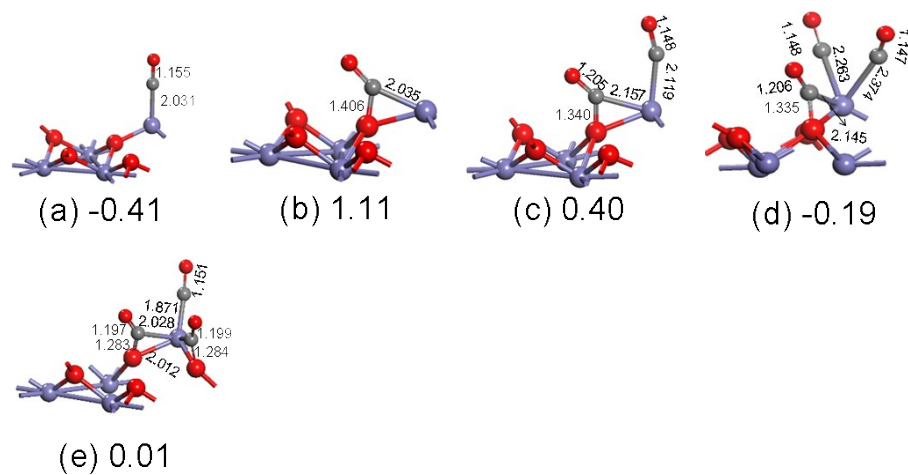


Figure S2. Configurations of least stable CO adsorption and oxidation on Fe<sub>oct2</sub> termination

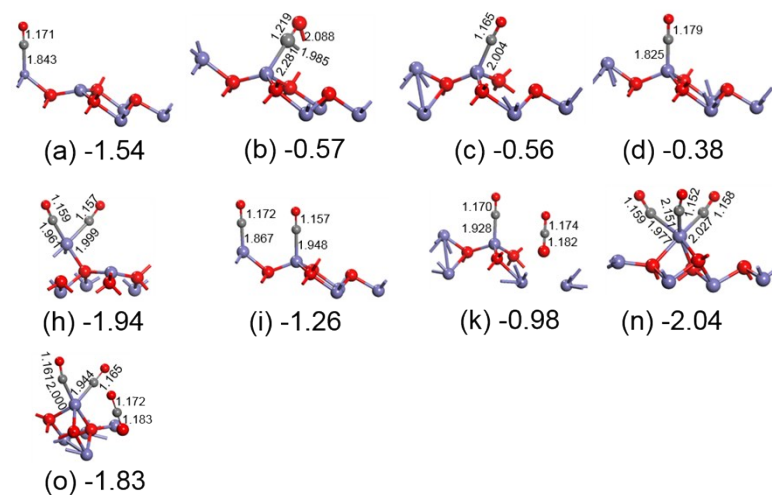


Figure S3. Configurations of least stable CO adsorption, oxidation and carbonate on  $\text{Fe}_3\text{O}_4(110)$  A layer.

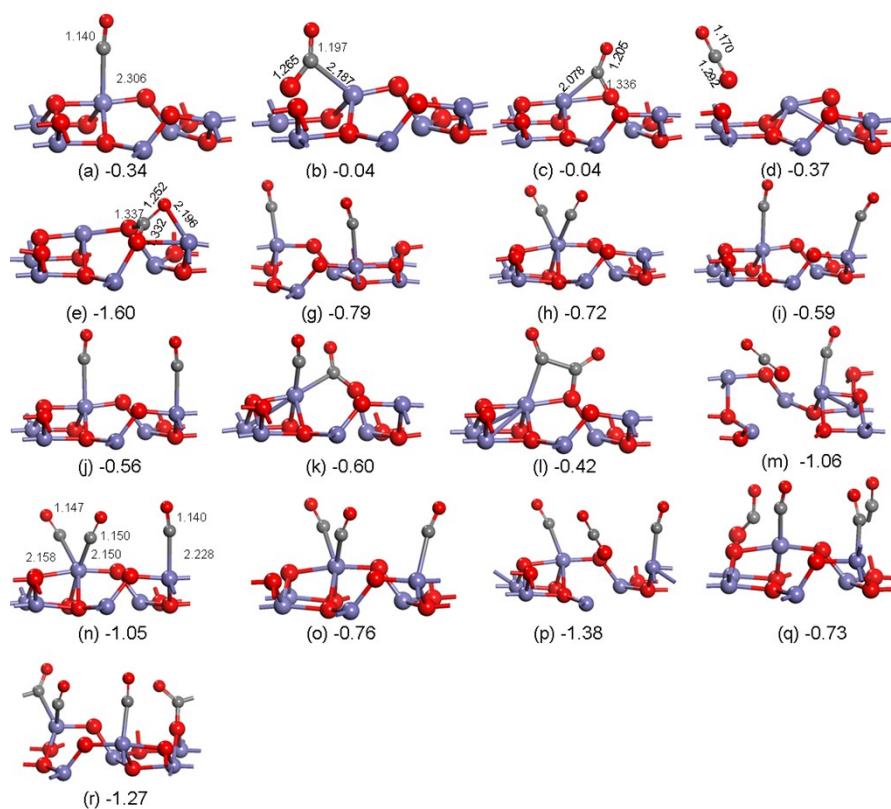


Figure S4. Configurations of least stable CO adsorption and oxidation on  $\text{Fe}_3\text{O}_4(110)$  B layer.

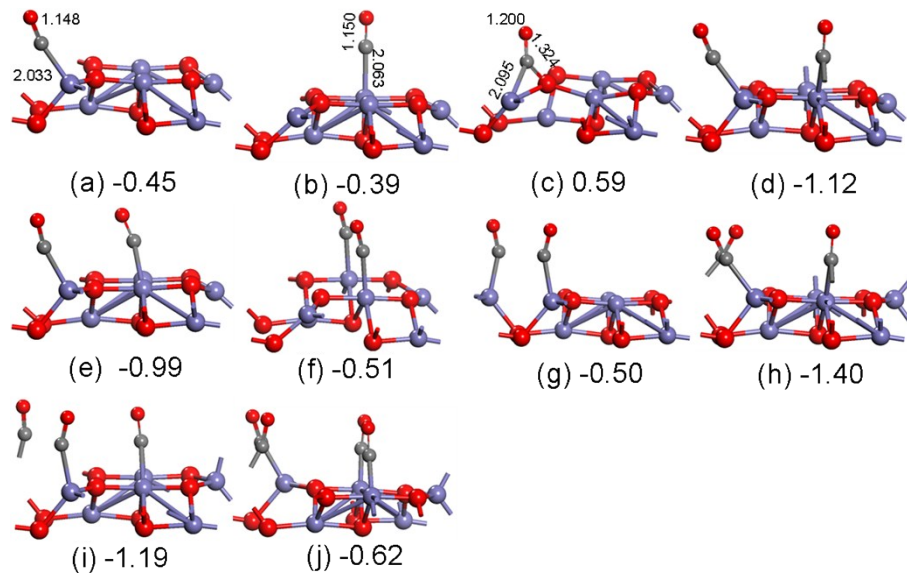


Figure S5. Configurations of least stable CO adsorption, oxidation and carbonate on on  $\text{Fe}_3\text{O}_4(001)$  B termination.

