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


# *Supporting Information*

**Iron-embedded $C_2N$ monolayer: a promising low-cost and high-activity single-atom catalyst for CO oxidation**

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**Table S1.** The adsorption energies ($E_{ad}$, in eV) and some selected structural parameters for $CO_2$ adsorbed on the $Fe/C_2N$ monolayer with different convergence criteria in Hellmann–Feynman force ($eVÅ^{-1}$). The units of the bond distance and bond angle are angstrom and degree, respectively.

| | 0.02 | 0.01 | 0.005 | 0.002 |
|---|---|---|---|---|
| $E_{ad}$ | 0.230 | 0. 228 | 0.227 | 0.227 |
| $d_{(C\text{-}Fe)}$ | 1.995 | 1.995 | 1.994 | 1.994 |
| $d_{(O\text{-}C)}$ | 1.252, 1.202 | 1.252, 1.202 | 1.252, 1.202 | 1.252, 1.202 |
| ∠(O-C-O) | 149.005 | 148.929 | 148.977 | 148.995 |

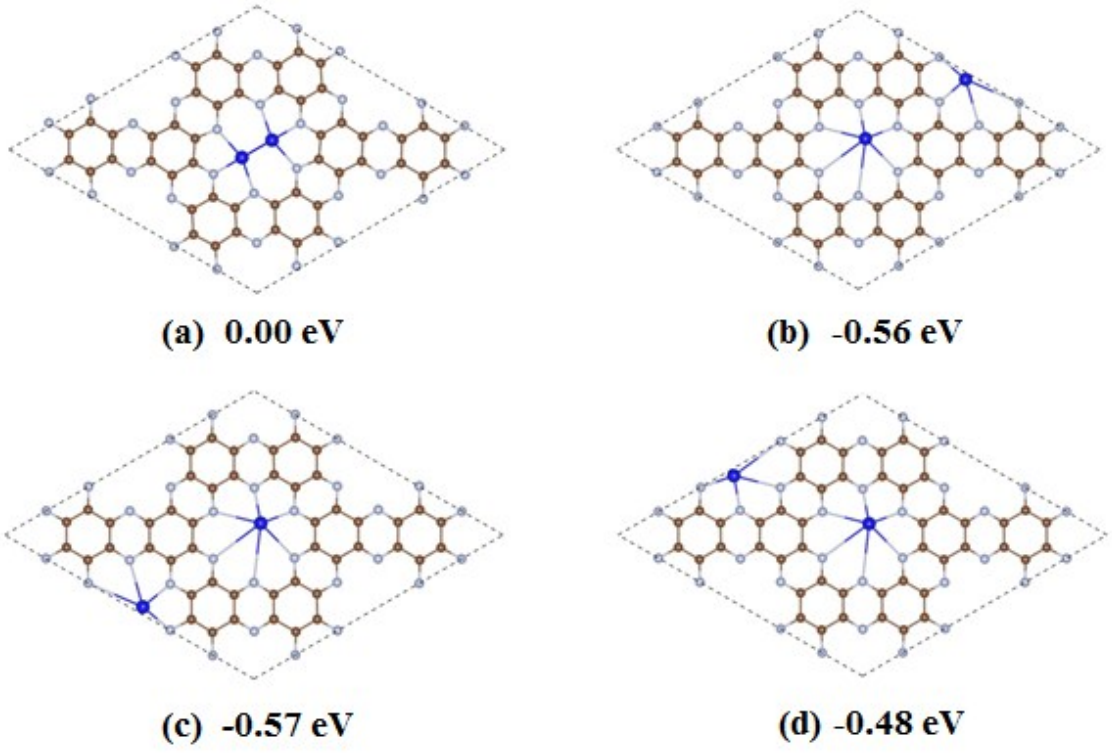


**Fig. S1.** The atomic structures of the most stable configuration of the $C_2N$ monolayer with the adsorbed Fe dimer and some configurations with two separate Fe atoms. The energies for these structures have been calculated with respect to the configuration shown in (a).

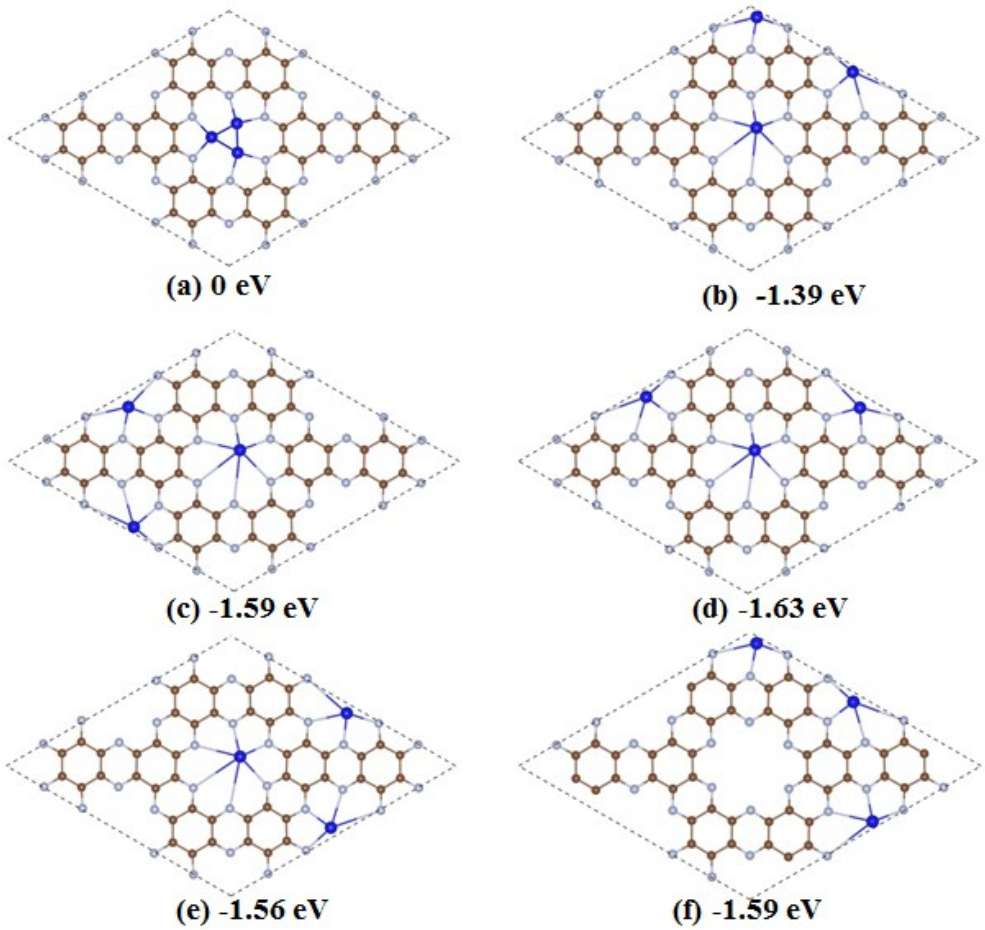


**Fig. S2.** The atomic structures of the most stable configuration of the $C_2N$ monolayer with the adsorbed Fe trimer and some configurations with three separate Fe atoms. The energies for these structures have been calculated with respect to the configuration shown in (a).