

## Supporting Information

### Coordination environment effect of single-atom catalysts on their nitrogen reduction reaction performance

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Table S1. The calculated magnetic moment of different configurations.

| configuration        | O <sub>4</sub> | NO <sub>3</sub> | N <sub>2</sub> O <sub>2</sub> | N <sub>3</sub> O | N <sub>4</sub> | N <sub>3</sub> C | N <sub>2</sub> C <sub>2</sub> | NC <sub>3</sub> | C <sub>4</sub> | C <sub>3</sub> O | C <sub>2</sub> O <sub>2</sub> | C <sub>1</sub> O <sub>3</sub> |
|----------------------|----------------|-----------------|-------------------------------|------------------|----------------|------------------|-------------------------------|-----------------|----------------|------------------|-------------------------------|-------------------------------|
| Magnetic moment (μB) | 2.92           | 3.01            | 3.14                          | 1.57             | 1.92           | 2.22             | 2.26                          | 2.68            | 2.24           | 2.45             | 1.98                          | 1.60                          |

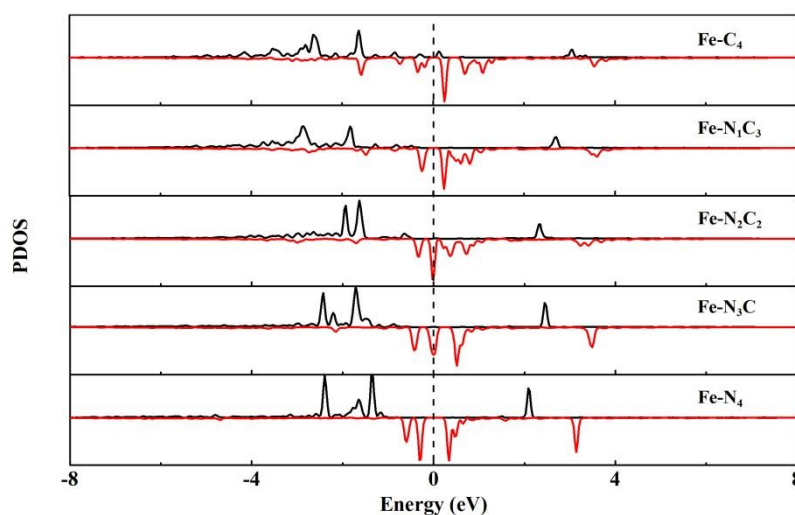


Fig. S1. PDOS of Fe-3d in Fe-N<sub>4-x</sub>C<sub>x</sub>-C, the Fermi level is denoted by the vertical dash line and set at 0 eV.

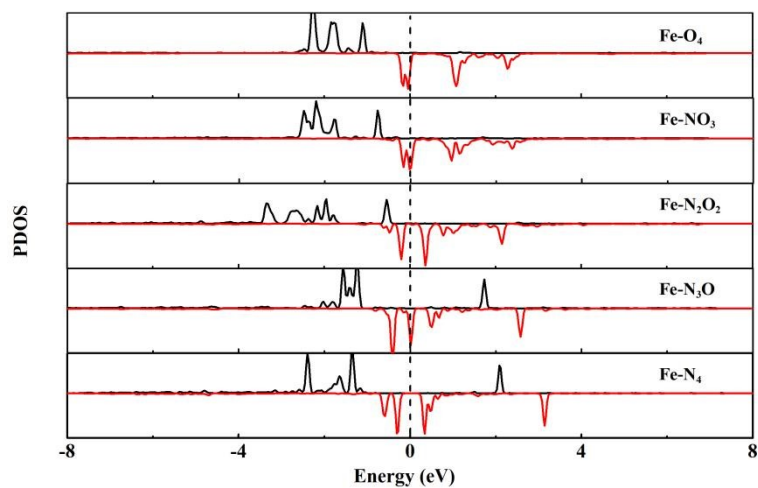


Fig. S2. PDOS of Fe-3d in  $\text{Fe-N}_x\text{O}_{4-x}\text{-C}$ , the Fermi level is denoted by the vertical dash line and set at 0 eV.

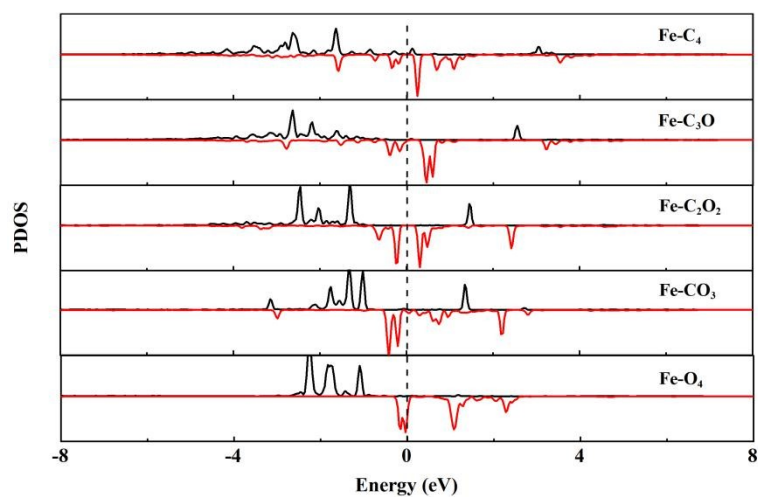


Fig. S3. PDOS of Fe-3d in  $\text{Fe-C}_{4-x}\text{O}_x\text{-C}$ , the Fermi level is denoted by the vertical dash line and set at 0 eV.