Supplementary Materials: Oxygen Reduction Electrocatalysts Based on Coupled Iron Nitride Nanoparticles with Nitrogen-Doped Carbon

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1. DFT calculations of XRD spectra

The stability of the structures are calculated by formation energy, defined as $E_f(x) = E_{tot}(Fe_xN_y) - E_{tot}(Fe) - x\ E_{tot}(N)$, where $E_{tot}(Fe_xN_y)$ is the total energy per Fe_xN_y unit, $E_{tot}(Fe)$ is the total energy per iron atom in the Fe crystal and $E_{tot}(N)$ is the energy per nitrogen atom in the N_2 molecule. Density functional theory (DFT) calculations were carried out with the Vienna ab-initio simulation package (VASP) [1,2] The exchange-correlation energy is described by generalized gradient approximation (GGA) proposed by Perdew, Burke and Ernzerhof (PBE) [3] The electronic wave functions were expanded on a plane wave basis set with a kinetic energy cutoff at 500 eV. Effects of the core electrons were replaced by projector augmented wave (PAW) potentials [4] After having obtained the most optimized structure from DFT calculation, a theoretical XRD pattern was generated by FullProf suite to match the experimental data.

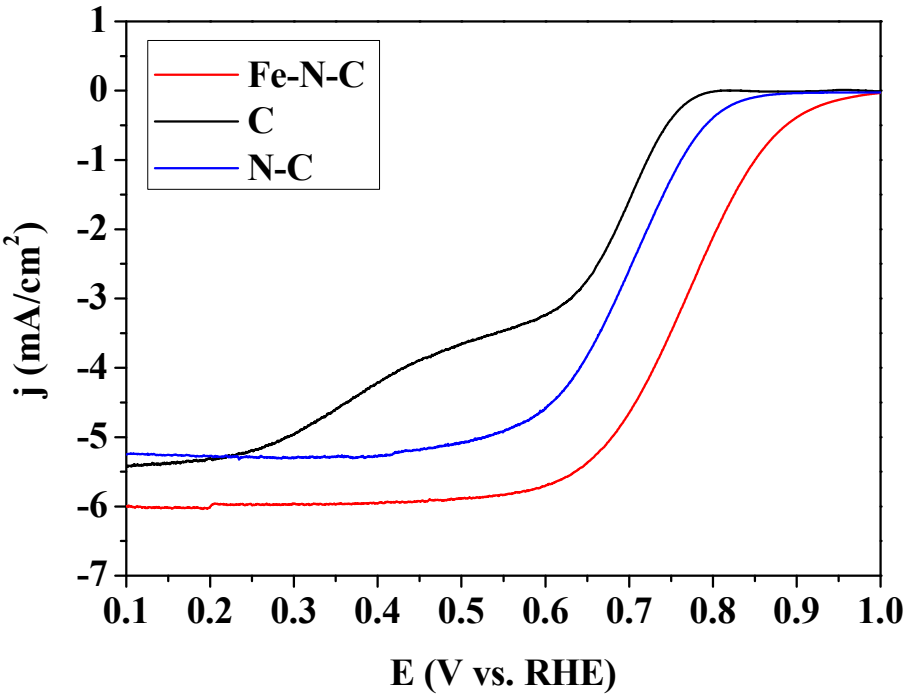

Figure S1. Linear sweep voltammetry curves of ORR in 0.1 M KOH catalyzed by Fe-N-C, C, and N-C.

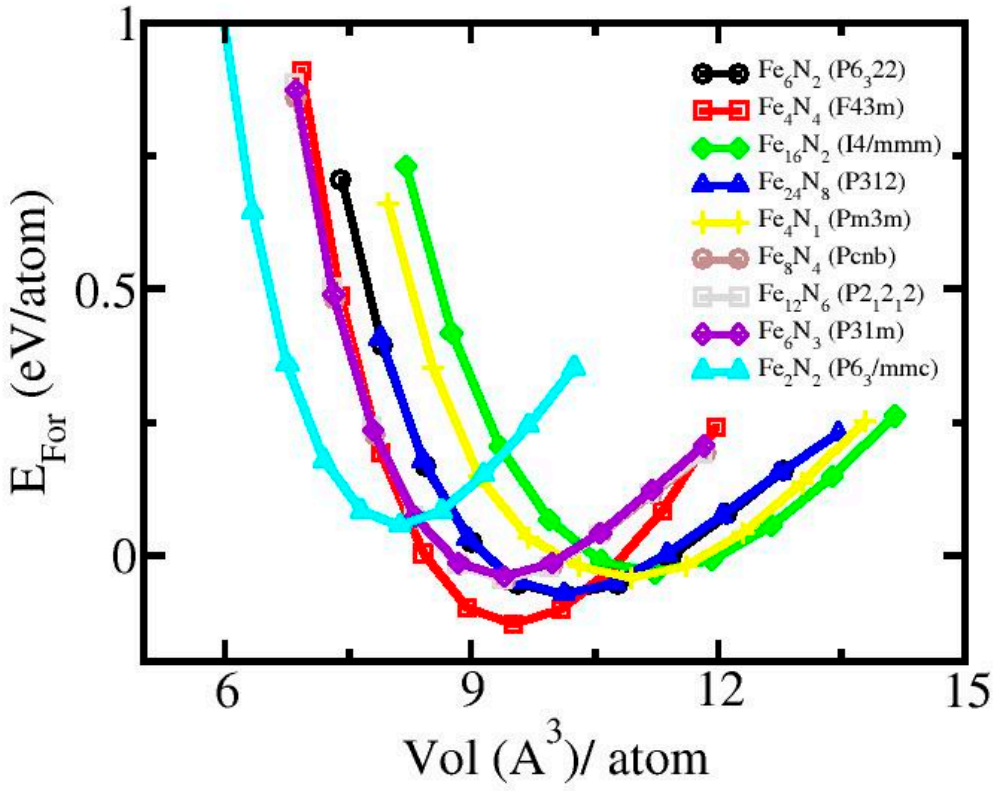

Figure S2. Calculated formation energy for different Fe_xN_y compounds.

References

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3. Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.
4. Blöchl, P.E. Projector augmented-wave method. *Phys. Rev. B* **1994**, *50*, 17953–17979.