Supporting Information

Modulating d-band center of boron doped single-atom site to boost oxygen reduction reaction

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1. Sample preparation

Synthesis of Fe\textsubscript{SA}/B,N-CNT, Fe\textsubscript{SA}/N-CNT, Fe\textsubscript{NP}/N-CNT and N doped carbon

Typically, polyvinylpyrrolidone (4 g), zinc nitrate (0.42 g), and 2-methylimidazole (3.36 g) were dissolved in 40 ml deionized water in a glass vial. The mixture was stirred at room temperature for 3 h. After adding ferric chloride (40 mg) into the solution, the vial was capped and 120 °C oven for 12 h. Lyophilization was performed to dry the mixture. 100 mg of the obtained powder and 250 mg of sodium borohydride were placed at two separate positions in a ceramic crucible with the sodium borohydride at the upstream side. The samples were heated at 900 °C for 2 h under argon atmosphere. The pyrolysis products were acid-washed with 1 M HCl solution at 80 °C overnight and then filtered and washed with plenty of deionized water. The final catalysts were obtained by vacuum drying. For comparison, the Fe\textsubscript{SA}/N-CNT was synthesized following the same procedure as Fe\textsubscript{SA}/B,N-CNT, but without involving sodium borohydride in the pyrolysis process. Fe\textsubscript{NP}/N-CNT was synthesized following the same procedure as Fe\textsubscript{SA}/N-CNT, except for the addition of 240 mg ferric chloride. The N doped carbon was synthesized following the same procedure as Fe\textsubscript{SA}/N-CNT, except for the addition of ammonium persulphate (100 mg) instead of ferric chloride.

2. Sample characterization

The morphologies were observed with a field emission scanning electron microscope (FESEM, SU8010, Japan) and a field emission transmission electron microscope (FETEM, Tecnai G2 F20, Hong Kong). The dispersion of single Fe atoms was characterized by atomic-resolution high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) on a JEOL JEM-ARM200F instrument equipped with probe spherical aberration corrector. The iron concentrations of the samples were conducted on the inductively coupled plasma atomic emission spectroscopy (ICP-OES). Surface elemental analysis was performed on XPS (Kratos Axis Ultra Dld, Japan). The X-ray absorption find structure spectra (Fe K-edge) were collected at 1W1B station in Beijing Synchrotron Radiation Facility (BSRF). The storage rings of BSRF was operated at 2.5 GeV with a maximum current of 250 mA. Using Si (111) double-crystal monochromator, the data collection was carried out.
in transmission mode using ionization chamber for Fe foil and in fluorescence excitation mode using a Lytle detector for FeSA/B,N-CNT. All spectra were collected in ambient conditions. The composition of the catalysts was characterized by X-ray diffraction pattern (XRD, D8 Advance, Bruker) and Raman spectroscopy (HR evolution, Horiba Jobin Yvon, France). N2-sorption analysis was performed by an ASAP 2020 accelerated surface area and porosimetry instrument (Micromeritics), equipped with automated surface area, at 77 K using BET calculations for the surface area.

3. Electrochemical measurements

All electrochemical measurements were carried out in a conventional three-electrode system using WaveDriver 20 bipotentiostat (Pine Instrument Company, USA). A Rotating Disk Electrode (RDE) with a glassy carbon disk served as the substrate was used as the working electrode, a Ag/AgCl and carbon rod were used as reference and counter electrode. The catalyst ink was prepared by dispersing 2 mg catalysts and 0.5 mg Acetylene Black in 380 μL ethanol and 20 μL Nafion solution (5 wt%) in an ultrasonic bath for at least 30 min. 8 μL of catalyst ink was then coated on glassy carbon disk. For comparison, Commercial Pt/C (20 wt%, Johnson Matthey) catalyst ink was prepared by dispersing 1 mg catalysts in 250 μL ethanol and 10 μL Nafion solution (5 wt%). 10 μL of catalyst ink was then coated on glassy carbon disk. The electrolyte was 0.1 M KOH. Before each experiment, electrolyte was saturated with N2/O2 by gassing with N2/O2 for at least 30 min. CV tests were performed in N2- and O2-saturated alkaline solution at 50 mV s⁻¹. LSV tests were performed in O2-saturated alkaline solution at 400, 625, 900, 1,225, 1,600, 2,025, 2,500 rpm with a scan rate of 10 mV s⁻¹. Unless noted otherwise, all the potentials mentioned in this paper were versus RHE. RRDE tests were conducted in O2-saturated 0.1 M KOH solution with the scan rate of 10 mV s⁻¹ under the rotation rate of 1,600 rpm. For the analysis of peroxide yield, the ring potential was held constant at 1.2 V vs. RHE. The percent of H2O2, the number of electron transfer (n) and kinetic current density (Jk) were determined by the following Koutecky–Levich equations:

\[
\% \text{(H}_2\text{O}_2) = \frac{I_r/N}{200I_d + I_r/N}
\]  

(1)
\[ n = 4\frac{I_d}{I_d + I_r/N} \] (2)

\[ \frac{1}{J} = \frac{1}{J_L} + \frac{1}{J_K} \] (3)

\[ J_K = nFkC_0 \] (4)

where \( I_d \) is the disk current, \( I_r \) is the ring current, and \( N (= 0.37) \) is the current collection efficiency of the Pt ring, \( J \) is the measured current density, \( J_L \) and \( J_K \) are the limiting and kinetic current densities. \( n \) is the overall number of electrons transferred in oxygen reduction, \( F \) is the Faraday constant \((F=96485 \text{ C mol}^{-1})\), \( C_0 \) is the bulk concentration of \( O_2 \), \( k \) is the electron-transfer rate constant.

The possible crossover effect caused by methanol was examined upon adding 3 M methanol into 0.1 M KOH electrolyte using the \( i-t \) technique. The durability of different samples were measured via chronoamperometric measurements in 0.1 M KOH with a rotation speed of 1,600 rpm.

Tafel slopes were obtained according to the Tafel equation:

\[ \eta = a + b \log j \] (5)

where \( \eta \) was the overpotential, \( j \) was the measured current density, and \( b \) was the Tafel slope. The electrochemical impedance spectroscopy (EIS) measurements were carried out in a frequency range of 0.01 Hz-100 KHz. The durability of different samples were measured via chronoamperometric measurements at 1,600 rpm in 0.1 M KOH.

The electrochemical surface areas (ECSA) values of different catalysts were determined by measuring the capacitive current associated with double-layer charging from the scan-rate dependence of CVs. The ECSA was measured on the same working electrode and electrolyte (0.1 M KOH). The potential window of CVs was 1.10–1.15 V vs. RHE, and the scan rates were 2, 4, 6, 8, and 10 mV/s. The double layer capacitance \((C_{dl})\) was estimated by plotting the current density at 1.14V vs. RHE against the scan rate. The slope is twice of \( C_{dl} \).
4. Simulation methods and computational modeling

4.1 Computational method.

The spin-polarized first-principle calculations were performed using the all-electron code Fritz-Haber Institute ab-initio molecules simulations package (FHI-aims). The exchange-correlation potentials were treated by the generalized gradient approximation (GGA) developed by Perdew, Burke, and Ernzerhof (PBE). The current work employs the armchair (6, 6) single-walled carbon nanotube (CNT). At least 10 Å of vacuum layer are exposed to the direction perpendicular to the CNT axis. The B-doped FeN\textsubscript{4}/CNT supercell has a hexagonal lattice with x, y = 20.00 Å and z = 14.76 Å. The Brillion zone was sampled by an appropriate Γ-centered Monkhorst-Pack grid with a density of at least 0.03 Å\textsuperscript{-1}. All geometrical structures were fully relaxed to its ground state until the charge density and the total energy were below of 10\textsuperscript{-4} eV/Å\textsuperscript{3} and 10\textsuperscript{-5} eV, respectively. To account for the weak van der Waals interaction, the functionals were augmented by the Tkatchenko and Scheffler scheme.

4.2 Formation energy

We compared formation energies of various possible models. Single B dopant could be generally classified into three different types, depending on the local chemical environment of carbon in the system: isolated B far away from FeN\textsubscript{4} moiety (B\textsubscript{iso}), B in a pentatomic ring bonded with FeN\textsubscript{4} moiety (B\textsubscript{pen}), B in a hexatomic ring bonded with FeN\textsubscript{4} moiety (B\textsubscript{hex}). With increasing B doping concentration, the situation of double B dopants incorporation of “Fe-porphyrin” into CNTs had been considered, affecting on the catalytic activity and electrical conducting of the system: two adjacent B dopants in a pentatomic or hexatomic ring (B\textsubscript{2}-adj-pen, B\textsubscript{2}-adj-hex), two opposite B dopants in different pentatomic or hexatomic rings (B\textsubscript{2}-opp-pen, B\textsubscript{2}-opp-hex), two adjacent B dopants bonded with the same N (B\textsubscript{2}-adj-N) and two interval B dopants in different rings (B\textsubscript{2}-pen-hex).

The formation energy (E\textsubscript{f}) of various B-doped FeN\textsubscript{4}/CNTs are calculated for comparing the relative stability of different B doped FeN\textsubscript{4}/CNT systems by the equation of
\[ E_f = E_{\text{tot}}(B_C) - E_{\text{tot}} + \sum_i n_i \mu_i \]  

where, \( E_{\text{tot}}(B_C) \) was the total energy of the supercell containing B substitutional carbon defects, \( E_{\text{tot}} \) was the total energy of the supercell without defects, \( n_i \) stood for the number of constituent element i being added/removed from the FeN_4/CNT supercell, \( \mu_i \) referred to the atomic chemical potential, \( E_{VBM} \) represented the valence band maximum (VBM) energy of the perfect supercell, \( E_F \) meant the Fermi energy measured from the VBM, varying in the range of the band gap (\( E_g \)), and \( \Delta V \) was the potential difference between the doped system and FeN_4/CNT supercell.

### 4.3 Gibbs free energy of each ORR steps

In alkaline media the overall ORR could be expressed as:

\[ 2H_2O + O_2 + 4e^- \rightarrow 4OH^- \]  

(7)

Since the ORR on FeN_4/CNT proceeded mainly along four-electron processes, we thus explored the reaction via four-electron pathways. The elementary reaction steps were listed as below:

\[ H_2O + O_2 + e^- \rightarrow HOO^* + OH^- \]  

(8)

\[ HOO^* + e^- \rightarrow O^* + OH^- \]  

(9)

\[ O^* + H_2O + e^- \rightarrow HO^* + OH^- \]  

(10)

\[ HO^* + e^- \rightarrow ** + OH^- \]  

(11)

where * represented an adsorption site. To quantitatively access the activity of the B-doped systems, we calculated the adsorption energies of ORR intermediates following the approach of Nørskov et al.
\[ \Delta E_{HOO^*} = E_{HOO^*} - E_* - \left[ 2E_{H_2O}(l) - 3/2E_{H_2}(g) \right] \]  

(12)

\[ \Delta E_{HO^*} = E_{HO^*} - E_* - \left[ E_{H_2O}(l) - 1/2E_{H_2}(g) \right] \]  

(13)

\[ \Delta E_{O^*} = E_{O^*} - E_* - \left[ E_{H_2O} - E_{H_2} \right] \]  

(14)

where, for example, \( E_{O^*} \) denoted the total energy of an oxygen atom adsorbed on the catalyst obtained by the calculations, \( H_2O \) and \( H_2 \) both referred to gas phases. To convert the adsorption energy at zero temperature into the adsorption Gibbs free energy at the room temperature (T) and standard pressure (\( p_0 \)), the electrode potential (U), entropy change (\( \Delta S \)) and zero-point energy corrections (\( \Delta ZPE \)) to the adsorption energy together with the solvation correction (\( \Delta G_{sol} + \Delta G_{PH} \)) were considered. Herein, the change in Gibbs free energy (\( \Delta G \)) for each reaction step of ORR could be given by the equation:

\[ \Delta G = \Delta E + \Delta ZPE - T\Delta S + ne(U - U_0) + \Delta G_{sol} + \Delta G_{PH} \]  

(15)

By setting the reference potential to be the standard hydrogen electrode, the free energy of 1/2\( H_2 \) could be used to replace that of (\( OH^- - e^- \)). The free energy of \( O_2 \) was obtained from the reaction \( 2H_2O \rightarrow O_2 + 2H_2 \) for which the free energy change is 4.92 eV. And a solvation correction with energy equals to -0.28 eV, +0.07 eV and -0.22 eV were applied to \( E_{HO^*}, E_{O^*} \) and \( E_{HOO^*} \) respectively. Therefore, for ORR intermediates, the adsorption Gibbs free energies could be expressed as following:

\[ \Delta G_{HOO^*} = \Delta E_{HOO^*} + \Delta ZPE - T\Delta S - 0.22 + 0.0591 \times PH - neU \]  

(16)

\[ \Delta G_{HO^*} = \Delta E_{HO^*} + \Delta ZPE - T\Delta S - 0.28 + 0.0591 \times PH - neU \]  

(17)

\[ \Delta G_{O^*} = \Delta E_{O^*} + \Delta ZPE - T\Delta S + 0.07 + 0.0591 \times PH - neU \]  

(18)

where, T was the room temperature (300K), entropy changes (\( \Delta S \)) and zero point energies (\( \Delta ZPE \)) were employing as implemented in prior works and tabulated values.\(^8,9\)
Through the DFT calculation, we carefully calculated the relationship of the boron-doped with the d-band center with the equation:

\[
E_{d\text{-band center}} = \frac{\int_{-\infty}^{E_F} E \cdot PDOS(E) dE}{\int_{-\infty}^{E_F} PDOS(E) dE}
\]  

(19)

5. Aqueous zinc-air battery assembly: All electrodes were directly used as the air cathodes, which were coated Fe\textsubscript{SA}/B,N-CNT and Pt/C+IrO\textsubscript{2} on Nickel foam with the loading 3 mg cm\textsuperscript{-2}, and zinc plates were polished to be used as the anodes. Rechargeable aqueous zinc-air batteries were prepared with addition of 0.2 M Zn(CH\textsubscript{3}COO)\textsubscript{2} into the 6 M KOH electrolyte.
Fig. S1. Schematic procedure for the synthesis of Fe₈N/B,N-CNT.
Fig. S2. SEM image of Fe$_{x}$/B,N-CNT.
**Fig. S3.** TEM image of Fe$_{NP}$/N-CNT, in which iron-based particles are encapsulated either at the tip or inside of carbon nanotubes.
Fig. S4. TEM image and HAADF-STEM image of Fe\textsubscript{3}N/C-CN. Fe\textsubscript{3}N/C-CN exhibits the nanotube morphology without Fe aggregation. A large number of isolated bright dots representing single Fe atoms uniformly disperse on the carbon support.
The results show no distinct differences between FeSA/B,N-CNT and FeSA/N-CNT, with two broad peaks assignable to the (002) and (101) planes of graphitic carbon. Notably, no peaks related to metallic Fe or other Fe species are observed. As for FeNP/N-CNT, it exhibits well-defined diffraction peaks associated with Fe-based carbides.
Fig. S6. Raman spectra of different samples. The D band (1360 cm$^{-1}$) and G band (1590 cm$^{-1}$) provide information on the disorder and crystallinity of carbon materials, respectively. Fe$_{NP}$/N-CNT shows the lowest $I_D/I_G$ value of 1.01. As for catalysts with single-atom dispersed Fe, the $I_D/I_G$ exhibits the same value of 1.03.
Fig. S7. XPS spectrum of Fe_{SA}/B,N-CNT. The survey scan indicates the presence of boron, carbon, nitrogen, and oxygen.
Fig. S8. High-resolution XPS spectra of C 1s of Fe$_{33}$/B,N-CNT. Four forms of carbon are observed including sp$^2$ at $\sim$284.3 eV, C=N at $\sim$285.5 eV, C-N at $\sim$286.5 eV, and $\pi-\pi^*$ at $\sim$288.4 eV.
Fig. S9. High-resolution XPS spectrum of N 1s of Fe_{SA}/B,N-CNT. Four forms of nitrogen are observed including pyridinic N at ~398.1 eV, pyrrolic N at ~398.9 eV, graphitic N at ~400.4 eV, and N-oxides at ~403.6 eV.
Fig. S10. High-resolution N 1s X-ray photoelectron spectra of the Fe_{x}/N-CNT and N-C. The N 1s spectra of N-C were deconvoluted into four peaks, assignable to the pyridinic N (397.8 eV), pyrrolic N (398.7 eV), graphitic N (400.4 eV), and pyridine N-oxides (403.6 eV), respectively. Once Fe was present in the catalyst, both pyridinic N and pyrrolic N shifted to higher binding energy of 398.1 and 398.9 eV, respectively, while no discernible peak shift was observed in graphitic N or pyridine N-oxides. This suggest strong chemical bond forming between Fe and pyridinic/pyrrolic N with a high electronegativity, leading to partial electron migration from Fe to pyridinic/pyrrolic N.
Fig. S11. (a) N₂ sorption isotherms and (b) pore size distribution curves of different samples. The specific surface area for each sample was calculated to be 399 m² g⁻¹ for Fe₃/N₄/C₄, 397 m² g⁻¹ for Fe₃/N₁/C₄, and 341 m² g⁻¹ for Fe₃/P₁/C₄. The typical mesopores centered at around 4 nm could facilitate the mass transfer during ORR process.
**Fig. S12.** Photographs of Fe$_{SA}$/B$_2$N-CNT (100 mg, right) and commercial Pt/C (20 wt. % Pt, 100 mg, left) in vials. Fe$_{SA}$/B$_2$N-CNT shows low volumetric density compared to commercial Pt/C catalyst.
Fig. S13. CV curves of different samples in O\textsubscript{2}-saturated (solid line) or N\textsubscript{2}-saturated (dash line) 0.1 M KOH. No redox peak was observed when the solution was saturated with N\textsubscript{2}. On the contrary, if the gas in the solution was replaced with O\textsubscript{2}, an obvious onset potential was observed at \(\sim 1.06\) V vs. RHE for Fe\textsubscript{SA}/B,N-CNT, suggesting the superior ORR performance.
Fig. S14. LSV curves at different rotation speeds and the corresponding K-L plots at different potentials of (a,b) Fe_{SA}/B,N-CNT, (c,d) Fe_{SA}/N-CNT, (e,f) Fe_{NP}/N-CNT and (g,h) Pt/C.
Fig. S15. Methanol resistance in O$_2$-saturated 0.1 M KOH tests without and with CH$_3$OH.
Fig. S16. ORR LSV curves of Fe₃₄/B,N-CNT before and after 20000 s i-t test.
Fig. S17. (a) AC HAADF-STEM image and (b) HRTEM image and corresponding element mapping of Fe$_{SA}$/B,N-CNT after durability test, demonstrating the atomically dispersed Fe atoms remain unchanged.
Fig. S18. XRD spectrum of the Fe$_{SA}$/B,N-CNT after test.
Fig. S19. Raman spectrum of the Fe$_{50}$/B,N-CNT after durability test. $I_D/I_G$ is the intensity ratio of the D peak to the G peak.
Fig. S20. ORR Tafel plots derived from the corresponding LSV curves. The much smaller Tafel slope of Fe\textsubscript{SA}/B,N-CNT (61.9 mV/dec) compared to other samples indicates a more favorable reaction kinetics.
**Fig. S21.** EIS spectra of different samples. $\text{Fe}_{\text{SA}}/\text{B,N-CNT}$ displays the smallest diameter of the semicircle and the largest slope among all the samples, confirming its fastest electron transport kinetics and ion diffusion rate.
Fig. S22. Cyclic voltammetry curves of different samples in 2 M KCl solution and a plot of the current density at 1.14 V vs. the scan rate of (a,b) Fe\textsubscript{SA}/B,N-CNT, (c,d) Fe\textsubscript{SA}/N-CNT, and (e,f) Fe\textsubscript{NP}/N-CNT. The double layer capacitance $C_{dl}$ increases in the order of Fe\textsubscript{NP}/N-CNT (10.14 mF cm\textsuperscript{-2}) < Fe\textsubscript{SA}/N-CNT (11.85 mF cm\textsuperscript{-2}) < Fe\textsubscript{SA}/B,N-CNT (13.06 mF cm\textsuperscript{-2}).
**Fig. S23.** The configurations and formation energies ($E_f$) of various possible B-doped FeN$_4$ active sites. A pentatomic ring consists of one Fe atom, two N atoms and two C atoms, the Fe and two N atoms together with three C atom compose a hexatomic ring. Purple, blue, pink, and grey represent Fe, N, B, and C atoms, respectively.
**Fig. S24.** The structure of (a) Fe$_{3}$A/N,CNT, (b) Fe$_{3}$/B$_{1}$/N-CNT, and (c) Fe$_{3}$/B$_{2}$/N-CNT. (d) The PDOS of Fe 3d band of the different catalysts. (e) The relation between d-band center and the O$_{2}$ adsorption of different catalysts. (f) The free energy of the catalysts at the equilibrium potential of $U = 1.23$ V.
Fig. S25. The charge-density variation wave of the Fe$_{SA}$/N-CNT, Fe$_{SA}$/B$_{1}$,N-CNT and Fe$_{SA}$/B$_{2}$,N-CNT. Light blue area represented charge density decrease ($\Delta \rho < 0$) and yellow area denoted charge density increase ($\Delta \rho > 0$). Purple, blue, pink, and grey represent Fe, N, B, and C atoms, respectively.
Fig. S26. The optimized structure of Fe₉₉/N-CNT. Purple, blue, and grey represent Fe, N, and C atoms, respectively.
Fig. S27. Linear sweep voltammetry OER curves of Fe$_{SA}$/B,N-CNT, Fe$_{SA}$/N-CNT and Fe$_{NP}$/N-CNT.
6. Supplementary Tables

**Table S1.** Elemental compositions (C, O, N, and B) obtained by XPS spectroscopy, and Fe contents measured by ICP-OES.

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>C (at%)</th>
<th>O (at%)</th>
<th>N (at%)</th>
<th>B (at%)</th>
<th>Fe (at%)</th>
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<td>Fe&lt;sub&gt;SA&lt;/sub&gt;/B,N-CNT</td>
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<td>Fe&lt;sub&gt;NP&lt;/sub&gt;/N-CNT</td>
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<td>6.68</td>
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**Table S2.** Comparison of ORR activity of various non-precious metal catalysts in 0.1 M KOH.

<p>| Catalyst    | $E_{\text{onset}}$ vs. RHE (V) | $E_{1/2}$ vs. RHE (V) | $J_{\text{k}|V=0.85,\text{V}}$ (mA cm&lt;sup&gt;-2&lt;/sup&gt;) | $K_{\text{tafel}}$ (mV dec&lt;sup&gt;-1&lt;/sup&gt;) | Ref.   |
|-------------|---------------------------------|-----------------------|-----------------------------------------------|------------------------------------------|--------|
| Fe&lt;sub&gt;SA&lt;/sub&gt;/B,N-CNT | 1.07                            | 0.933                 | 62.57                                         | 61.9                                      | This work |
| Fe&lt;sub&gt;SA&lt;/sub&gt;/N-CNT     | 1.04                            | 0.890                 | 13.17                                         | 65.6                                      | This work |
| Fe-ISAs/CN                | 0.986                           | 0.900                 | 37.85                                         | 58                                        | 10      |
| SA-Fe-HPC                 | /                               | 0.890                 | 3.72                                          | 49                                        | 11      |
| FeCl&lt;sub&gt;1&lt;/sub&gt;N&lt;sub&gt;4&lt;/sub&gt;/CNS | /                                | 0.921                 | 41.11                                         | 51                                        | 12      |
| N-GCNT/FeCo               | 1.03                            | 0.920                 | /                                             | 66.8                                      | 13      |</p>
<table>
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<th>Material</th>
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<th>M (%)</th>
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<td>/</td>
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S38
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<th>mD</th>
<th>E</th>
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<th>IMPS (V)</th>
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<td>Fe−N−CC</td>
<td>0.94</td>
<td>0.83</td>
<td>18.3</td>
<td>0.58V</td>
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<td>Fe-NMCSs</td>
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<td>1.01</td>
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<td>Fe/N/G-0.25</td>
<td>0.98</td>
<td>0.84</td>
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<td>Meso/micro-PoPD</td>
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<td>4.23</td>
<td>0.8V</td>
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<td>0.910</td>
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<td>25% Cu-N/C</td>
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<td>Co SAs/N-C(900)</td>
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<td>22</td>
<td>0.8 V</td>
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<td>Co–Nₓ/C NRA</td>
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<td>NC@Co-NGC DSNC</td>
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<td>0.71 V</td>
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<td>1.03</td>
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<td>0.86</td>
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<td>Co-ISAS/p-CN</td>
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<td>0.838</td>
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Table S3. Free energy change (ΔG) for the 4-electron transfer processes during ORR at T = 298 K, PH = 13 and U = 0 V.

<table>
<thead>
<tr>
<th>Elementary steps</th>
<th>ΔG Fe_{NP}/CNT</th>
<th>ΔG Fe_{SA}/N-CNT</th>
<th>ΔG Fe_{SA}/B,N-CNT</th>
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<tr>
<td>* +O\textsubscript{2}\rightarrow OO*</td>
<td>5.22</td>
<td>4.71</td>
<td>4.78</td>
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<tr>
<td>OO*+H\textsubscript{2}O+e^-\rightarrow HOO*+OH\textsuperscript{-}</td>
<td>4.85</td>
<td>4.06</td>
<td>3.97</td>
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<tr>
<td>HOO*+e^-\rightarrow O*+OH\textsuperscript{-}</td>
<td>2.50</td>
<td>1.73</td>
<td>1.85</td>
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<tr>
<td>O*+H\textsubscript{2}O+e^-\rightarrow HO*+OH\textsuperscript{-}</td>
<td>1.68</td>
<td>1.00</td>
<td>1.05</td>
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<tr>
<td>HO* +e^-\rightarrow * +OH\textsuperscript{-}</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
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References


