Single-Atom Iron Catalyst Based on Functionalized Mesophase Pitch Exhibiting Efficient Oxygen Reduction Reaction Activity

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Supporting Information

Table S1: Elemental compositions of SA-Fe@NC catalysts determined by XPS.

Entry	C [at%]	O [at%]	Fe [at%]	Total N [at%]
SA-Fe@NC_{800}	90.22	5.98	0.43	3.71
SA-Fe@NC_{950}	92.44	5.24	0.26	2.05
SA-Fe@NC_{1100}	93.65	4.62	0.14	1.59
SA-Fe@NC_{800-1}	90.42	6.45	0.34	2.79
SA-Fe@NC_{800-2}	88.31	9.86	0.19	1.63

Table S2: N contents of SA-Fe@NC catalysts pyrolyzed at different temperatures obtained from XPS N 1s spectra.

Entry	Total N [at%]	Pyridinic [at%]	Pyrrolic [at%]	Quaternary [at%]	Graphitic [at%]	Fe-N_x [at%]
SA-Fe@NC_{800}	3.71	0.83	1.96	0.29	0.24	0.39
SA-Fe@NC_{950}	2.05	0.32	1.41	0.13	0.10	0.10
SA-Fe@NC_{1100}	1.59	0.17	1.06	0.19	0.07	0.06

Table S3: Structural parameters extracted from the Fe K-edge EXAFS fitting.

Entry	Shell	Bond length (Å)	Coordination Number	σ^2 ($Å^2$)	E_0 shift (eV)	R-factor ($\times10^{-3}$)
SA-Fe@NC_{800}	Fe-N(O)	2.17	5.1	0.008	1.4	9.8
Fe Foil	Fe-Fe	2.43	12	0.003	3.2	8.7
Fe_2O_3	Fe-O	2.04	6.0	0.009	0.1	0.9
-	Fe-Fe	2.97	5.9	0.007	0.1	0.9
-	Fe-Fe	3.39	4.3	0.007	0.1	0.9
-	Fe-Fe	3.71	5.6	0.007	0.1	0.9

σ^2 is the Debye-Waller factor; R factor is used to value the goodness of the fitting.

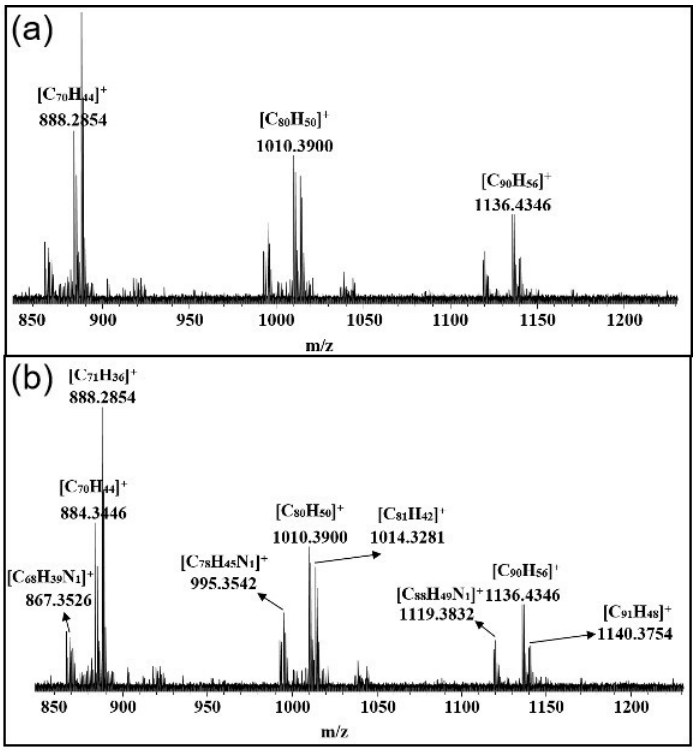

Figure S1: FT-ICR-MS results under the atmospheric pressure photo ionization (APPI) mode, (a) peaks show the presence of the naphthalene polymers and (b) peaks show the presence of the dehydrogenized co-polymers of indole-naphthalene.

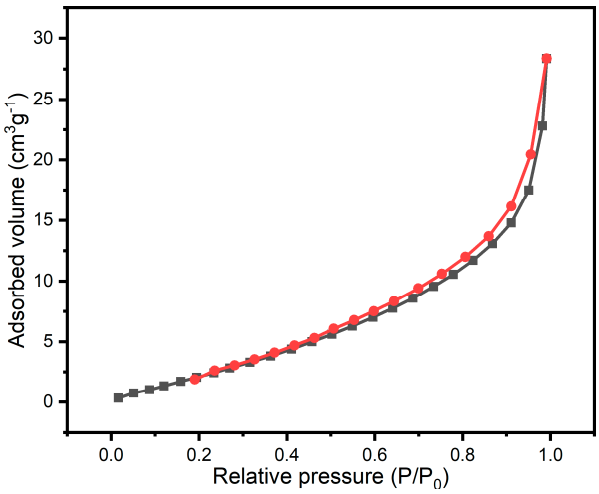

Figure S2: BET results for the control sample using $AlCl_3$ as polymerization catalyst.

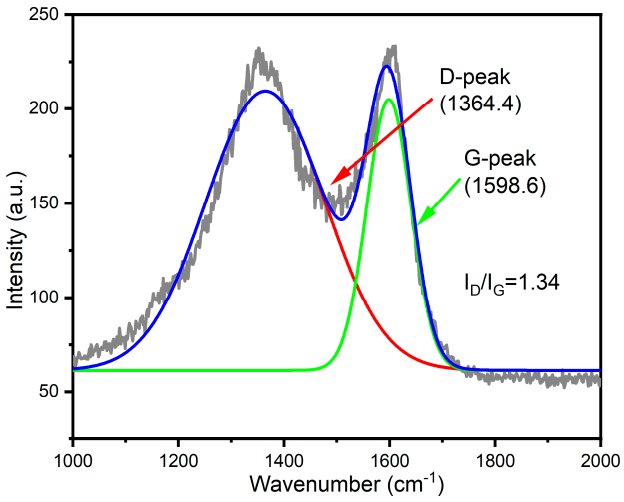

Figure S3: Raman of SA-Fe@NC_{950}.

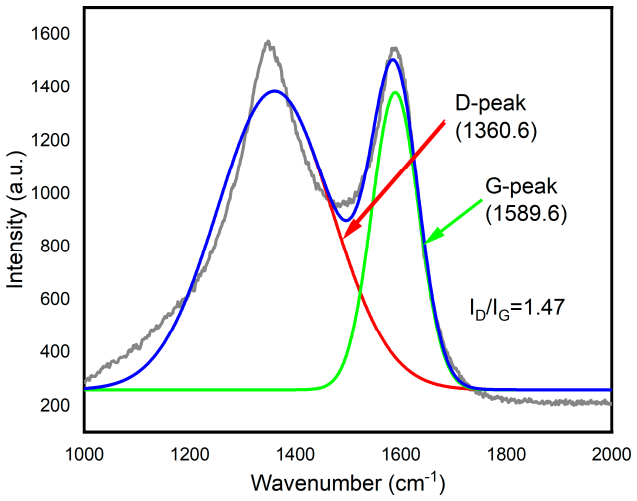

Figure S4: Raman of SA-Fe@NC_{1100}.

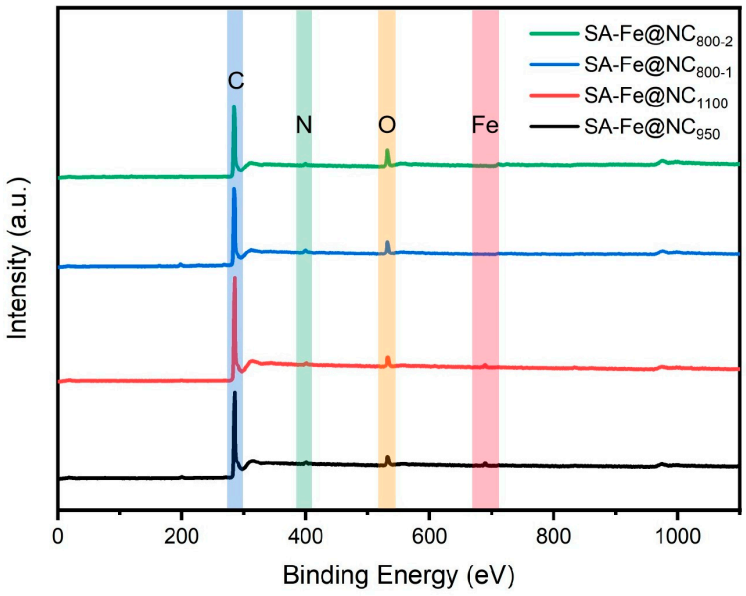

Figure S5: XPS survey scan spectra of SA-Fe@NC_{950}, SA-Fe@NC_{1100}, SA-Fe@NC_{800-1} and SA-Fe@NC_{800-2}

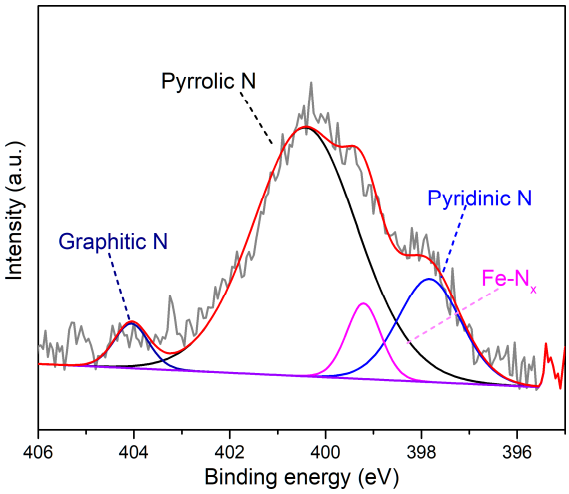

Figure S6: XPS of SA-Fe@NC$_{950}$.

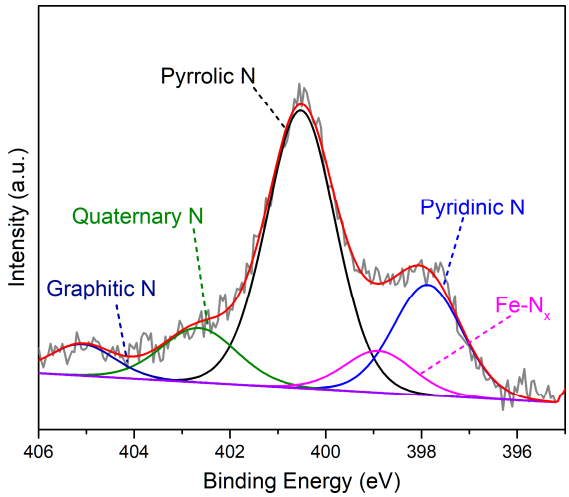

Figure S7: XPS of SA-Fe@NC$_{1100}$.

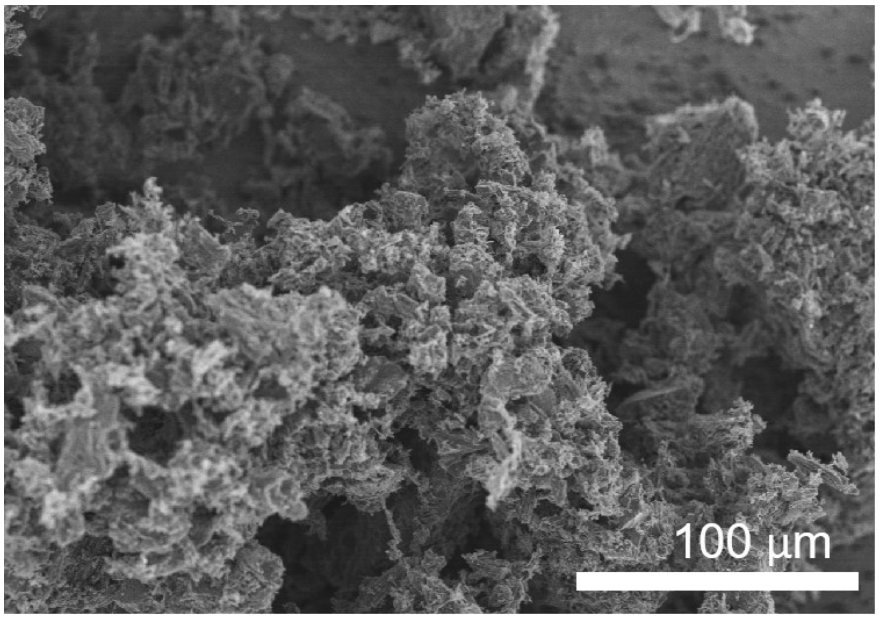

Figure S8: SEM of SA-Fe@NC_{800} showing structures with hierarchical pores.

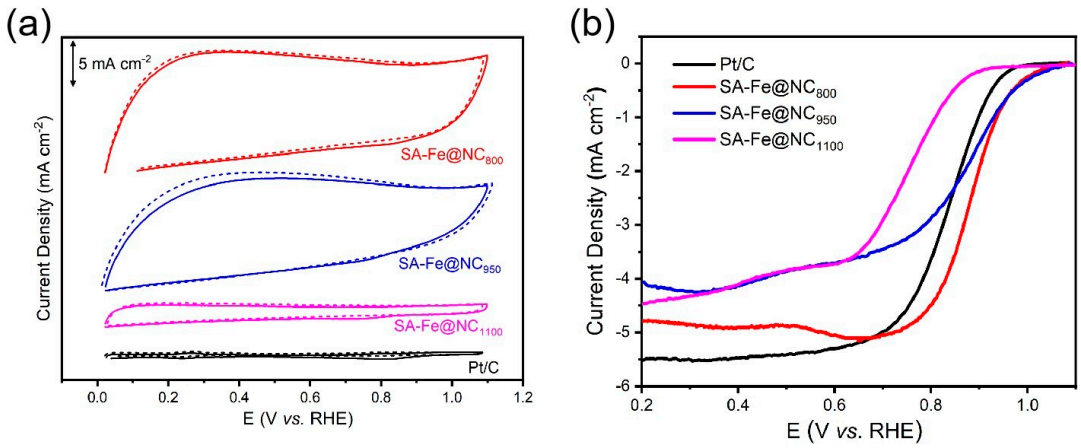

Figure S9: (a) CV curves of SA-Fe@NC_{800}, SA-Fe@NC_{950}, SA-Fe@NC_{1100} and Pt/C catalysts in O_2-saturated (solid line) and N_2-saturated (dashed line) in 0.1 M KOH solutions at a sweep rate of 50 mv s^{-1}. (b) LSV curves of above catalysts in O_2-saturated 0.1 M KOH electrolyte at 10 mV s^{-1} with a rotation rate of 1600 rpm.

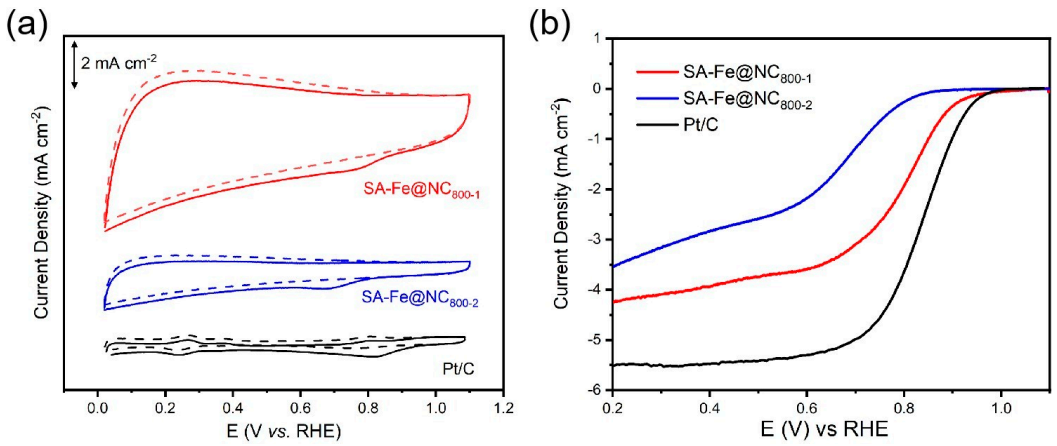

Figure S10: (a) CV curves of SA-Fe@NC_{800-1}, SA-Fe@NC_{800-2} and Pt/C catalysts in O_2-saturated (solid line) and N_2-saturated (dashed line) in 0.1 M KOH solutions at a sweep rate of 50 mV s^{-1}. (b) LSV curves of above catalysts in O_2-saturated 0.1 M KOH electrolyte at 10 mV s^{-1} with a rotation rate of 1600 rpm.

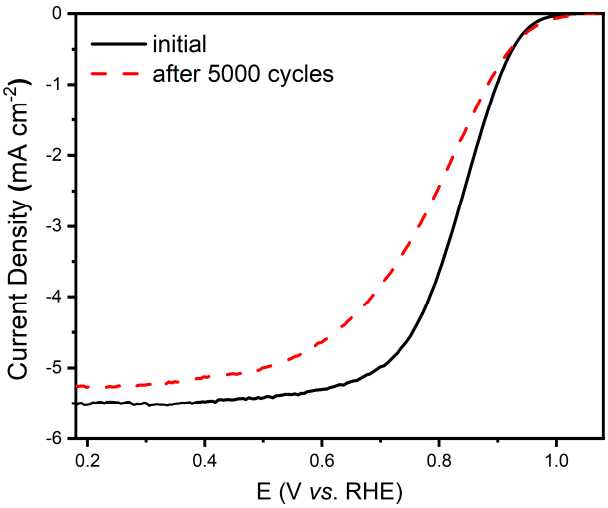

Figure S11: LSV curves for Pt/C before and after 5000 CV cycles between 0.6 and 1.0 V.

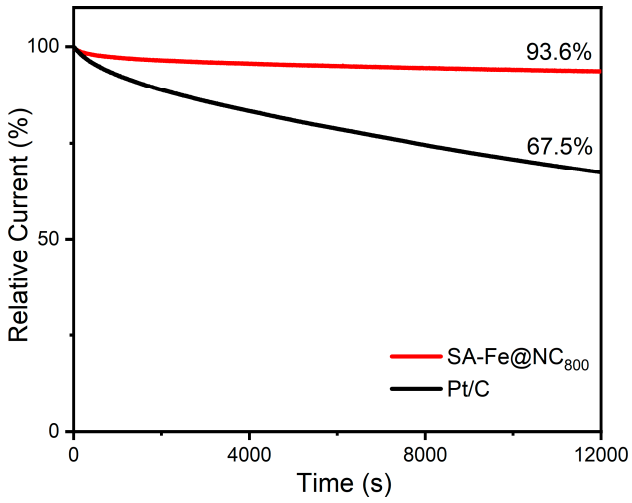

Figure S12: Stability test of the SA-Fe@NC_{800} and the commercial Pt/C in the O_2-saturated 0.1M KOH solution at 0.8 V under a rotation rate of 1600 rpm.