

Supporting Information

Constructing B and N separate codoped carbon nanocapsules wrapped Fe/Fe₃C for oxygen reduction reaction with high current density

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Table S1. The detailed experimental parameters for all the compared samples.

samples	The dosage of melamine (g)	The dosage of H ₃ BO ₃ (g)	The dosage of Fe(NO ₃) ₃ •9H ₂ O (g)	Pyrolysed temperature (°C)
NGFe-800	3	0	3	800
B ₁ NGFe ₂ -800	3	0.4	3	800
B ₂ NGFe ₂ -800	3	0.6	3	800
B ₃ NGFe ₂ -800	3	0.8	3	800
BNC-800	3	0.6	0	800
B ₂ NGFe ₁ -800	3	0.6	2	800
B ₂ NGFe ₃ -800	3	0.6	4	800
B ₂ NGFe ₂ -700	3	0.6	3	700
B ₂ NGFe ₂ -900	3	0.6	3	900

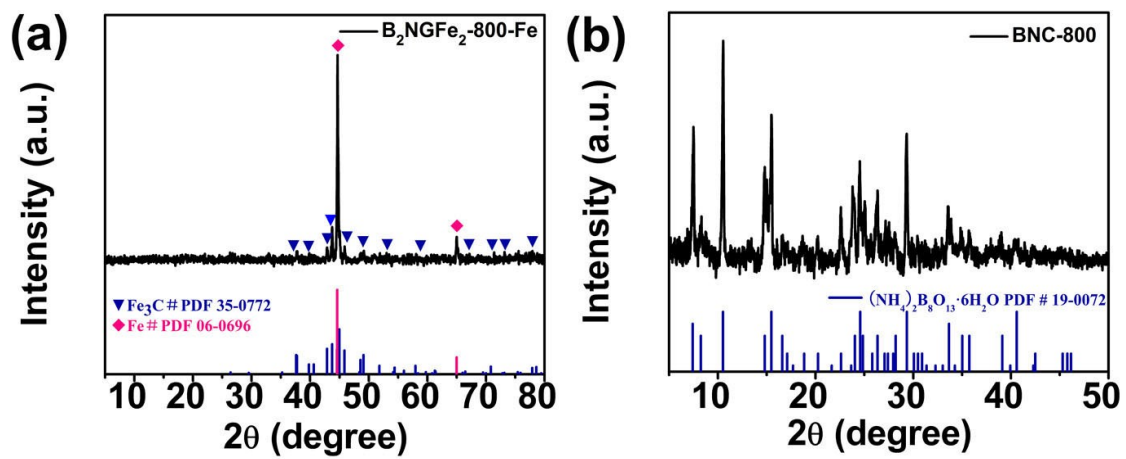


Fig. S1 XRD patterns of (a) $B_2NGFe_2-800-Fe$ and (b) the BNC-800 composites.

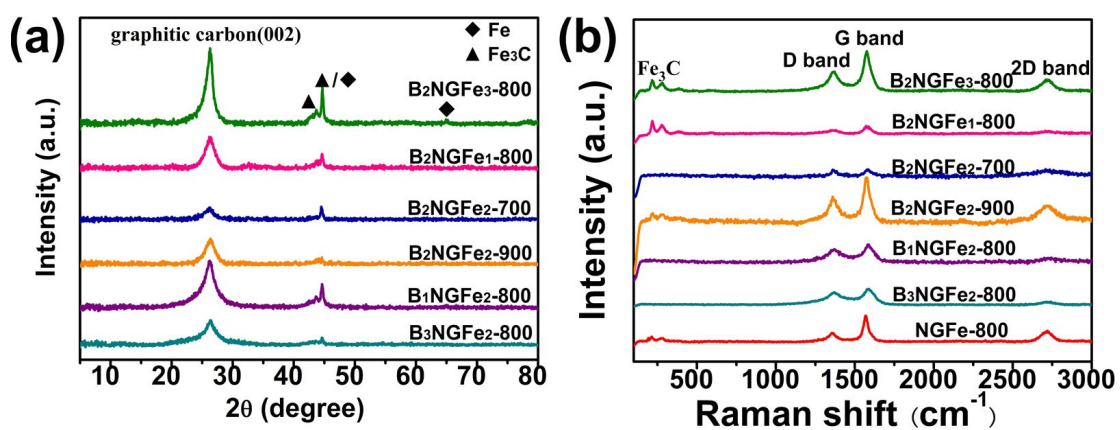


Fig. S2 (a) XRD patterns and (b) Raman spectra of all the compared samples synthesized from different dosages of boric acid and iron nitrate, and different pyrolysed temperatures.

Table S2. The high-resolution XPS spectrum analytic results of B1s, N1s and Fe2p for B₂NGFe₂-800 and other compared samples.

samples	B content (at.%)	C content (at.%)	N content (at.%)	O content (at.%)	Fe content (at.%)	B/N	B/Fe
B ₂ NGFe ₂ -800	1.35	90.11	2.77	4.87	0.89	0.49	1.5
B ₁ NGFe ₂ -800	1.00	86.34	5.44	6.77	0.44	0.18	2.3
B ₃ NGFe ₂ -800	9.97	69.59	11.55	8.64	0.26	0.86	38
B ₂ NGFe ₁ -800	1.62	87.30	4.41	5.90	0.78	0.37	2.1
B ₂ NGFe ₃ -800	1.84	87.36	5.83	3.91	1.05	0.32	1.8
B ₂ NGFe ₂ -700	2.62	78.52	10.06	7.99	0.80	0.26	3.3
B ₂ NGFe ₂ -900	10.84	66.71	11.40	10.79	0.26	0.95	42
NGFe-800	0.00	90.17	3.23	6.04	0.56	0	0

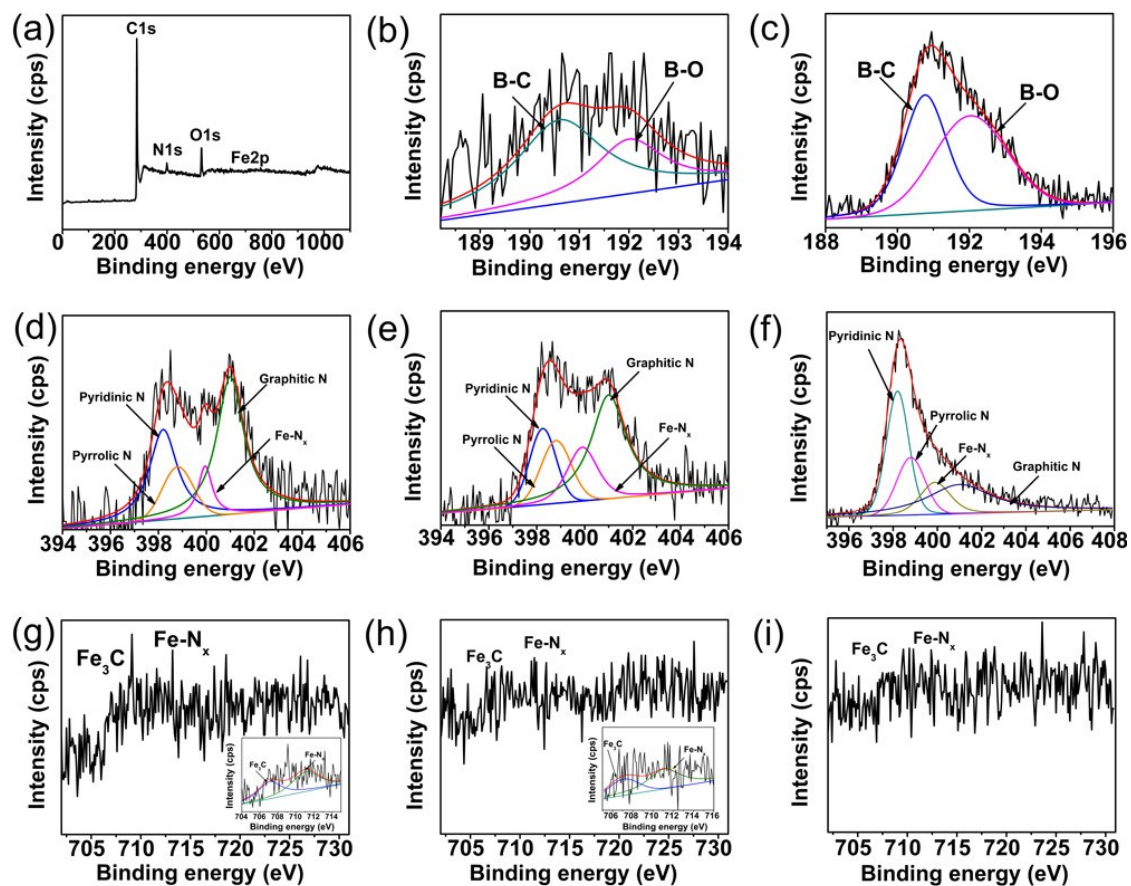


Fig. S3 (a) Survey XPS spectrum, (d) N1s and (g) Fe2p XPS spectra of NGFe-800 composite; (b) B1s, (e) N1s and (h) Fe2p XPS spectra of B₁NGFe₂-800 composite; Survey XPS spectrum, (c) B1s, (f) N1s and (i) Fe2p XPS spectra of B₃NGFe₂-800 composite.

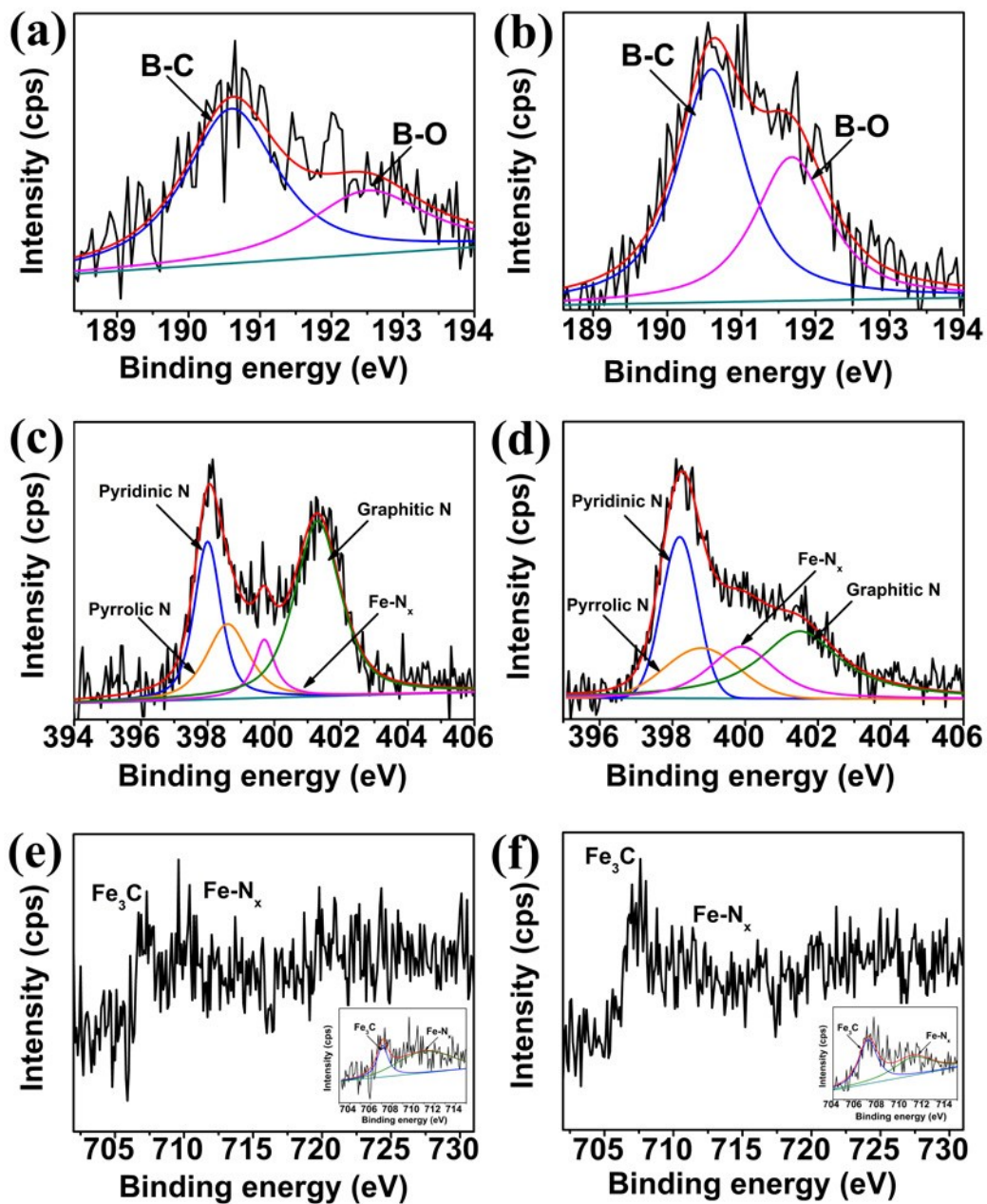


Fig. S4 (a) B₁s, (c) N₁s and (e) Fe₂p XPS spectra of B₂NGFe₃-800 composite; (b) B₁s, (d) N₁s and (f) Fe₂p XPS spectra of B₂NGFe₁-800 composite.

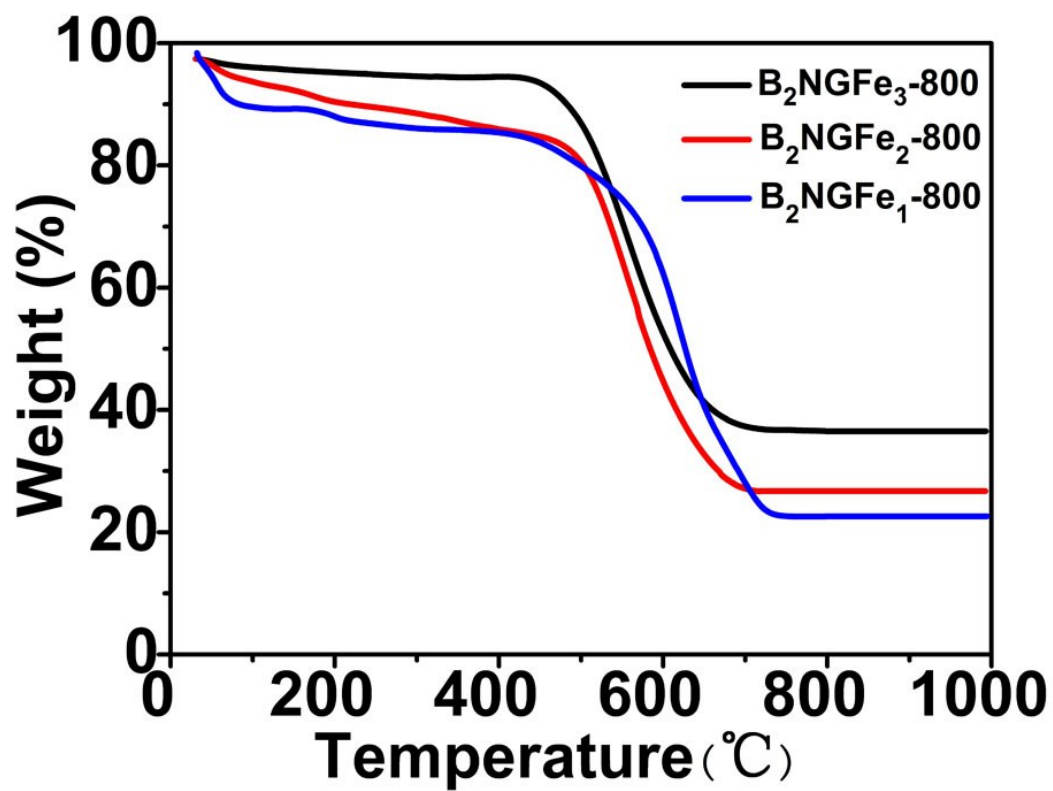


Fig. S5 TGA curves of B₂NGFe₁-800, B₂NGFe₂-800 and B₂NGFe₃-800 composites.

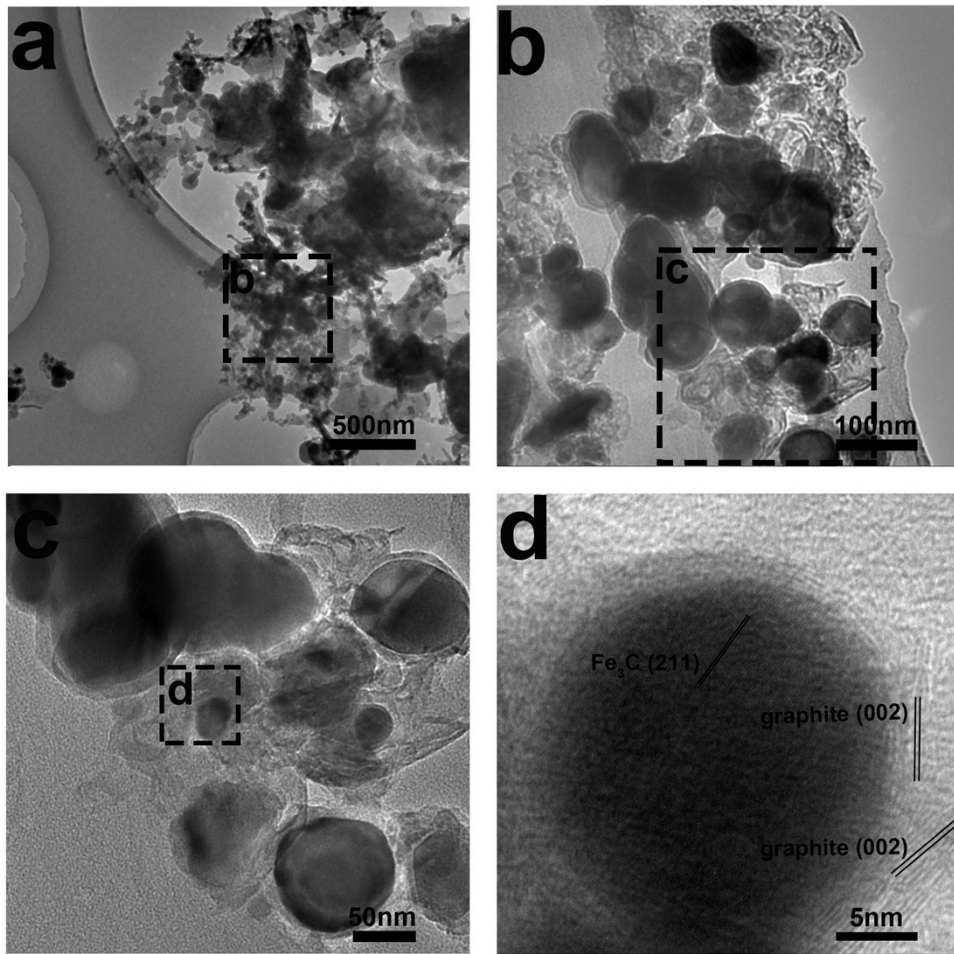


Fig. S6 TEM and HRTEM images of $B_2NGFe_2-800-Fe$ composite without treating by HCl.

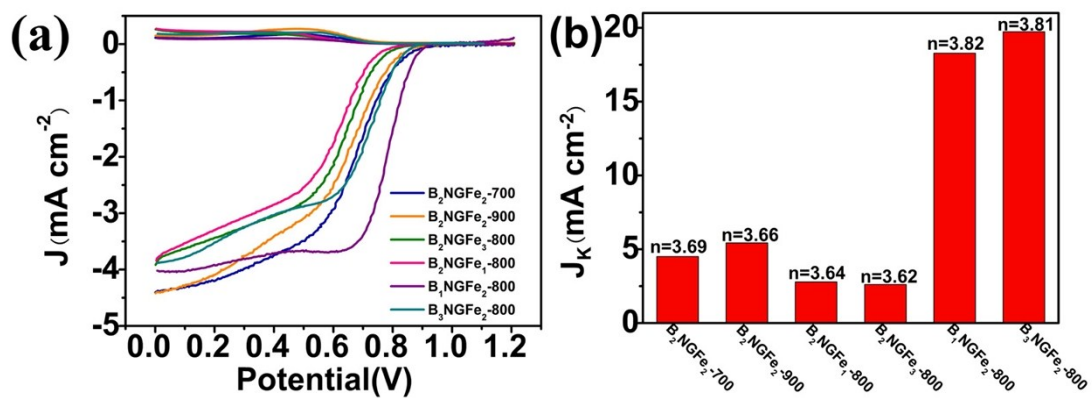


Fig. S7 (a) RRDE voltammetric response in O₂-saturated 0.1 M KOH electrolyte at a scan rate of 5 mV s⁻¹ and (b) electrochemical activity given as the kinetic current density (J_k) at 0.6 V for compared electrodes; The electrode rotation rate was 1600 rpm, and the Pt ring electrode was polarized at 1.2 V.

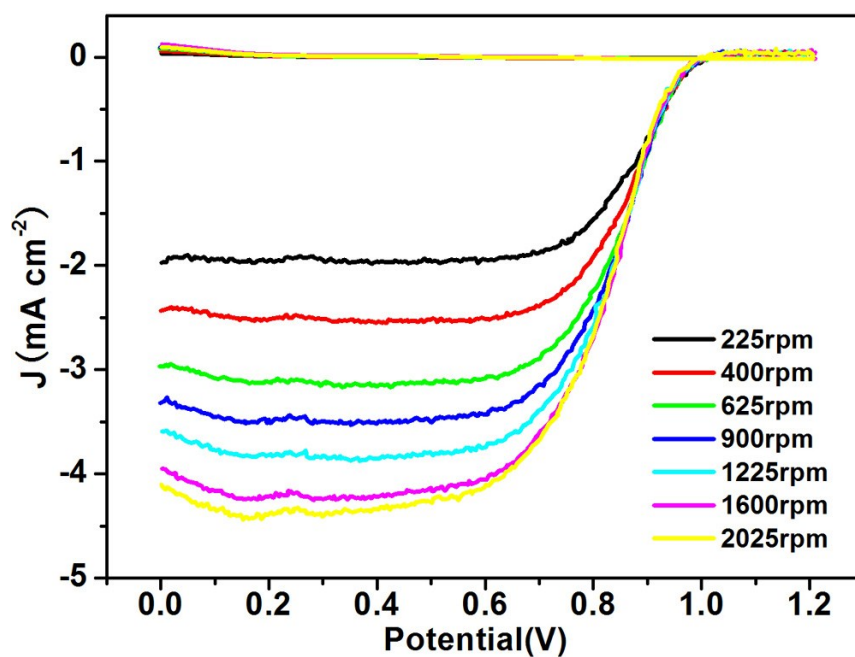


Fig. S8 RRDE curves of Pt/C on a RRDE in an O₂-saturated 0.1 M KOH electrolyte with various rotating speeds at scan rates of 5 mV s⁻¹.

Table S3. Current densities of B₂NGFe₂-800 and Pt/C for ORR at different potentials.

Current density (m A cm ⁻²)	0.1V	0.2V	0.3V	0.4V	0.5V	0.6V	0.7V	0.8V	0.9V
B ₂ NGFe ₂ -800	4.8	4.9	4.9	4.9	4.9	4.8	4.6	2.9	0.5
Pt/C	4.2	4.2	4.2	4.2	4.2	4.1	3.7	2.6	0.4

Table S4. The comparison of ORR performance of B₂NGFe₂-800 with other Pt-free ORR electrocatalysts (vs. RHE)

Catalysts	Loading (mg cm ⁻²)	electrolyte	$E_{1/2}$ (V)	E_{Onset} (V)	J_{K} (mA cm ⁻²)	Ref
B ₂ NGFe ₂ -800	0.3 mg cm ⁻²	0.1M KOH	0.83	0.98	72.7	This work
Fe@C-FeNCs	0.7 mg cm ⁻²	0.1M KOH	0.899	1.0	41.6 A/g at 0.80 V	1
Fe-N/C-800	0.1 mg cm ⁻²	0.1M KOH	0.809	0.923	Not mentioned	2
Fe ₃ C/C hollow spheres	0.6 mg cm ⁻²	0.1M KOH	0.83	1.05	Not mentioned	3
Fe@N-C/SiC@N-C	1.0 mg cm ⁻²	0.1M KOH	0.84	0.88	Not mentioned	4
Fe-N-Doped Carbon Capsules	0.1 mg cm ⁻²	0.1M KOH	0.83	0.94	18.3 mA cm ⁻²	5
N-doped mesoporous carbons with a trace amount of Fe	0.08 mg cm ⁻²	0.1M KOH	Not mentioned	0.98	Not mentioned	6
B and N isolate-doped graphitic nanosheets	0.2 mg cm ⁻²	0.1M KOH	Not mentioned	0.95	11.9 mA cm ⁻² @0.7V	7

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