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基于金属有机框架衍生的 Fe-N-C 纳米复合材料作为高效的氧还原催化剂

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Metal-Organic Framework-Derived Fe-N-C Nanohybrids as Highly-Efficient Oxygen Reduction Catalysts

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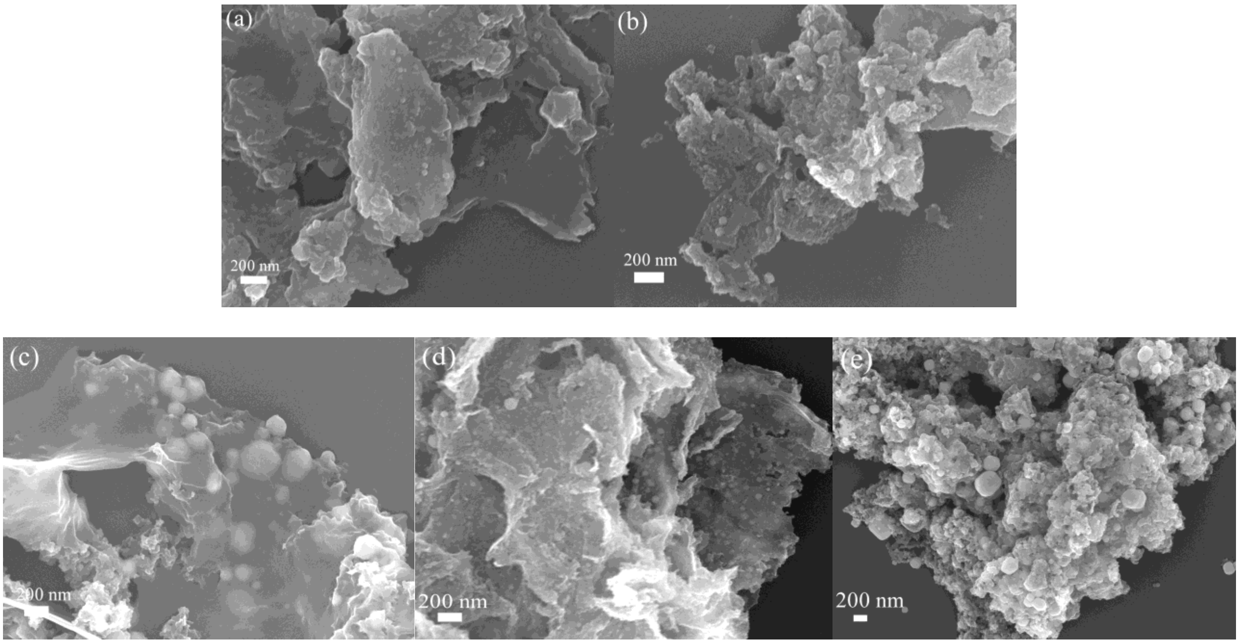

Fig. S1 SEM images of (a) Fe-N-C-800, (b) Fe-N-C-1000, (c) Fe-C-900, (d) Fe-N-900 and (e) MIL-900.

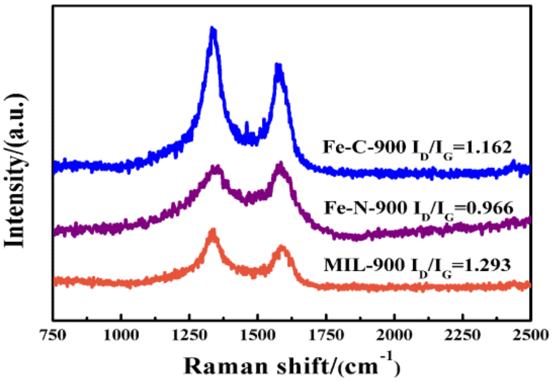

Fig. S2 Raman spectra of Fe-C-900, Fe-N-900 and MIL-900.

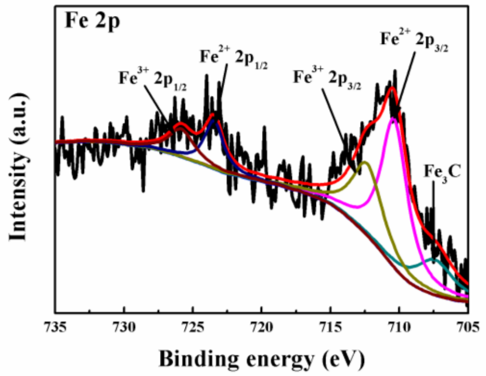

Fig. S3 Fe 2*p* spectrum of Fe-N-C-900.

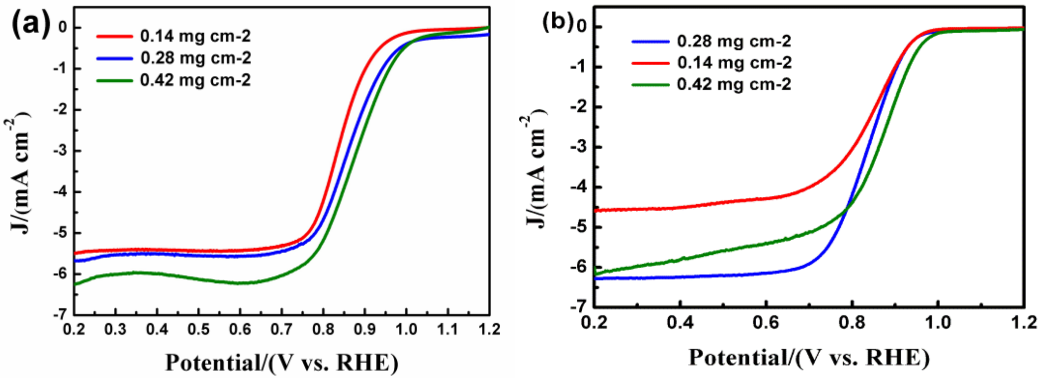

Fig. S4 LSV curves of Pt/C and Fe-N-C-Tcatalysts at a rotation speed of 1600 r·min^{-1} with a scan rate of 10 mV s^{-1} the different catalyst loadings.

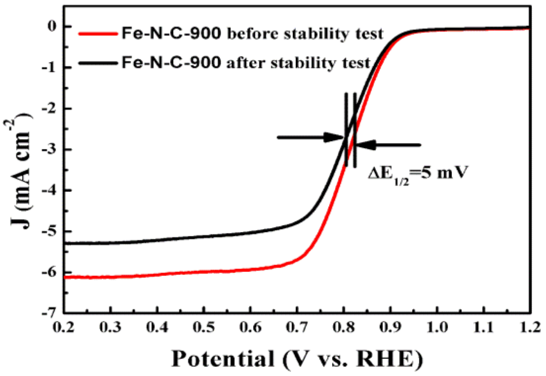

Fig. S5 LSV curves of Fe-N-C-900 before and after stability tests.

Table S1 The crystallite size of Fe-N-C-T, Fe-C-900, Fe-N-900, and MIL-900 calculated form their I_D/I_G rations based on Tuinstra-Koeng relation.

Samples	I_D/I_G ratio	L_a/nm
Fe-N-C-800	1.032	18.629
Fe-N-C-900	1.000	19.225
Fe-N-C-1000	0.980	19.617
Fe-C-900	1.162	16.544
Fe-N-900	0.966	19.901
MIL-900	1.293	14.868

The crystallite size L_a of as-obtained samples can be estimated from Tuinstra-Koeng relation as follows. L_a (in nm) = $(2.4 \times 10^{-10})\lambda^4(I_D/I_G)^{-1}$

Where λ is Raman excitation wavelength (532 nm). The higher values of L_a reflect the increase in the average size of sp^2 domains in carbon-based materials.

Table S2 Nitrogen sorption data of Fe-N-C-800, Fe-N-C-900, Fe-N-C-1000, Fe-C-900, Fe-N-900 and MIL-900.

Samples	S_{BET}/(m^2·g^{-1})	Pore volumes/(cm^3·g^{-1})
Fe-N-C-800	465	0.973
Fe-N-C-900	502	2.662
Fe-N-C-1000	437	0.954
Fe-C-900	435	1.531
Fe-N-900	428	0.928
MIL-900	112	0.385

Table S3 The elemental analysis of Fe-N-C-800, Fe-N-C-900 and Fe-N-C-1000.

Samples	C (at.%)	N (at.%)	O (at.%)	Fe (at.%)
Fe-N-C-800	86.38	5.69	6.82	1.11
Fe-N-C-900	89.79	4.2	4.45	1.56
Fe-N-C-1000	90.85	3	5.26	0.89

Table S4 The percentage contents of various chemical states of N in Fe-N-C-800, Fe-N-C-900 and Fe-N-C-1000.

samples	N content (at.%)	Pyridinic N content (at.%)	Fe-N content (at.%)	Pyrrolic N content (at.%)	Graphitic N content (at.%)	Oxidized N content (at.%)
Fe-N-C-800	5.69	33.6	22.4	16.2	15.5	12.3
Fe-N-C-900	4.2	25.3	16.6	11.1	27.0	20.0
Fe-N-C-1000	3.0	15.2	16.3	5.7	33.8	29

Table S5 Comparison of the ORR performance of Fe-N-C-900 and other state-of-the-art catalysts reported in literatures in 0.1 mol·L^{-1} KOH.

Catalyst	E_{onset}/V	$E_{1/2}$/V	J/(mA·cm^{-2})	Electron transfer numbers	References
Co-CoO/N-rGO	0.88	0.78	～5.7	3.7–3.9	(1)
CoN-GCI	～0.94	0.857	～5.6	4	(2)
VB12/Silica colloid	～0.88	0.78	～4.8	3.8	(3)
Fe_3C/b-NCNT	0.96	～0.82		4	(4)
C-Fe-Z8-Ar	0.95	0.82		3.98	(5)
Fe-N/G	0.874	～0.79	～5.2	3.77–3.99	(6)
Fe-N/C-900	0.98	～0.79	～4.8	3.95	(7)
C-FeZIF-900-0.84	0.95	0.84		3.8	(8)
Fe-N/C-700	0.956	0.84			(9)
Fe-N-C900	0.96	0.83	6.28	4	this work

[a] All the potential values here are relative to RHE for comparison.

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