

Electronic Supplementary Material

Carboxylate Trapping Engineering to Fabricate Monodispersed Dual-Atom Iron Sites for Efficient Oxygen Reduction

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1. Figures

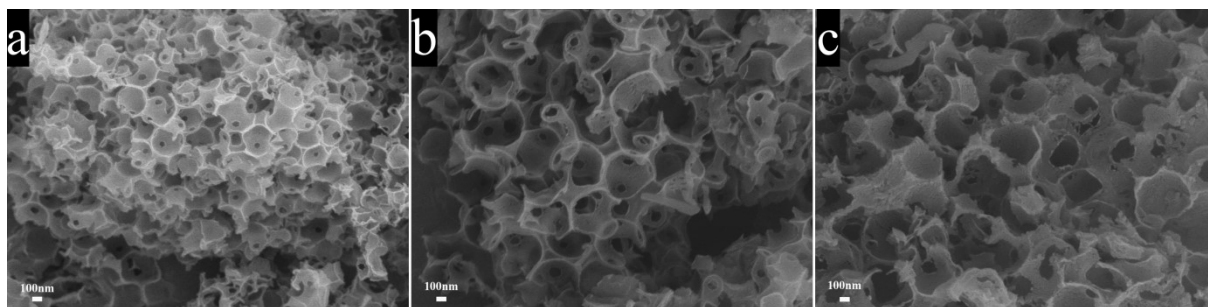


Fig. S1. SEM images of (a) 0.05FeNC-OAc, (b) 0.8FeNC-OAc, and (c) 1.6FeNC-OAc.

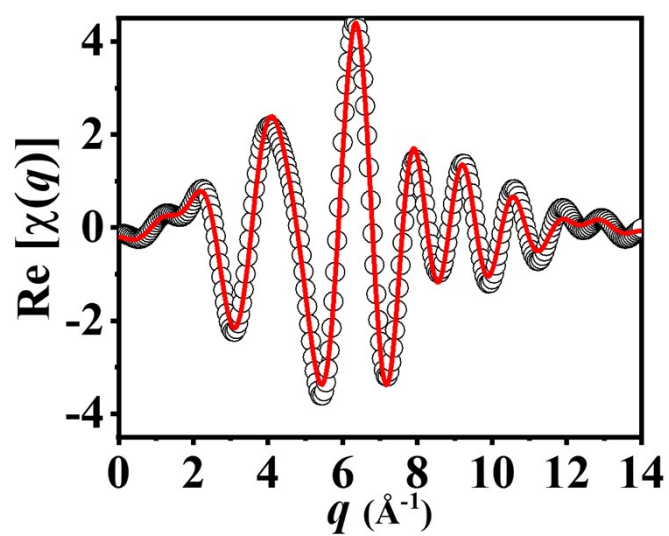


Fig. S2. The fitting curves in q-space

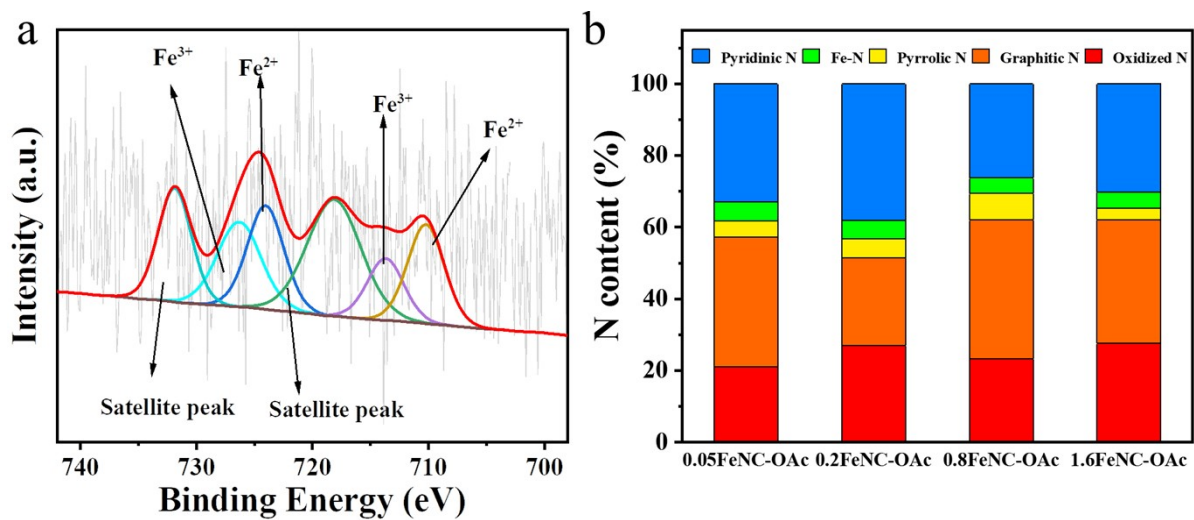


Fig. S3 XPS of 0.2FeNC-OAc: (a) Fe 2p high-resolution spectra and (b) Nitrogen content of the different N species from XPS.

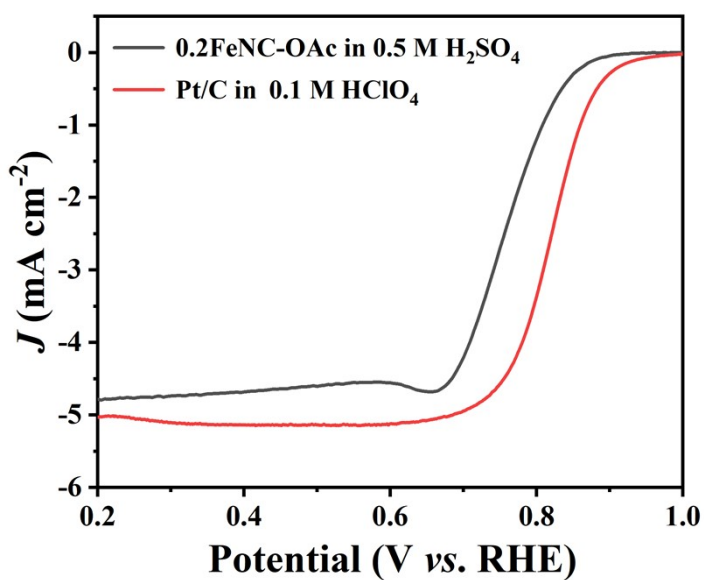


Fig. S4 ORR polarization curves of 0.2FeNC-OAc catalysts in 0.5 M H₂SO₄ and Pt/C in 0.1 M HClO₄

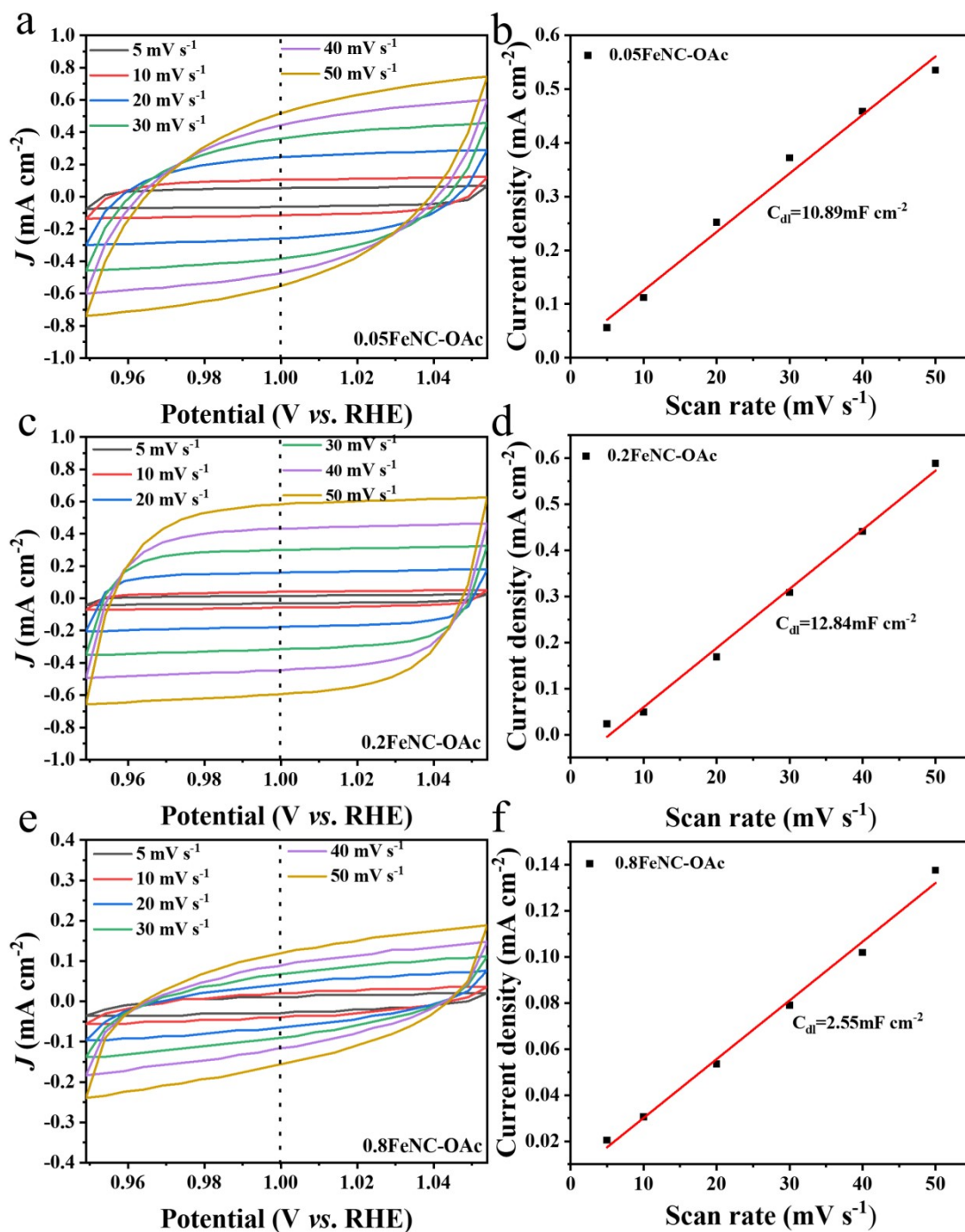


Fig. S5 (a, c, and e) Corresponding capacitive Δj at the potential of 1.00 V (vs. RHE) plots to estimate the electrochemical double-layer capacitances (C_{dl}) for (b) 0.05FeNC-OAc, (d) 0.2FeNC-OAc, and (f) 0.8FeNC-OAc.

2. Tables

Table S1 Fitting parameters of EXAFS for 0.2FeNC-OAc and FePc reference.

Catalysts	Path	Coordination	Bond length	ΔE_0 [eV]	R factor
		Number [N]	R [\AA]		
0.2FeNC-OAc	Fe-N	4.2	2.03	1.28	0.021
	Fe-Fe	0.9	2.54	1.28	0.021
	Fe-O	0.7	1.49	1.28	0.021
FePc	Fe-N	3.84	1.92	6.51	0.0196

Note: ΔE_0 is inner potential correction; R factor is the goodness of fitting result.

Table S2. Textural parameters of all n FeNC-OAc catalyst according to N_2 sorption isotherms.

Catalysts	BET SSA ^a [$\text{m}^2 \cdot \text{g}^{-1}$]			$S_{\text{ext}}/S_{\text{micro}}^e$	V_{total}^f [$\text{cm}^3 \cdot \text{g}^{-1}$]	APD ^g [nm]
	S_{total}^b	S_{micro}^c	S_{ext}^d			
0.2FeNC-OAc	664	416	248	62.7%	0.74	4.47
0.8FeNC-OAc	676	213	463	31.5%	0.85	5.00
1.6FeNC-OAc	656	104	552	15.9%	0.88	5.39

^a Brunauer-Emmett-Teller specific surface (BET SSA); ^b total specific surface; ^c micropore ratio surface; ^d external surface; ^e Proportion of the micropore surface area in the total SSA; ^f total pore capacity; ^g average pore size.