

Electronic supplementary information

Encapsulation of Co nanoparticles with single-atomic Co sites into nitrogen-doped carbon for electrosynthesis of hydrogen peroxide

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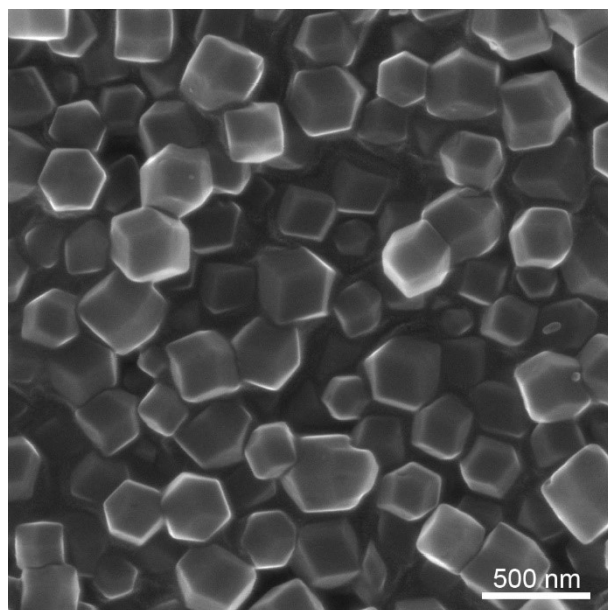


Fig. S1. SEM image of the resultant ZIF-67.

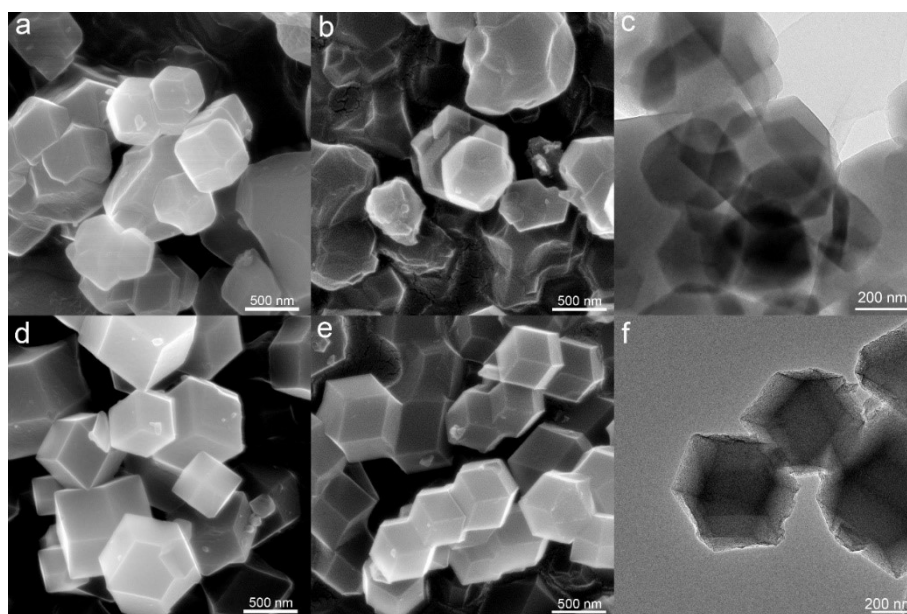


Fig. S2. (a, b, d, e) SEM images, (c, f) TEM images of the resultant ZIF-8 (a), NC-900 (b-c), Co/Zn-ZIF (d), and Co SACs-900 (e-f).

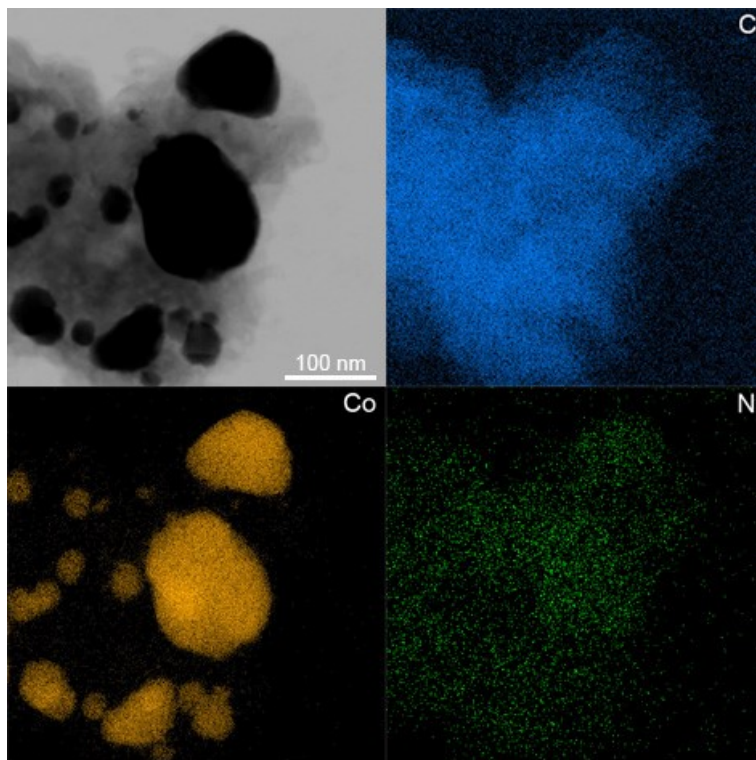


Fig. S3. EDX mappings of the resultant CoNC-900.

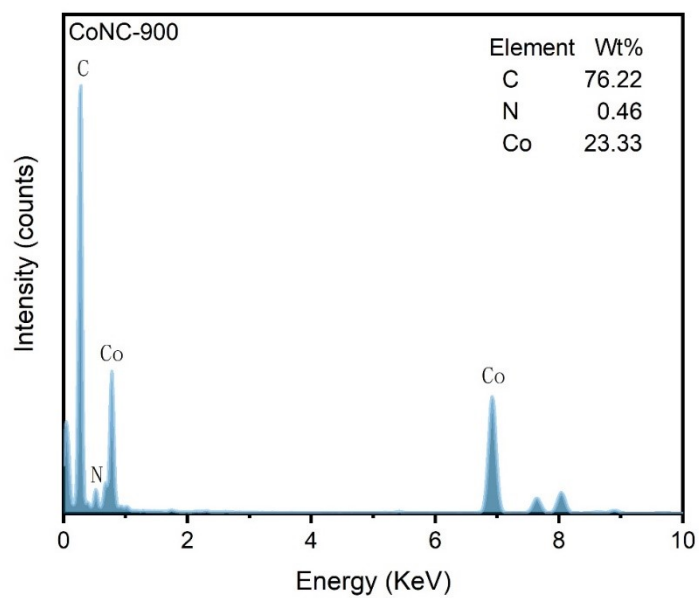


Fig. S4. The corresponding EDS spectrum of CoNC-900.

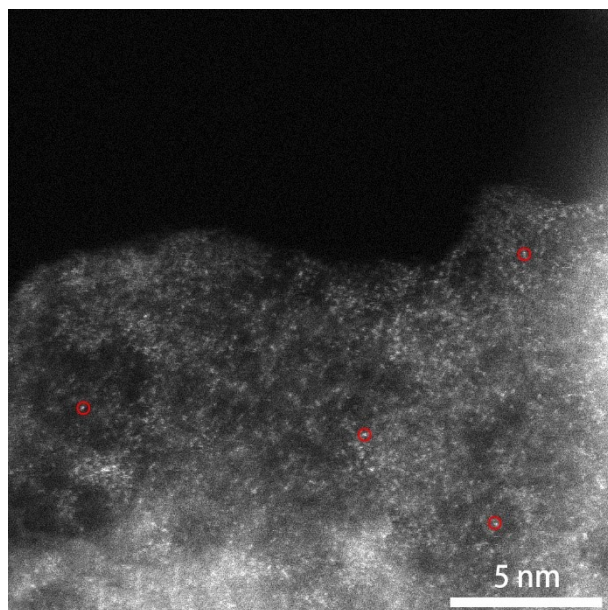


Fig. S5. AC HAADF-STEM images of the resultant Co SACs-900.

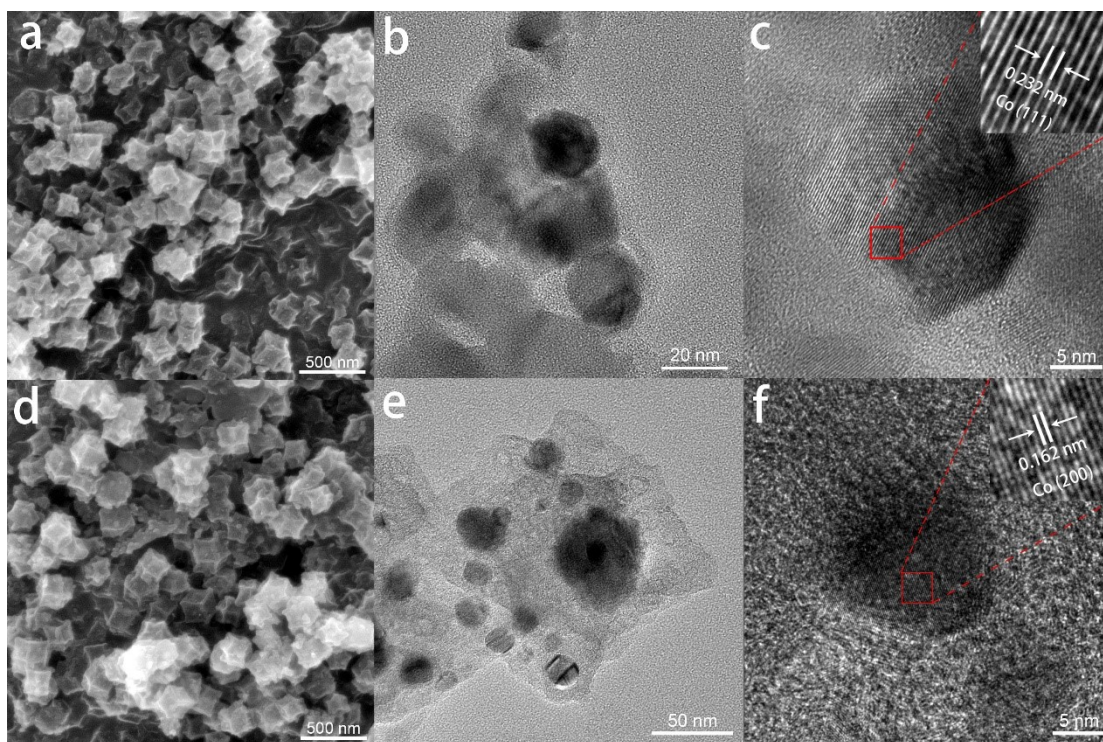


Fig. S6. (a, d) SEM, (b, e) TEM, (c, f) HRTEM images of the resultant CoNC-700 (a-c) and CoNC-800 (d-f).

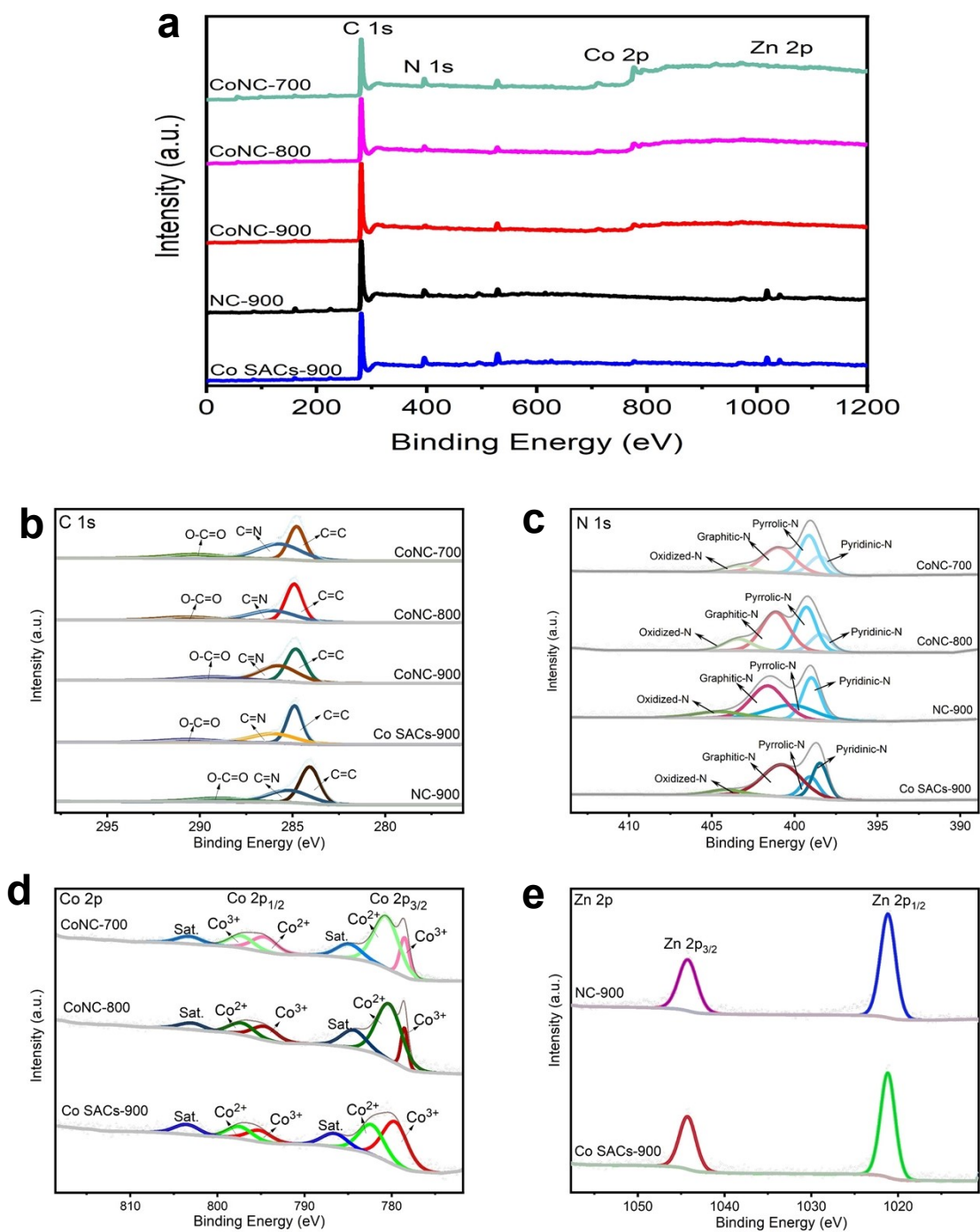


Fig. S7. (a) The survey XPS spectrum, (b) high resolution C 1s XPS spectra, (c) high resolution N 1s XPS spectra, (d) high resolution Co 2p XPS spectra, and (e) high resolution Zn 2p XPS spectra of the resultant catalysts.

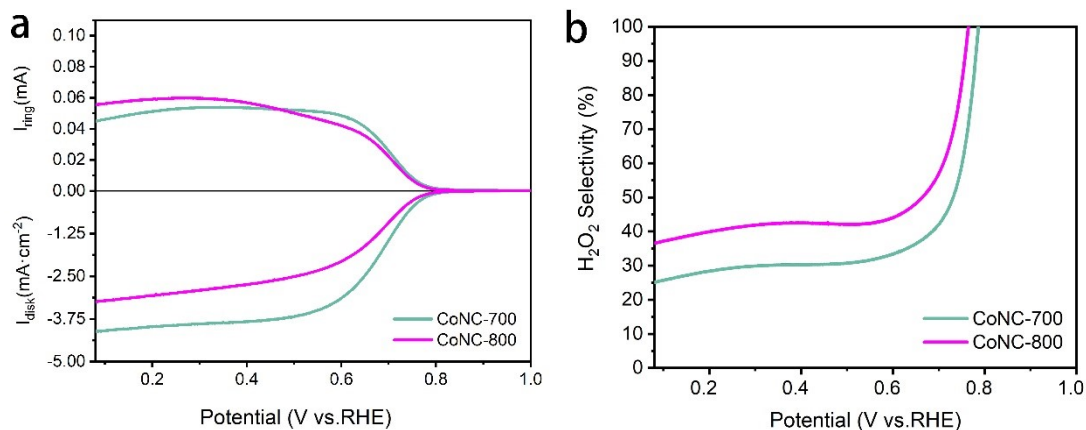


Fig. S8. (a) LSV curves and (b) H₂O₂ selectivity of CoNC-700, CoNC-800 in 0.5 M H₂SO₄.

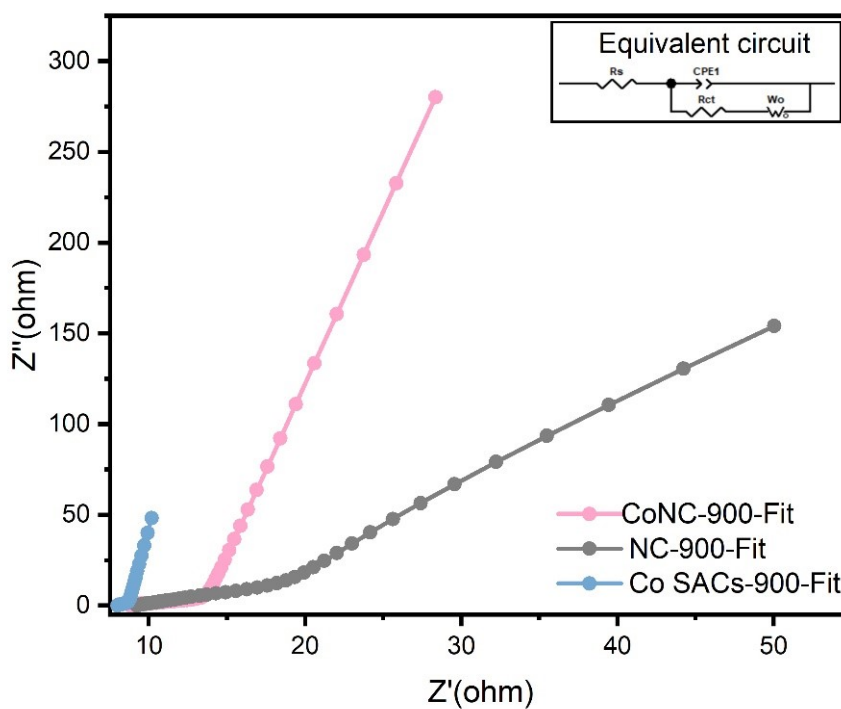


Fig. S9. The EIS fit results' curves for CoNC-900, NC-900, and Co SACs-900. Note: R_s : Solution resistance; $CPE1$: Constant phase element; R_{ct} : Charge transfer resistance; W_o : Warburg element (open).

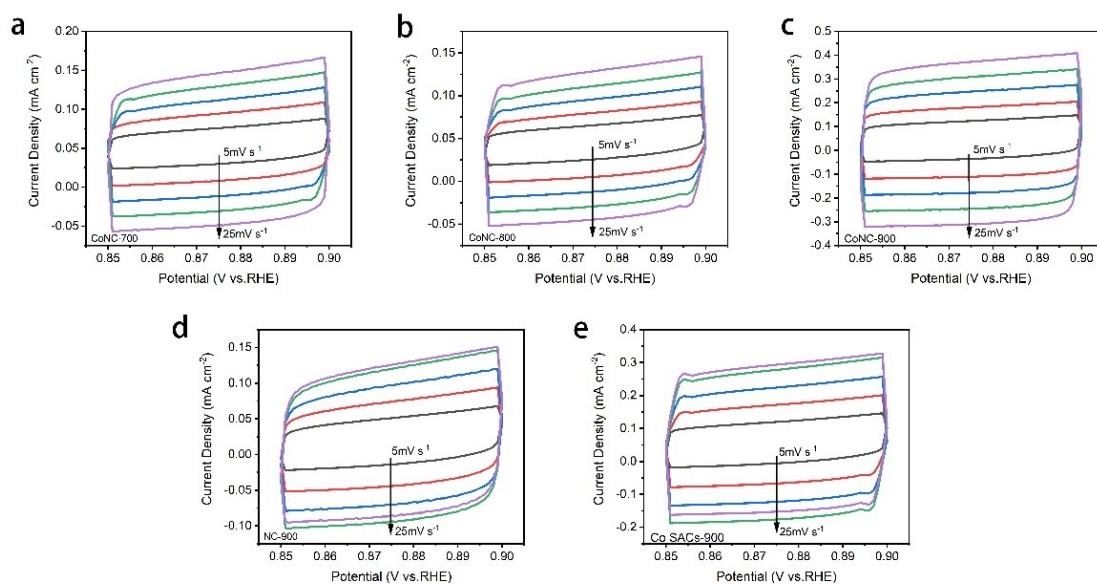


Fig. S10 CV curves at different scan rates of 5, 10, 15, 20 and 25 mV s^{-1} over the resultant (a) CoNC-700, (b) CoNC-800, (c) CoNC-900, (d) NC-900, and (e) Co SACs-900 in 0.5 M H_2SO_4 .

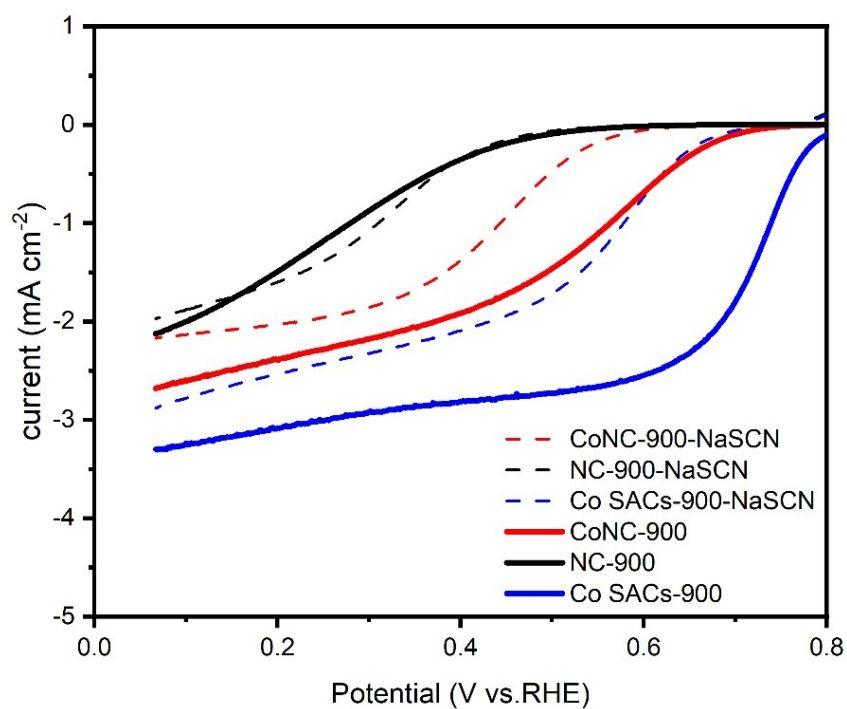


Fig. S11 LSV curves as a function of scan rates for CoNC-900, NC-900, and Co SACs-900 in 0.5 M H_2SO_4 with and without 10mM NaSCN.

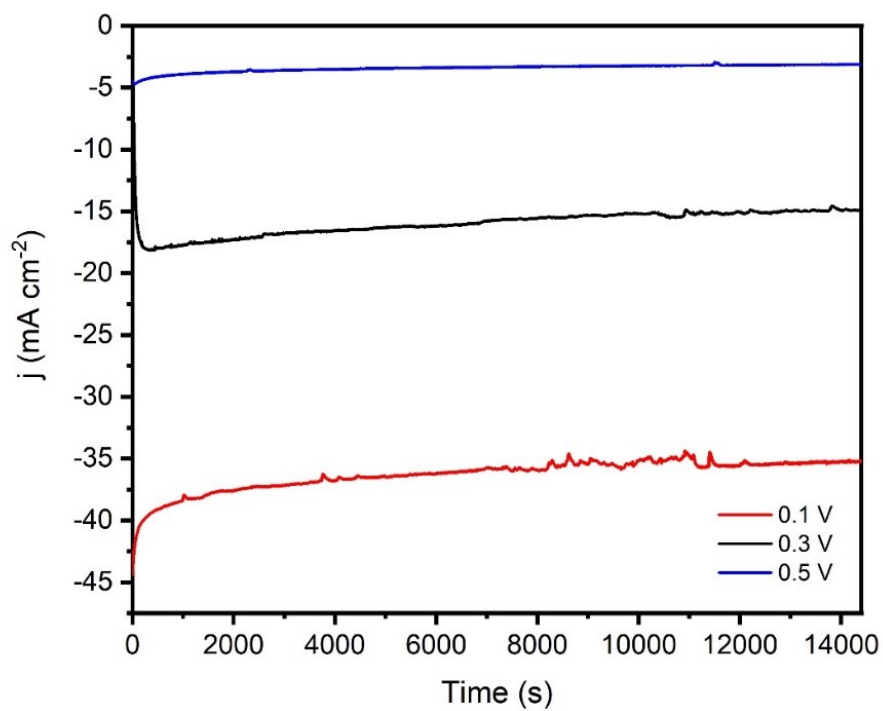


Fig. S12 Chronoamperometry curves of CoNC-900/CP were obtained at 0.1 V, 0.3 V, and 0.5 V for 4 hours at each potential in 0.5 M H₂SO₄.

Table S1 Peak fitting data of Raman spectra for the resultant catalysts.

Catalyst	Band	Peak Area	Center	Maximum Intensity	FWHM
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CoNC-900	D	36464.58	1343.72	170.73	200.65
	G	23085.09	1582.30	203.57	106.53
NC-900	D	119989.54	1349.36	583.68	193.14
	G	95657.97	1569.95	573.69	156.64
Co SACs-900	D	24440.98	1349.96	114.30	200.88
	G	18262.05	1570.28	118.52	144.74

Table S2 The relative content of each element of the resultant catalysts from XPS analysis.

Table S3 The fitted relative content of nitrogen species within the resultant catalysts.

Catalyst	Catalyst	C (at%)	Configuration of N (%)			
			Oxidized-N	Graphitic-N	Pyrrhic-N	Pyridinic-N
CoNC-700	CoNC-700	85.2	13.28 ^{6.2}	36.86 ^{5.9}	32.71 ^{2.7}	17.15
CoNC-800	CoNC-800	91.5	18.79 ^{4.2}	38.03 ^{3.0}	30.50 ^{1.3}	12.67
CoNC-900	CoNC-900	94.4	9.50 ^{4.0}	69.45 ^{1.0}	6.98 ^{0.6}	14.07
NC-900	NC-900	91.1	10.34 ^{5.3}	38.50 ^{3.0}	24.05	27.11 ^{0.7}
CoSACs-900	CoSACs-900	86.8	6.08 ^{6.6}	52.78 ^{5.5}	13.94 ^{0.4}	27.21 ^{0.8}

Table S4 BET surface area and pore volume of the resultant catalysts.

Table S5 EIS fitting results of the resultant catalysts.

Catalyst	Rs/ Ω	CPE1-T/s	CPE1-P/F	Rct/ Ω	Wo-R/ Ω	Wo-T/s	Wo-P
CoNC-900	7.30	3.85E-8	1.55	0.25	13.28	6.78E-3	0.48
NC-900	9.18	7.78E-4	0.72	1.20	50.37	0.03	0.49
CoSACS-900	8.90	1.29E-3	0.98	0.01	5.13	0.01	0.50

Catalyst	Surface Area /m ² g ⁻¹	Pore Volume /cm ³ g ⁻¹
CoNC-900	228.9075	0.232735
NC-900	1,092.0055	0.193640
Co SACs-900	890.0014	0.062090

Note: Rs: Solution resistance; CPE1: Constant phase element; Rct: Charge transfer resistance; Wo: Warburg element (open).