

Atomic and Nanosized Co Species Functionalized N-Doped Porous Carbon Hybrid for Boosting Electrocatalytic Oxygen Reduction

Supporting Information

The computation detail of Bader charge analysis

All the DFT computation is conducted within VASP package under periodic boundary conditions. The configuration of Co₄-decorated Co-N₄-C has been optimized. The interaction between atoms and electrons are described by projected augmented wave method (PAW). The exchange and correlation energy are approximated with the PBE functional under the generalized gradient approximation. A vacuum layer of 20 Å is applied between the two monolayers of Co₄-decorated Co-N₄-C to avoid layer-to-layer interaction. The kinetic energy cutoff for the plane wave is set to 400 eV. The Monkhorst-Pack method is applied for sampling within the Brillouin zone, and the generated 4×4×1 k-points are adopted. The structural optimization is conducted until the force on each atom is less than 0.01 eV Å⁻¹. Between two consecutive electronic steps, the energy convergence is set to 1×10⁻⁵ eV. Van der Waals forces are considered by applying a dispersion corrected framework (DFT-D2).

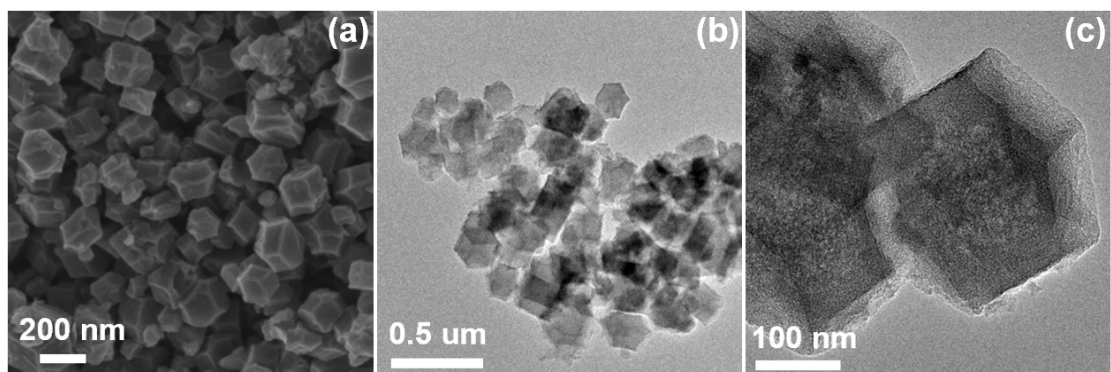


Figure S1 (a) SEM and (b, c) TEM images of Co@NPC.

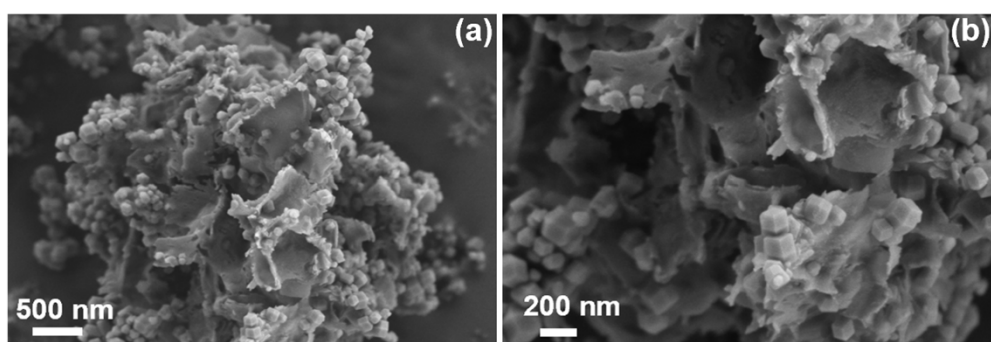


Figure S2 SEM images of CoZn-ZIF/CN precursor.

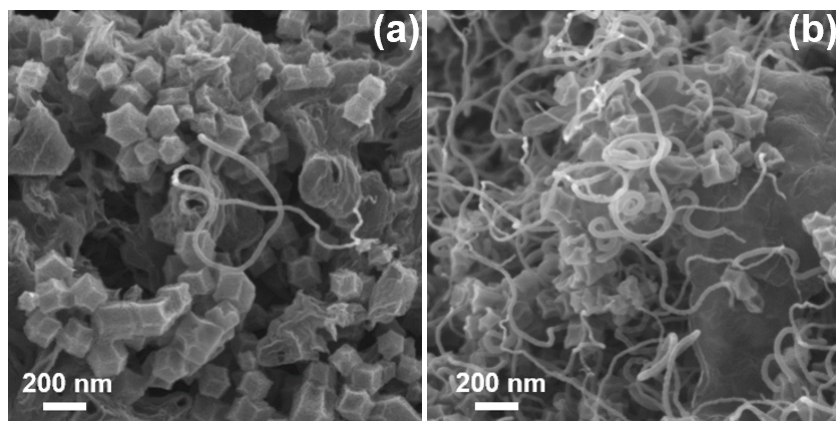


Figure S3 SEM images of Co@NRPC-30 (a) and Co@NRPC-150 (b).

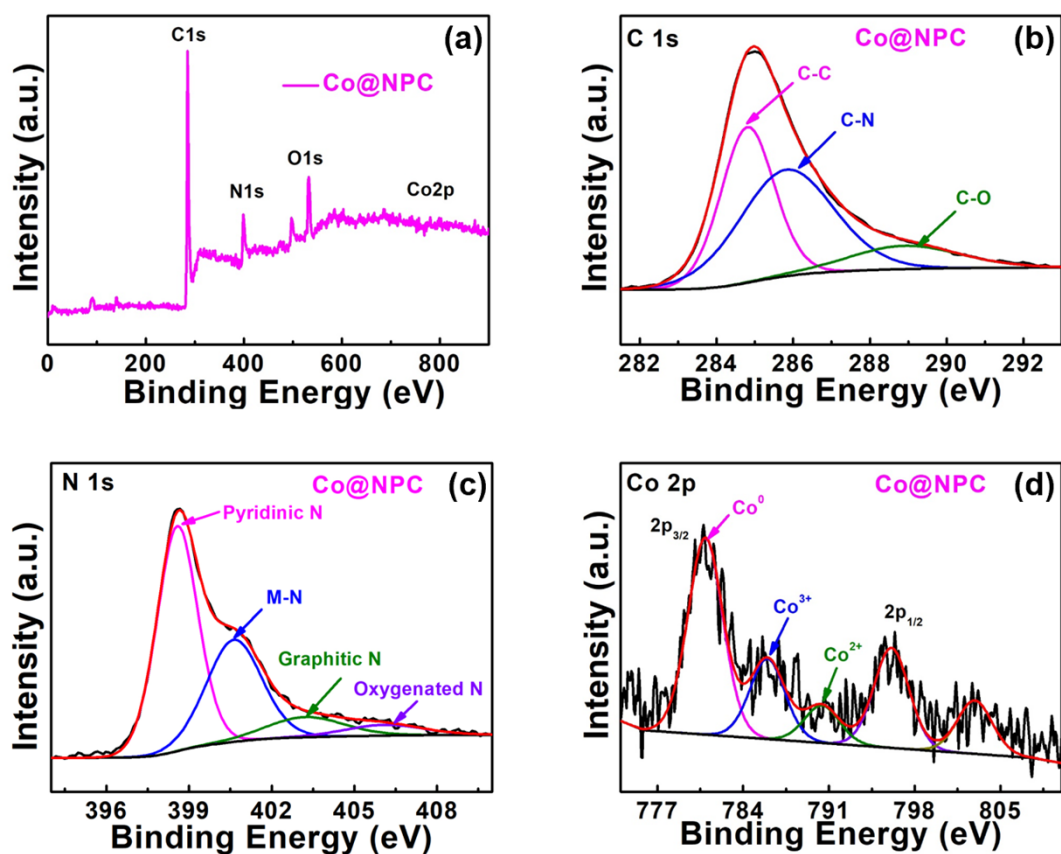


Figure S4 (a) Full, (b) C 1s, (c) N 1s, and (d) Co 2p XPS spectra of Co@NPC.

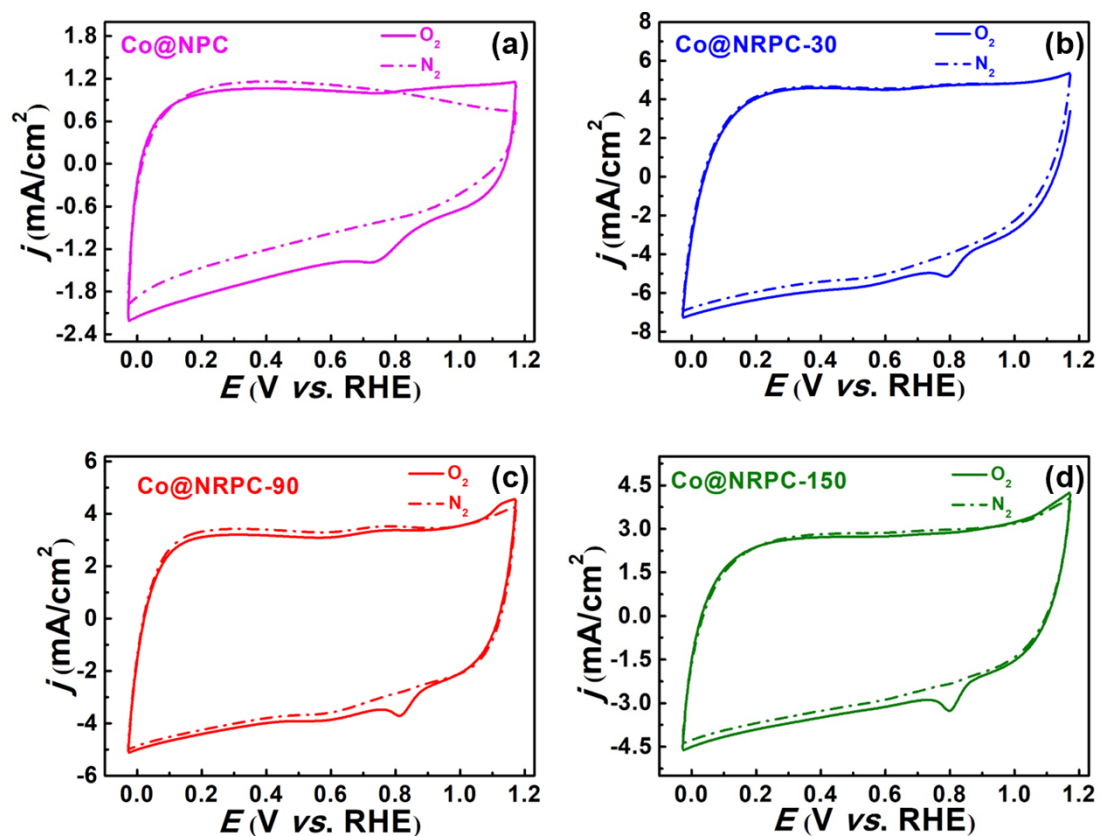


Figure S5 Cyclic voltammograms (CVs) of Co@NPC and Co@NRPC-x (x = 30, 90, and 150).

in the N_2 - or O_2 -saturated 0.1 mol L^{-1} KOH electrolyte at a scan rate of 10 mV s^{-1} .

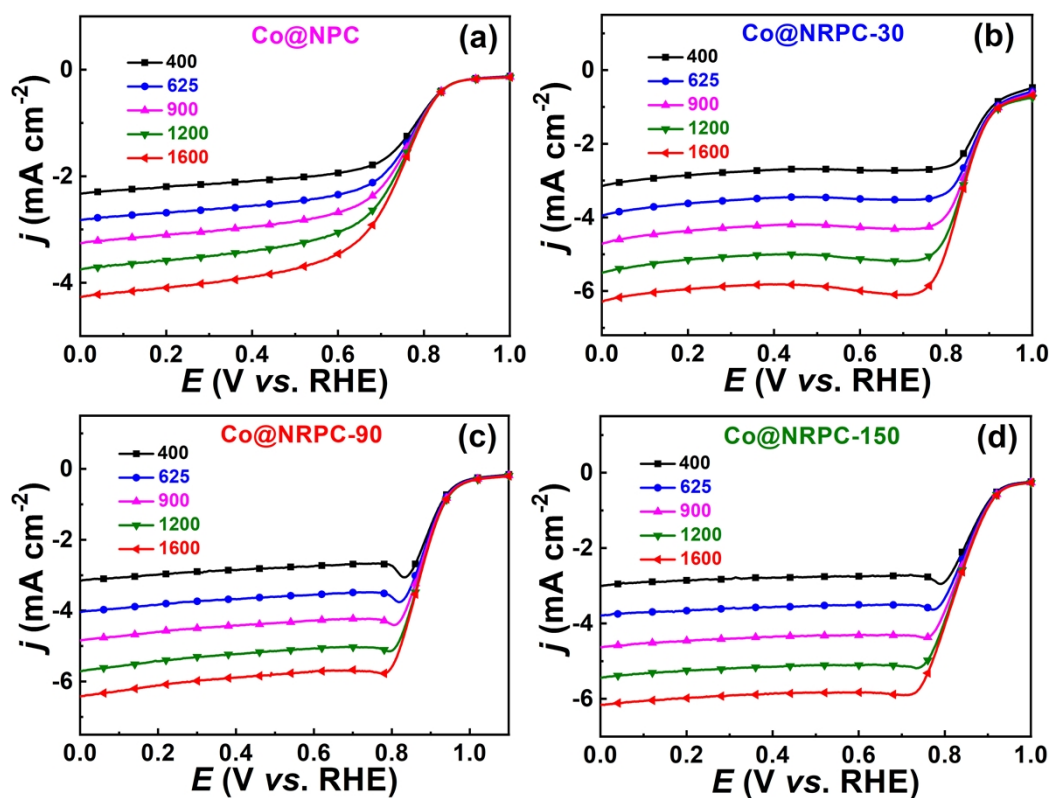


Figure S6 RDE measurements of Co@NPC and Co@NRPC-x (x = 30, 90, and 150) under different rotating speeds from 400 to 1600 rpm.

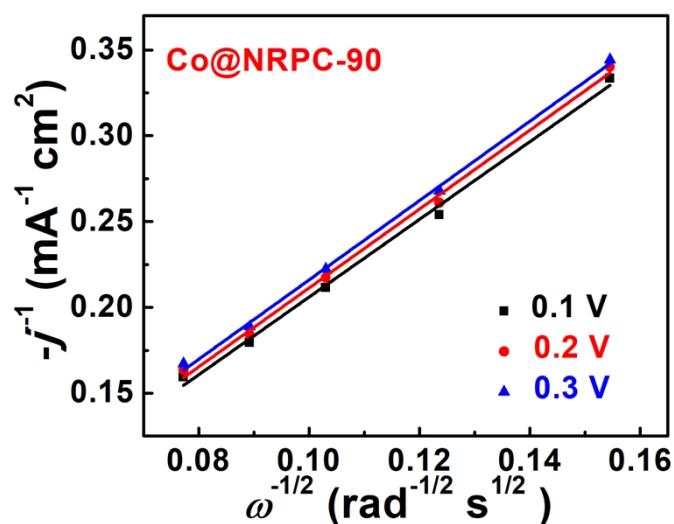


Figure S7 K-L plots of Co@NRPC-90 under different potentials.

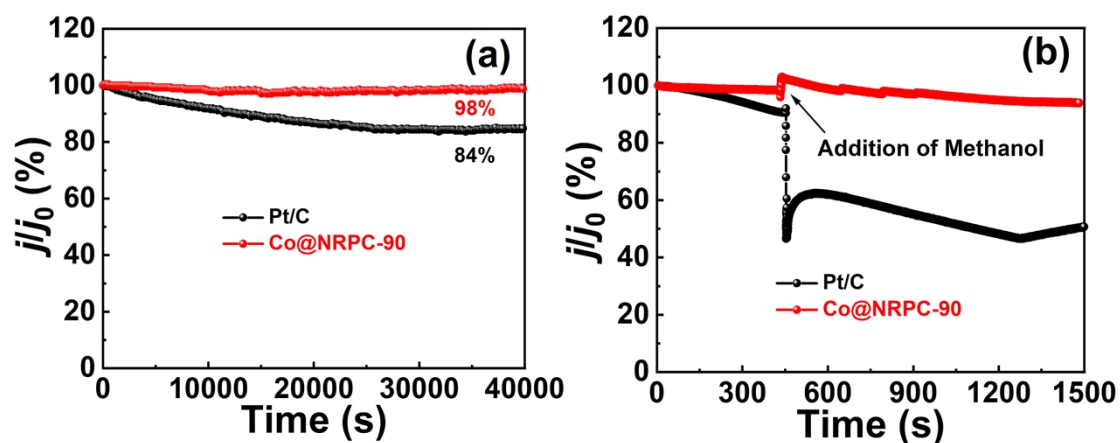


Figure S8 (a) *i-t* chronoamperometric responses of Co@NRPC-90 and Pt/C in O₂-saturated 0.1 mol L⁻¹ KOH electrolyte, and (b) with addition of methanol.

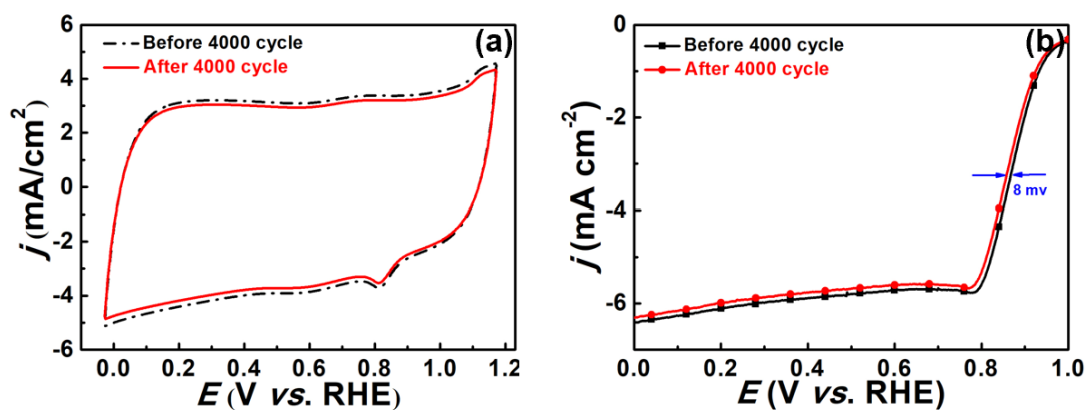


Figure S9 CV (a) and LSV (b) curves of Co@NRPC-90 before and after 4000 cycles.

Table S1 Pore size distribution of Co@NPC and Co@NRPC-90

Sample	Pore volume (cm ³ g ⁻¹)				Percentage of pore volume (%)			
	<2 nm	2~10 nm	10~50 nm	>50 nm	<2 nm	2~10 nm	10~50 nm	>50 nm
Co@NPC	0.024649	0.028841	0.356724	0	6.01	7.03	86.96	0
Co@NRPC-90	0.020433	0.139627	0.597579	0.137178	2.28	15.60	66.78	15.33