Supporting Information

Probing heteroatomic dopant-activity synergy over Co_3O_4/doped carbon nanotube electrocatalysts for oxygen reduction reaction

Aiai Zhang,† Jinfang Wu,† Lei Xue,† Shan Yan,‡ Shanghong Zeng*†*

†Inner Mongolia Key Laboratory of Chemistry and Physics of Rare Earth Materials, School of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot 010021, China

‡Department of Chemistry, State University of New York at Binghamton, Binghamton, New York 13902, United States

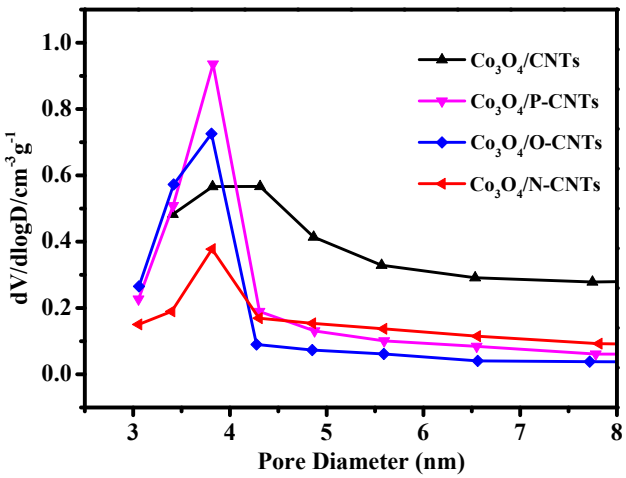

Figure S1. Pore size distribution curves of Co_3O_4/CNTs, Co_3O_4/P-CNTs, Co_3O_4/O-CNTs, Co_3O_4/N-CNTs.

Table S1 Pore structure parameters of the samples

Sample	BET surface area(m^2/g)	Pore volume(cm^3/g)
Co_3O_4/CNTs	178.48	0.64
Co_3O_4/P-CNTs	123.94	0.14
Co_3O_4/O-CNTs	102.46	0.11
Co_3O_4/N-CNTs	80.00	0.11

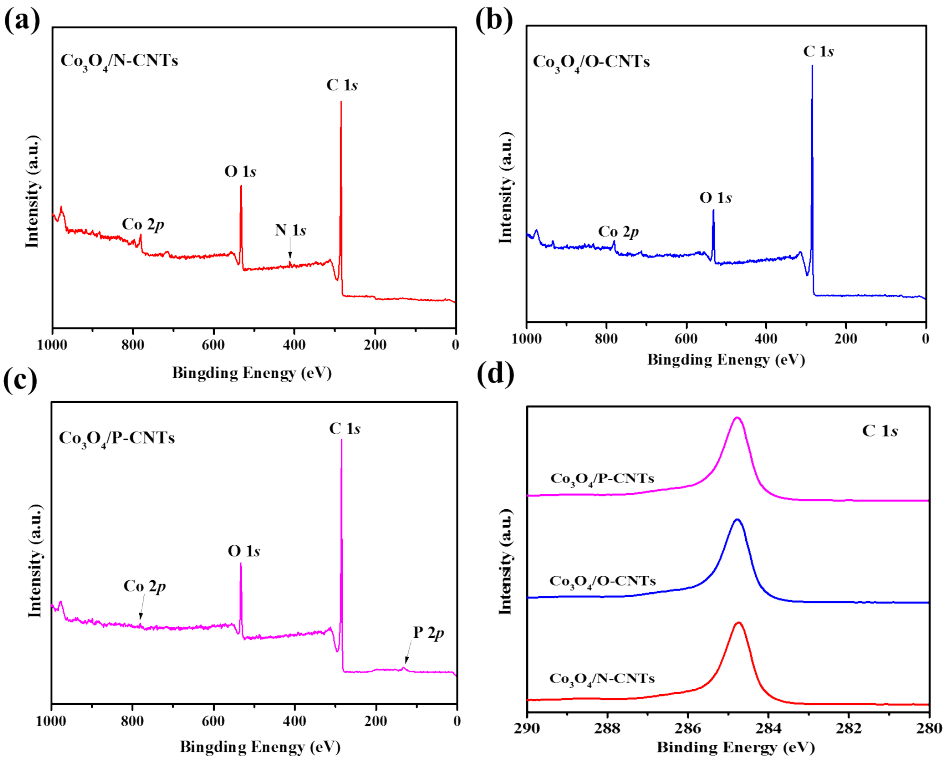

Figure S2. Wide-scan XPS spectra of (a) Co_3O_4/N-CNTs, (b) Co_3O_4/O-CNTs, (c) Co_3O_4/P-CNTs, and XPS spectra of (d) C 1s.

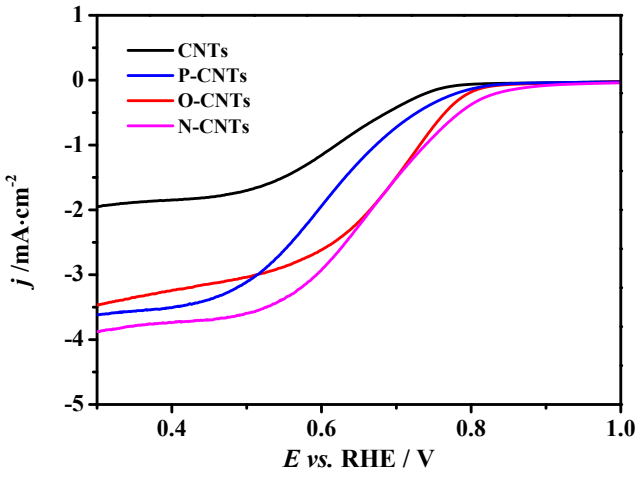

Figure S3. LSV polarization curves of CNTs, P-CNTs, O-CNTs and N-CNTs.

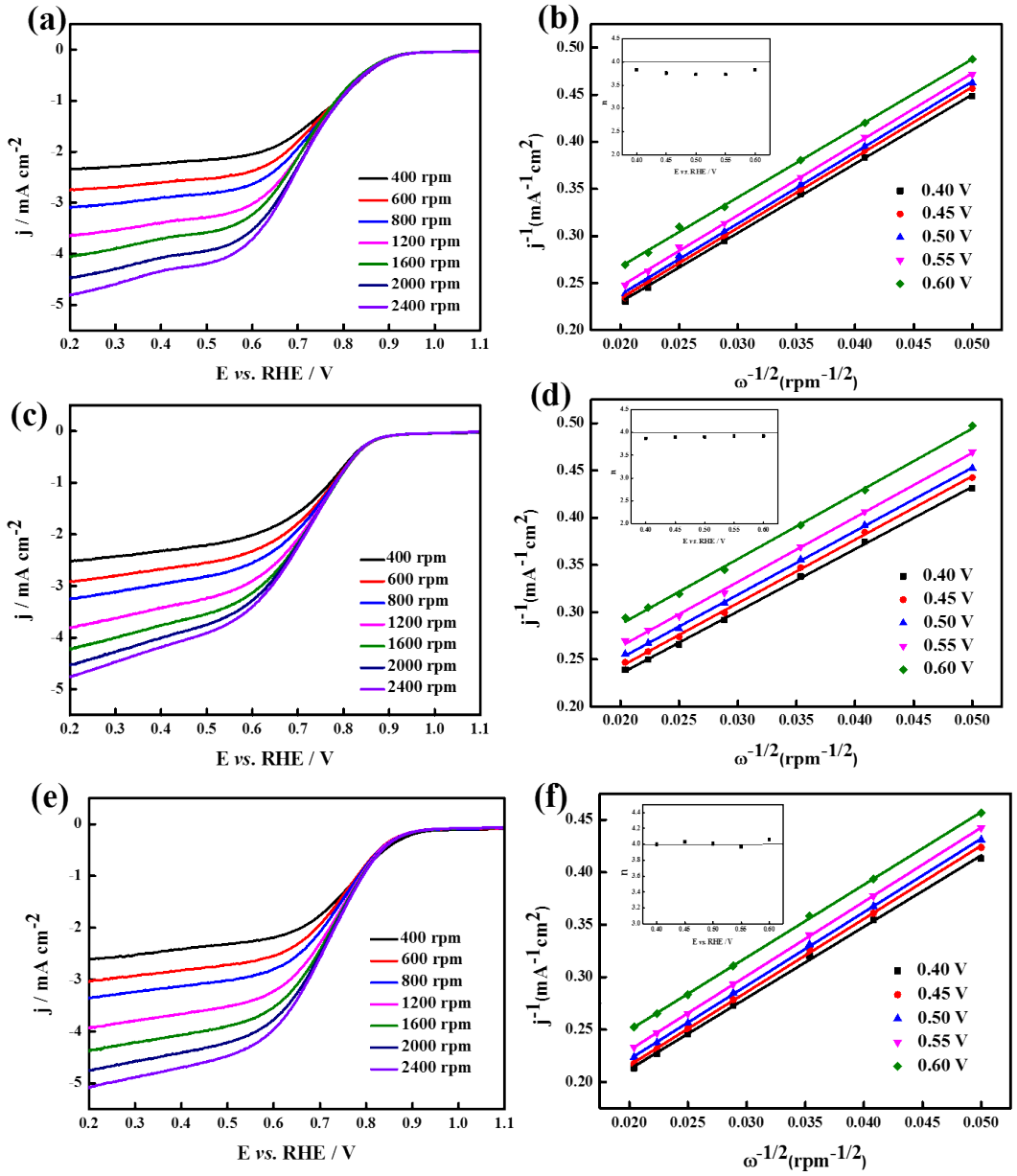

Figure S4. LSV polarization curves for ORR with various rotation rates and the corresponding K-L plots (j^{-1} vs $\omega^{-1/2}$) at different potentials of (a, b) Co_3O_4/CNTs, (c, d) Co_3O_4/P-CNTs and (e, f) Co_3O_4/O-CNTs.

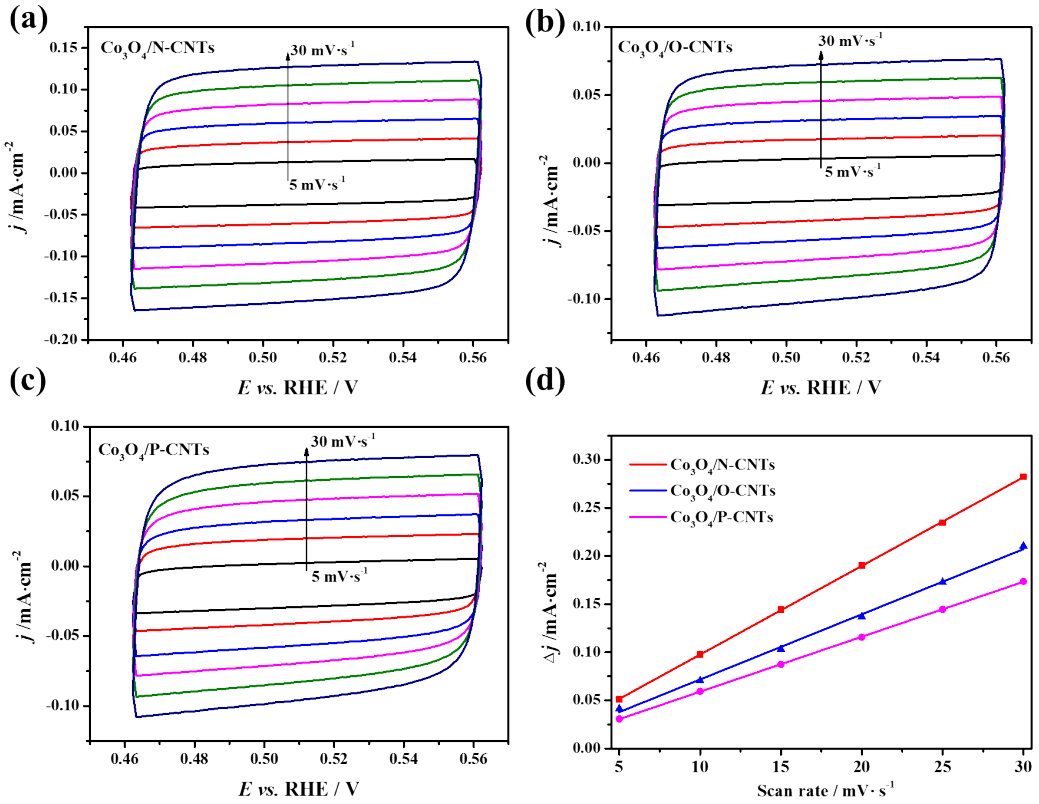

Figure S5. The electric double layer capacitance (C_{dl}) test of Co_3O_4/N-CNTs, Co_3O_4/O-CNTs Co_3O_4/P-CNTs with different scan rate.

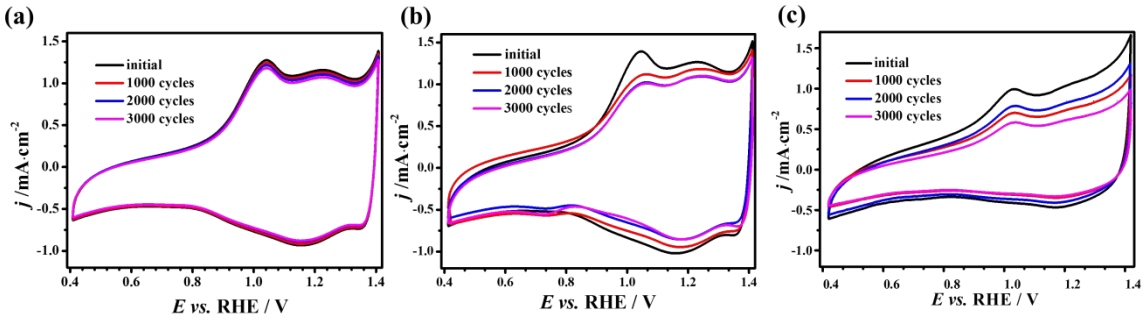

Figure S6. CV curves of (a) Co_3O_4/N-CNTs, (b) Co_3O_4/O-CNTs and (c) Co_3O_4/P-CNTs after accelerated stability tests.

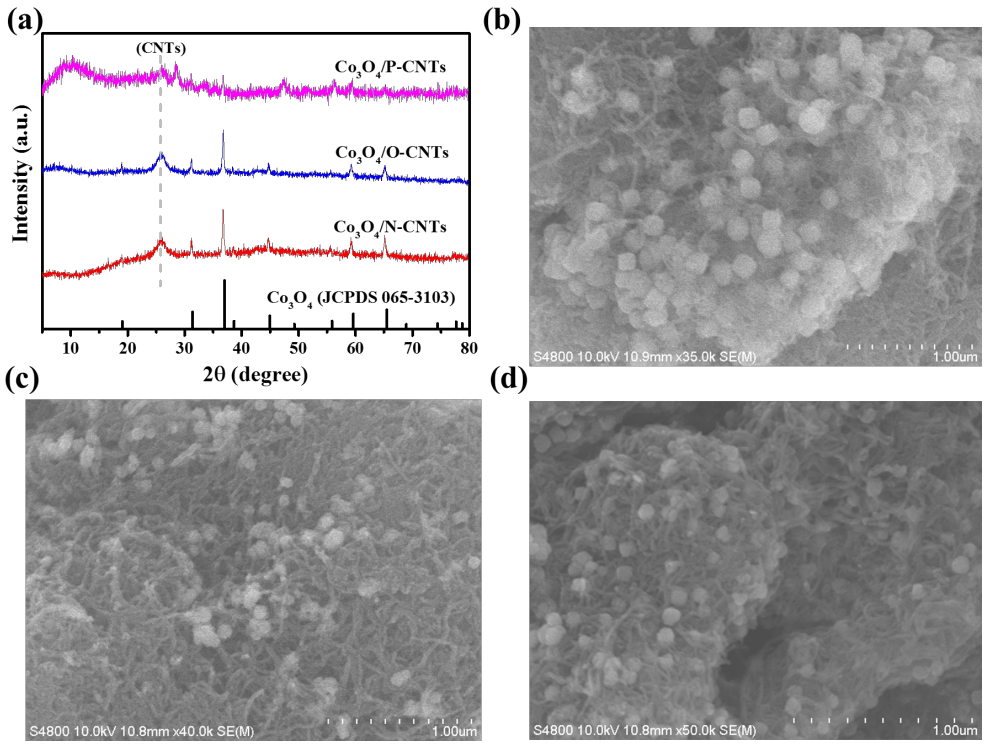

Figure S7. XRD patterns of (a) the catalysts and SEM images of (b) Co_3O_4/N-CNTs, (c) Co_3O_4/O-CNTs and (d) Co_3O_4/P-CNTs after potential cycling of 10000 cycles.

Table S2 The energy of LUMO, HOMO and LUMO-HOMO energy gap of pure CNTs and doped CNTs.

	HOMO (eV)	LUMO (eV)	$\Delta E_{\text{LUMO-HOMO}}$
CNTs	-4.767	-4.029	0.738
P-CNTs	-4.450	-3.906	0.544
O-CNTs	-4.286	-3.779	0.507
N-CNTs	-4.848	-4.220	0.628

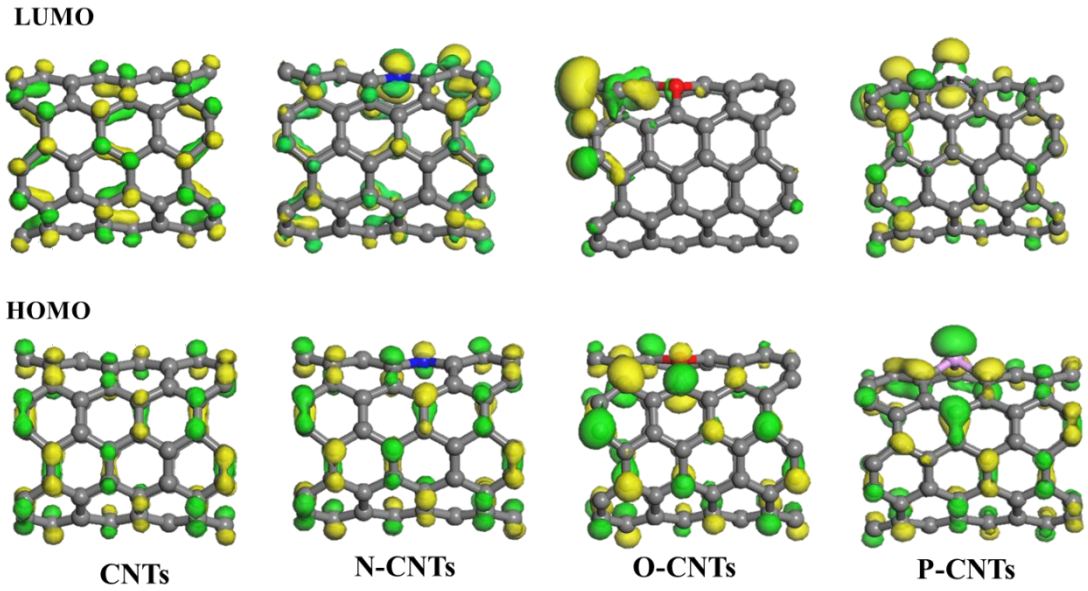

Figure S8. LUMO and HOMO shapes of pure CNTs and doped CNTs**.**