Supporting Information

Density Functional Theory Optimization of Cobalt- and Nitrogen-Doped Graphene Catalysts for Enhanced Oxygen Evolution Reaction

Jiatang Wang [1], Huawei He [1], Weiwei Cai [1,*], Chao Yang [2], Yu Wu [3], Houcheng Zhang [4,*], Rui Liu [1] and Hansong Cheng [1]

[1] Sustainable Energy Laboratory, Faculty of Materials Science and Chemistry, China University of Geosciences, Wuhan 430074, China
[2] Shanghai Frontiers Science Center of "Full Penetration" Far-Reaching Offshore Ocean Energy and Power, Merchant Marine College, Shanghai Maritime University, Shanghai 201306, China
[3] College of Engineering Science and Technology, Shanghai Ocean University, Shanghai 201306, China
[4] College of New Energy, Ningbo University of Technology, Ningbo 315211, China
* Correspondence: willcai1985@gmail.com (W.C.); hczhang@nbut.edu.cn (H.Z.)
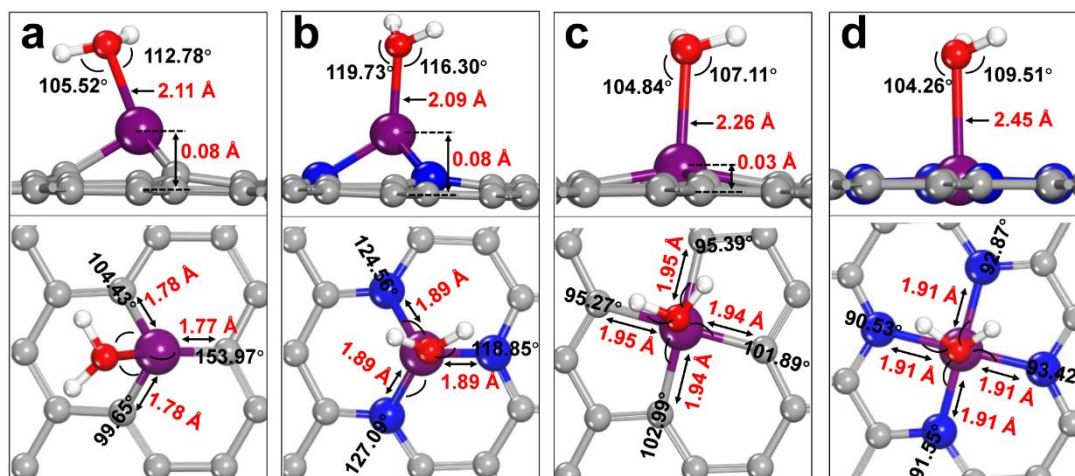
Supplementary Figures:

Figure S1. Bond lengths and bond angles of the stable Co-N-g catalyst of (a) SV-GN, (b) SV-N3, (c) DV-GN, and (d) DV-N4.
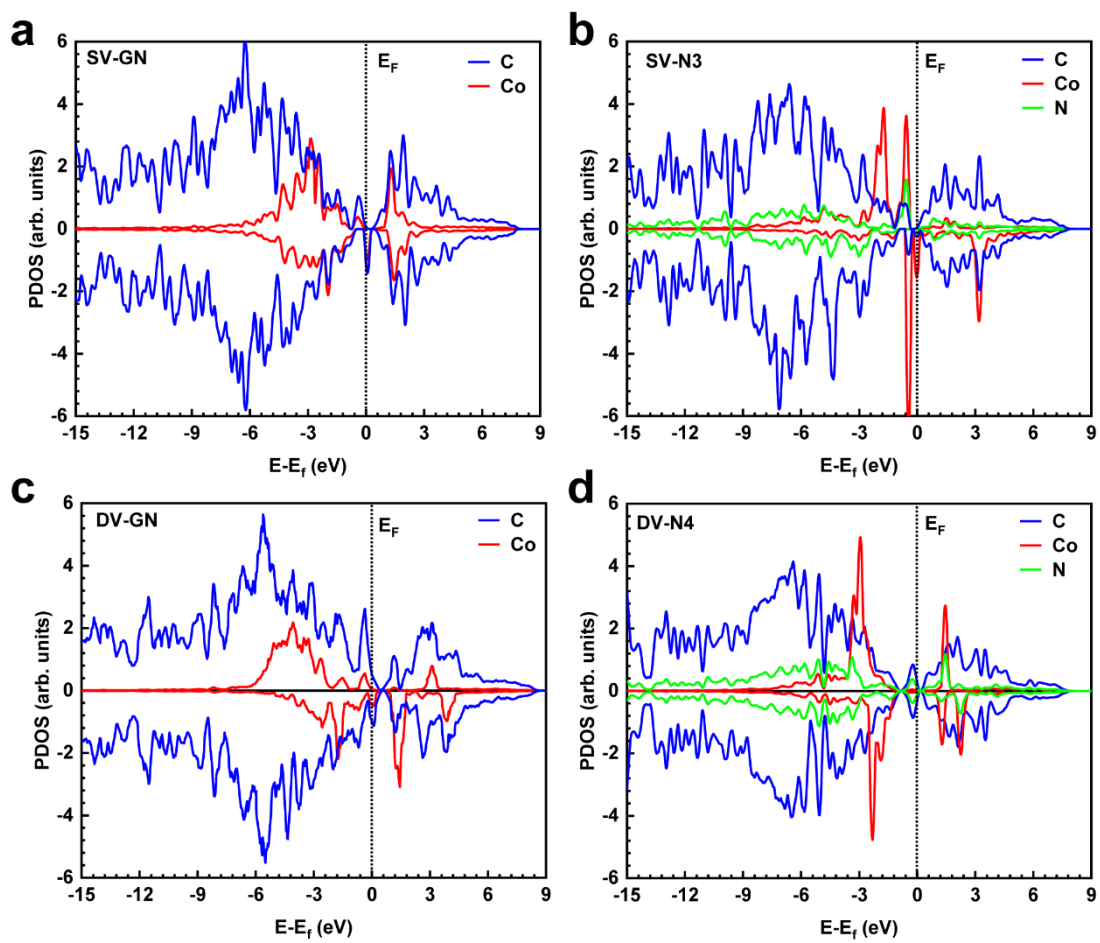
Figure S2. PDOS of specified elements C (blue), Co (red) and N (green), for Co-N-g catalyst of (a) SV-GN, (b) SV-N3, (c) DV-GN, and (d) DV-N4.
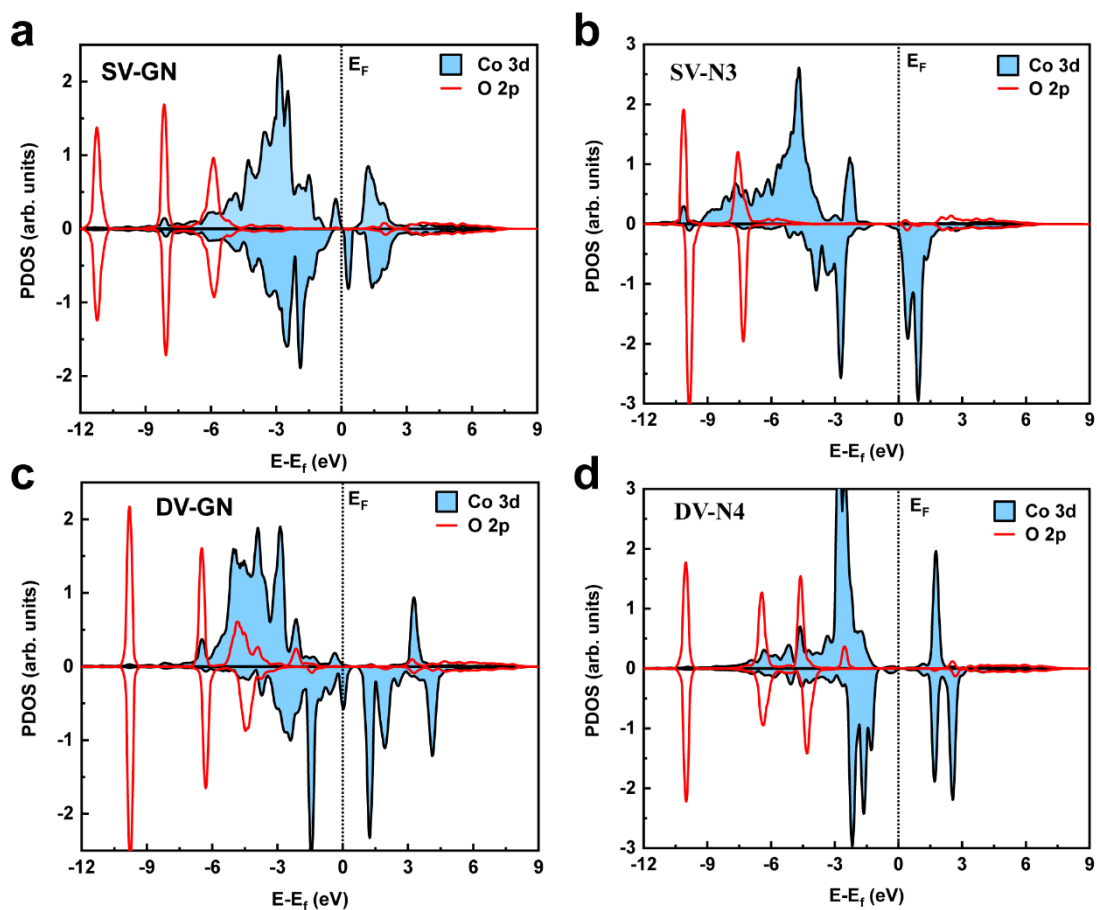
Figure S3. PDOS of Co-3d (blue) and O-2p states (red) after H_2O adsorption on the catalyst surface.

Table S1. Bader charge and d-band center values of SV-GN, SV-N3, DV-GN, and DV-N4 catalysts with H_2O adsorbed.

Catalysts	Bader charge (eV)			d-band center (eV)
	Co of catalysts	Co of H_2O adsorbed on catalysts	O of H_2O adsorbed on catalysts	Co of H_2O adsorbed on catalysts
SV-GN	0.50	0.63	-1.19	-2.45
SV-N3	0.73	1.06	-1.24	-5.22
DV-GN	0.84	0.92	-1.29	-3.39
DV-N4	0.95	0.98	-1.25	-2.68

Table S2. HOMO, LUMO, and HOMO-LUMO gap[a] of α electrons and β electrons for SV-GN, SV-N3, DV-GN, and DV-N4 catalysts with H_2O adsorbed. The unit is eV.

	SV-GN		SV-N3		DV-GN		DV-N4	
	α electron	β electron	α electron	β electron	α electron	β electron	α electron	β electron
HOMO	-7.99	-8.79	-6.41		-8.95	-8.29	-8.46	-7.32
LUMO	-0.10	-0.13	-3.27		-0.79	-0.99	-0.13	-0.04
HOMO-LUMO gap	7.89	8.66	3.14		8.16	7.30	8.33	7.28

[a] HOMO-LUMO gap is the difference between LUMO and HOMO energy levels.