Supplementary Information

Metal-Organic Framework-Derived Atomically Dispersed Co-N-C Electrocatalyst for Efficient Oxygen Reduction Reaction

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XPS analysis

In a survey spectrum, the peak area is characterized using a quantification table based upon values computed from regions. The primary objectives of the quantification region are to define the range of energies over which the signal can be attributed to the transition of interest and to specify the type of approximation appropriate for the removal of background signals not belonging to the peak. Then, the elemental contents are extracted from the survey spectrum based on peak areas.

The high-resolution spectra were collected with a narrow banding energy range focused on one element. Moreover, an increased dwell time and sweep numbers were applied to the high-resolution spectra.

The curve fitting was conducted using CasaXPS software, with a model created from a set of Gaussian/Lorentzian line shapes. Peak models were created using the Components property page on the Quantification Parameters dialog window. A range of line shapes is available for constructing the peak models including both symmetric and asymmetric functional forms.

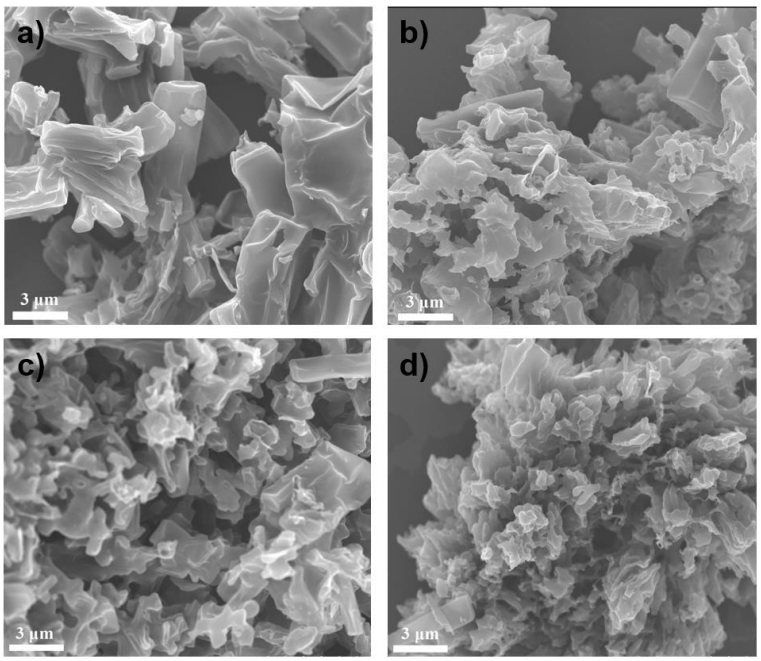

Figure S1. SEM images of (a) N-C, (b) Co-N-C-1, (c) Co-N-C-2, and (d) Co-N-C-3.

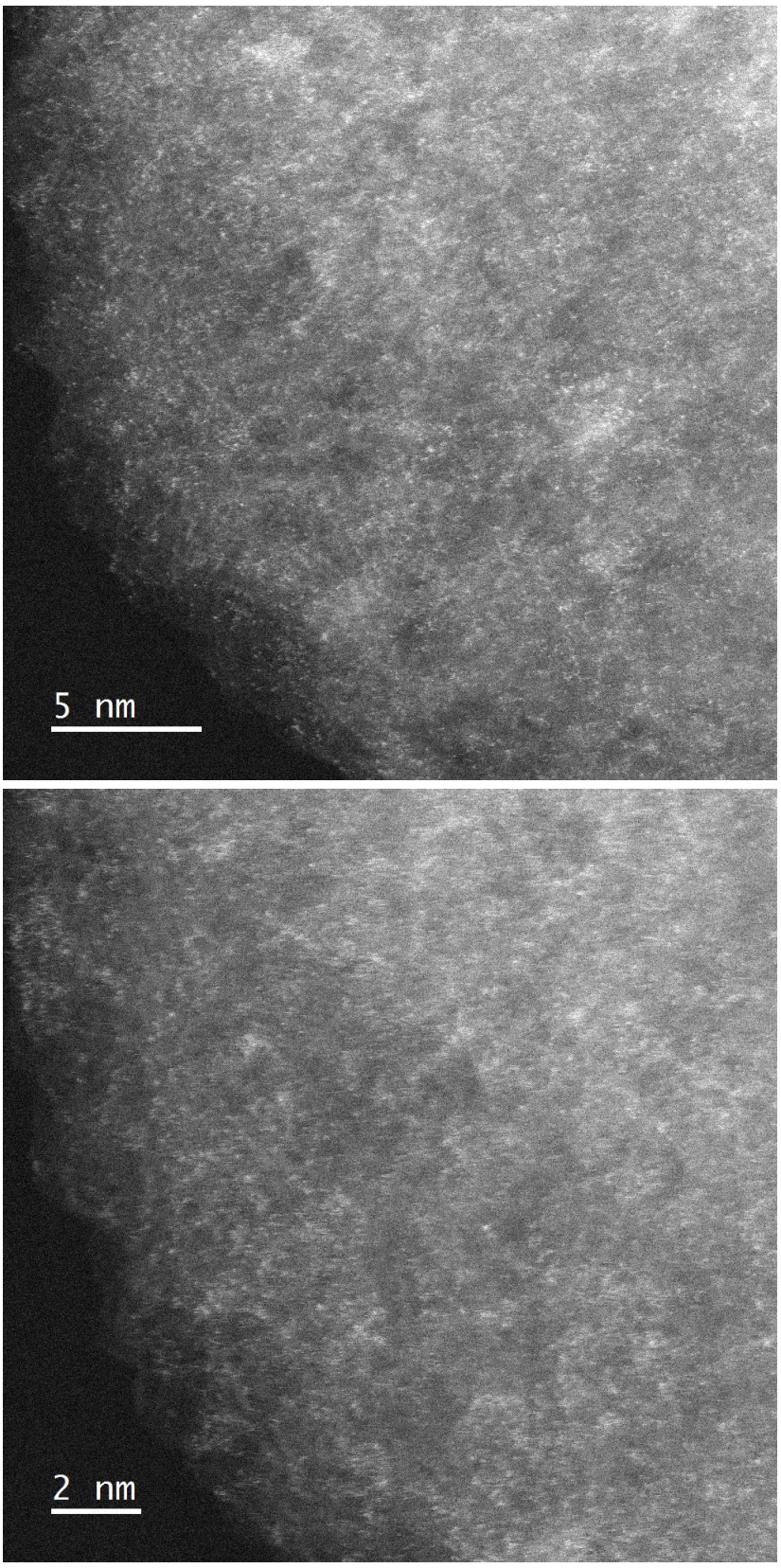

Figure S2. HAADF-STEM images of the Co-N-C-2 catalyst.

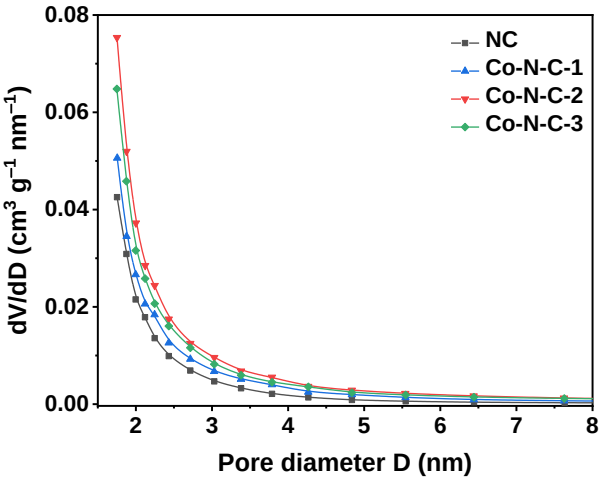

Figure S3. Pore size distribution of the obtained NC and Co-N-C catalysts.

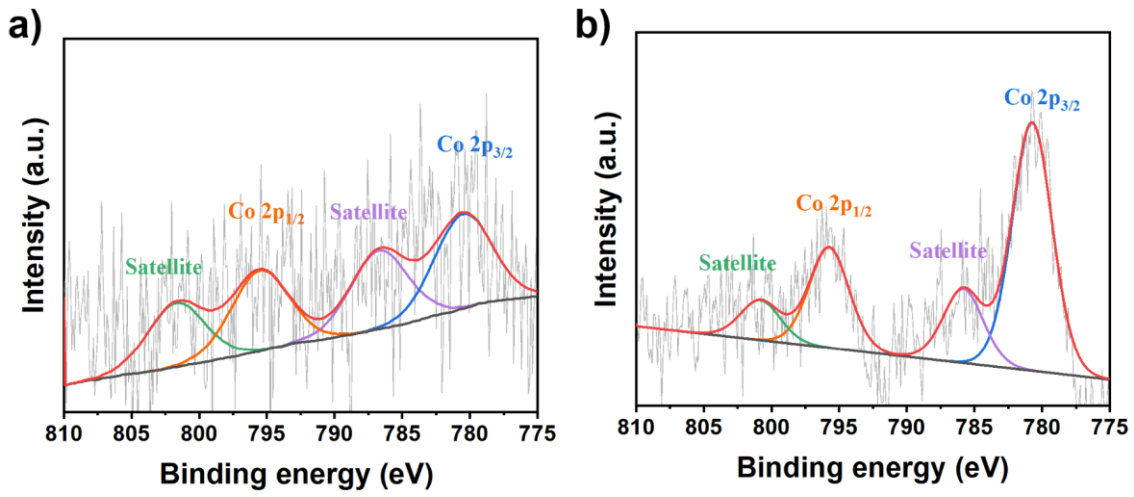

Figure S4. Co 2p peaks and fitting results of (a) Co-N-C-1 and (b) Co-N-C-3.

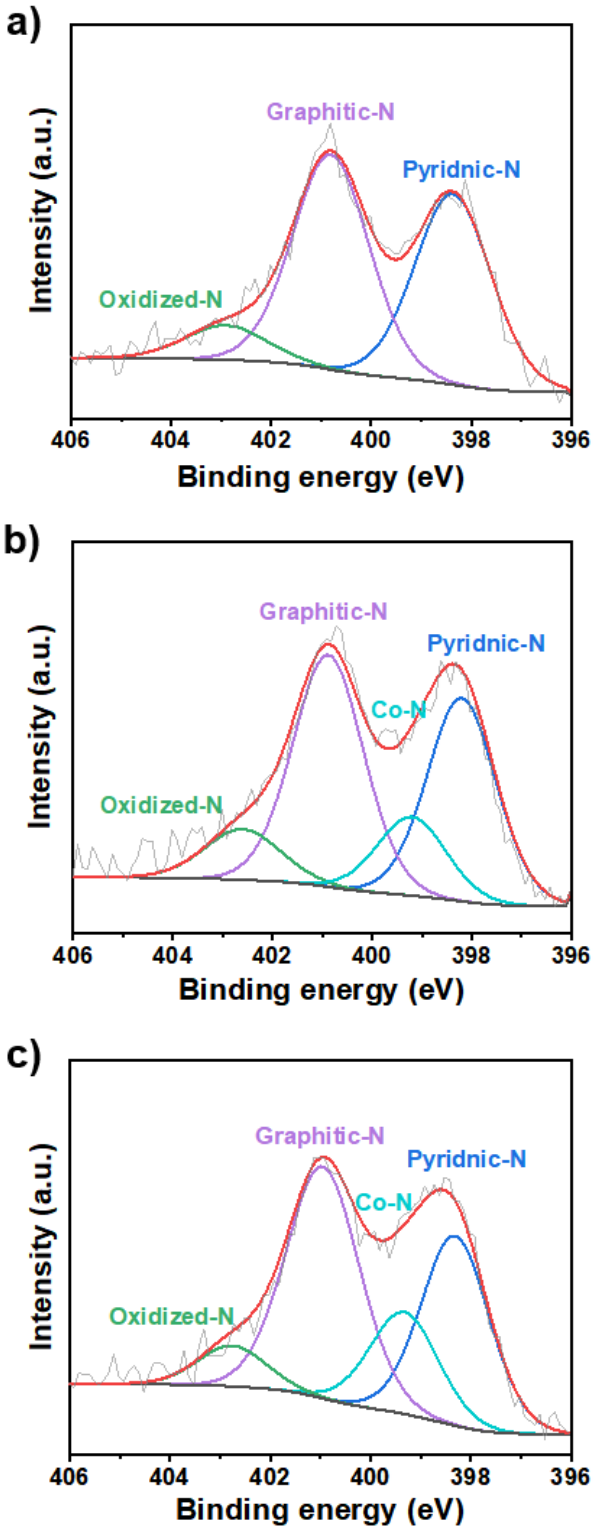

Figure S5. N 1s peaks and fitting results of (a) N-C, (b) Co-N-C-1, and (c) Co-N-C-3.

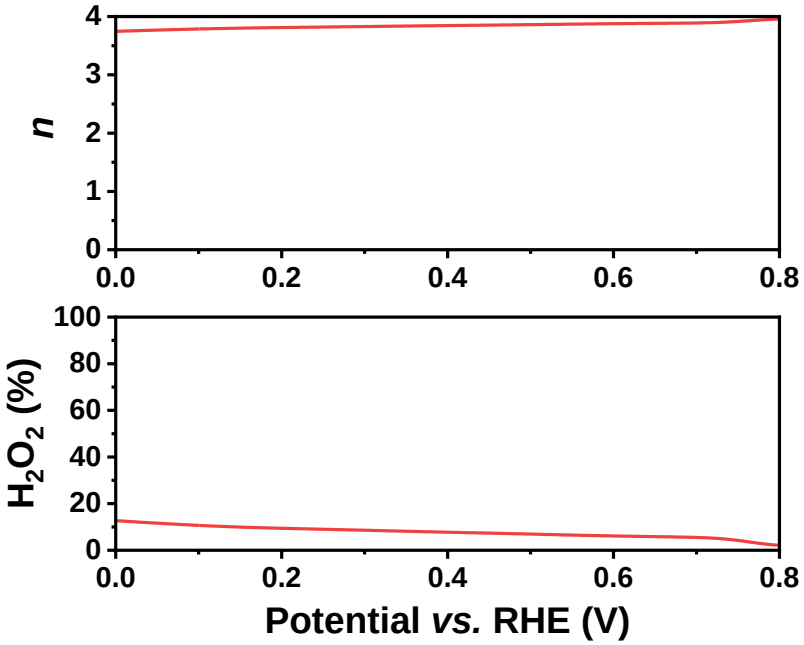

Figure S6. Yield of hydrogen peroxide (%) and electron transfer number of the Co-N-C-2 catalyst toward ORR.

Table S1. Pore features of the N-C and Co-N-C catalysts.

Sample	A_{BET} (m^2 g^{-1})	A_{Micro} (m^2 g^{-1})	A_{Meso} (m^2 g^{-1})
N-C	840	785	55
Co-N-C-1	888	816	72
Co-N-C-2	1076	976	100
Co-N-C-3	1003	913	90

Table S2. Surface elemental composition (wt.%) of the obtained materials measured by XPS.

Sample	C	N	O	Zn	Co
N-C	87.23	3.71	8.58	0.49	-
Co-N-C-1	87.29	3.87	7.42	0.76	0.66
Co-N-C-2	85.07	5.31	7.44	1.20	0.98
Co-N-C-3	86.32	4.48	6.65	0.93	1.61

Table S3. Content of each nitrogen component (%) of the N-C and Co-N-C catalysts.

Sample	Pyridinic-N	Co-N	Graphitic-N	Oxide-N
N-C	43.12	-	48.56	8.32
Co-N-C-1	35.32	13.68	41.29	9.70
Co-N-C-2	33.93	17.86	41.07	7.14
Co-N-C-3	32.63	17.54	42.83	7.00

Table S4. Comparison of the ORR catalytic performance of the Co-N-C-2 SACs catalyst and the other M-N-C catalysts reported in the literature in 0.1 M KOH.

Catalysts	E_{onset} (V vs. RHE)	$E_{1/2}$ (V vs. RHE)	References
Co-N-C-2	**0.96**	**0.89**	**This work**
Co-BM-800	0.89	0.82	[1]
SSM/Co_4N/CoNC	0.91	0.83	[2]
FeNC-$TPTZ_{0.5}DAN_{0.5}$	1.03	0.90	[3]
Fe-PpPD-800	1.01	0.89	[4]
Hm-LDH-700	1.13	0.86	[5]
CoO/Co-N-C/MC	0.90	0.78	[6]
OLC/Co-N-C	0.93	0.86	[7]
Co/N-C_{Zn}	0.96	0.88	[8]
Co-N-C(A)	1.01	0.89	[9]
Co-N-PC-800	1.12	0.83	[10]
CoO/Co/N-C-10-700	0.97	0.92	[11]
CoO_x/Co-N-C (800)	0.95	0.88	[12]
Co/C-N@CNFs	0.95	0.85	[13]
Co@NC-5	0.95	0.86	[14]
Co@NCB	0.93	0.85	[15]
Co-pyridinic N-C	0.99	0.87	[16]
Co@Co-N-C-A NHs	0.98	0.85	[17]
CoSAs/PTF-600	0.92	0.81	[18]
Co-N-C-900	0.93	0.88	[19]
C-MOF-C2-900	0.91	0.82	[20]

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