Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Pyridinium Functionalized Coordination Containers as a Highly Efficient Electrocatalyst for Sustainable Oxygen Evolution

N. Bhuvaneswari,[a,b] K. P. Annamalai,[a] Feng-Rong Dai,[a]* and Zhong-Ning Chen[a]*

[a]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China.

[b]University of Chinese Academy of Sciences, Beijing, 100039, P. R. China.

Table S1. Crystallographic Data for Compounds **1-Co** and **1-Ni.**

	1-Co	**1-Ni**
Empirical formula	$C_{160}H_{186}N_{12}O_{50}Co_8S_8Br_2$	$C_{136}H_{130}N_4O_{42}Ni_8S_8Br_2$
Formula weight	3964.94	3378.41
Temperature (K)	298(2) K	298(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic
space group	*P*-1	*P*-1
a (Å)	13.420(7)	13.404(8)
b (Å)	14.187(6)	13.953(7)
c (Å)	26.269(14)	26.278(17)
α(°)	80.00(2)	79.49(3)
β(°)	81.54(2)	81.51(3)
γ(°)	66.431(16)	65.614(19)
V (Å^3)	4498(4)	4387(5)
Z	1	1
D(calcd) (g cm^{-3})	1.464	1.279
μ (Mo K_α) (mm^{-1})	1.337	1.457
F(000)	2044	1732
θ range (°)	2.088 - 24.998	2.104 - 25.000
Limiting indices	-15<=h<=15 -16<=k<=16 -31<=l<=31	-15<=h<=15 -16<=k<=16 -31<=l<=31
Reflections collected / unique	40439 / 15768 [R_{int} = 0.0575]	40053 / 15420 [R_{int} = 0.0686]
Data / restraints / parameters	15768 / 42 / 1081	15420 / 13 / 929
GOF	1.063	1.005
R_1 (I>2σ(I))	0.1021	0.0989
wR_2 (I>2σ(I))	0.2987	0.2727
R_1 (all data)	0.1266	0.1498
wR_2 (all data)	0.3256	0.3053
$\Delta\rho$ / e A$^{\circ-3}$	2.461, -1.347	1.041, -0.597

Table S2. Comparison of OER performance of recently reported catalysts and our functionalized coordination containers.

Samples	Electrolyte	η (V) at 10 mA/cm^2	Tafel values (mV/dec)	Capacitance mF/cm^2	Stability	Reference
1-Co	**1.0 M KOH**	**0.290**	**75**	**133**	**>48 h**	**This work**
1-Ni	**1.0 M KOH**	**0.302**	**110**	**40**	**>48 h**	**This work**
MAF-X-27 OH	1.0 M KOH	0.292	127	-	>24 h	1
Co-NU-1000	0.1M Na_2SO_4/NaOH	>0.4	90	-	>10 h	2
Pb-TCPP	1.0 M KOH	1.70 vs RHE	106	-	>100 cycles	3
Co/Co_9S_8@ S,N doped porous graphene	0.1 M KOH	0.29	96	-	>1000 cycles	4
Co_2P/CNT-900	1.0 M KOH	0.292	68	25	>2000 cycles	5
CoN nanowire	1.0 M KOH	0.29	72	92	>30 h	6
$Ni_{0.5}Co_{0.5}$-Nanocarbon	1.0 M KOH	0.3	91	26	>10 h	7
Co-MOF/CNT	1.0 M KOH	0.34	69	22.3	>25 h	8
Ni-Mo_2C/PC	1.0 M KOH	0.368	-	11.2	>10 h	9

Note: TCPP=Tetra(carboxyphenyl)porphyrin); CNT= Carbon nanotube; PC= Porous carbon.

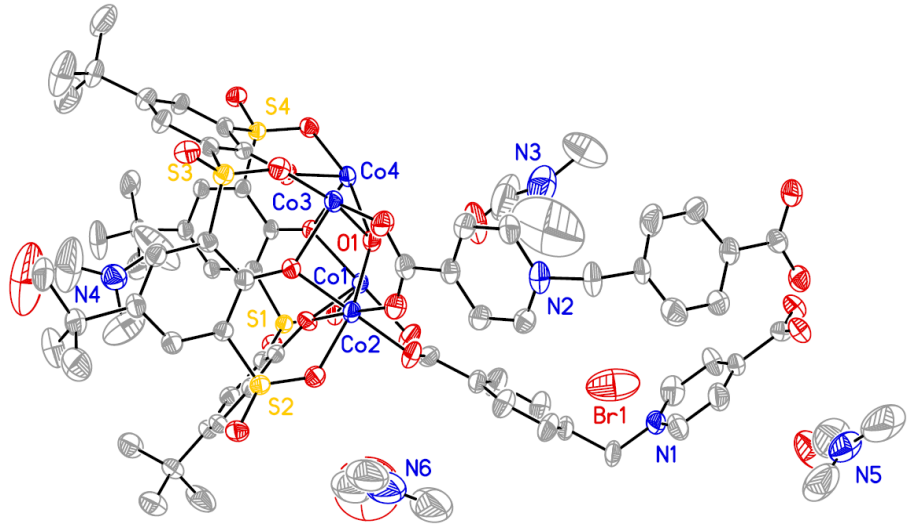

Fig. S1. ORTEP drawing of the asymmetric unit of **1-Co** (thermal ellipsoids with 30% probability).

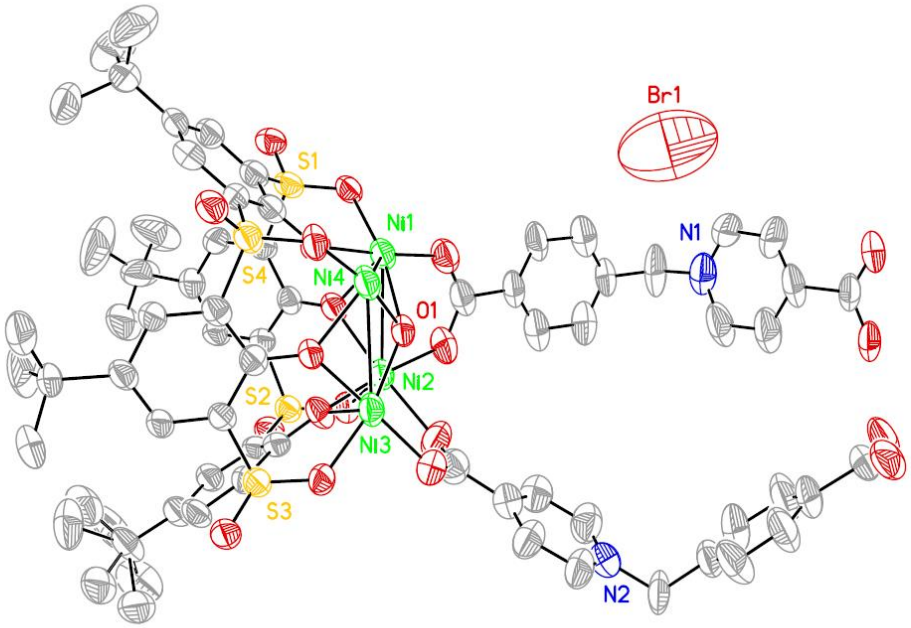

Fig. S2. ORTEP drawing of the asymmetric unit of **1-Ni** (thermal ellipsoids with 30% probability).

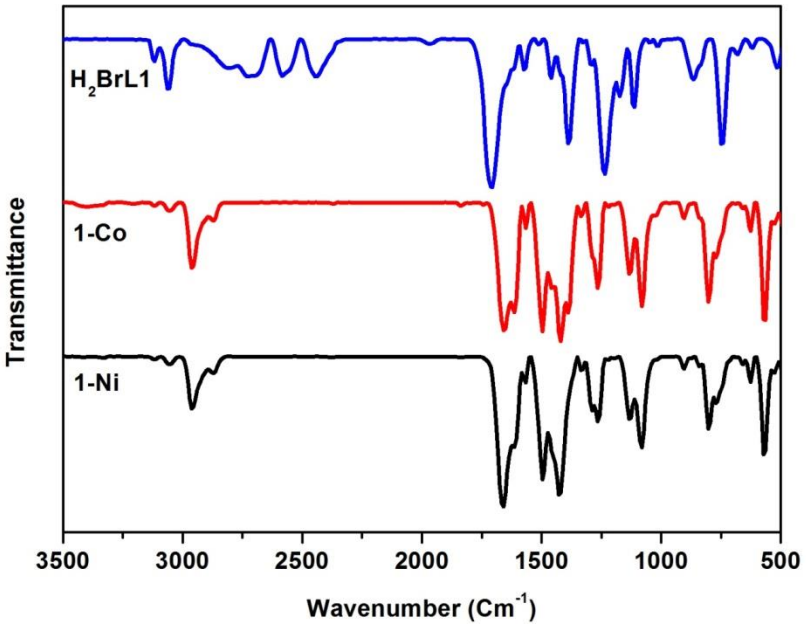

Fig. S3. FT-IR spectra of as-synthesized samples **1-Co**, **1-Ni** and H_2Br**L1** linker.

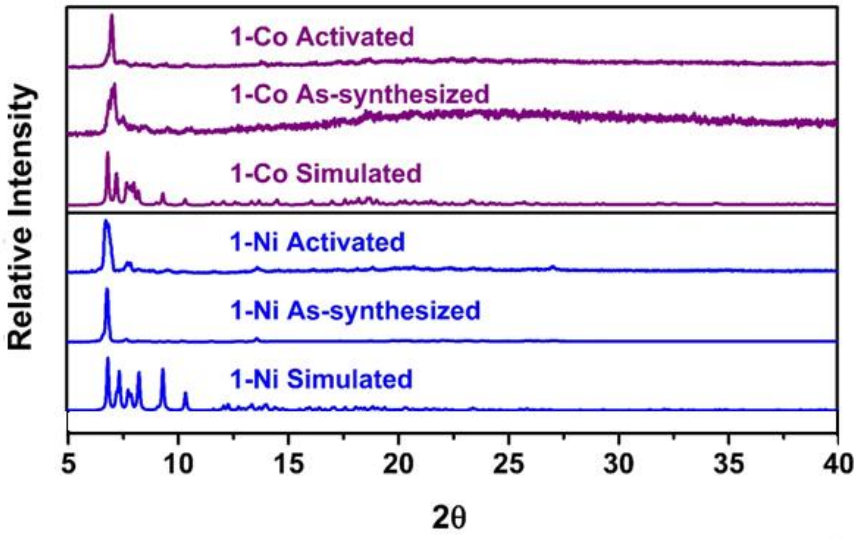

Fig. S4. PXRD Pattern of **1-Co** and **1-Ni**.

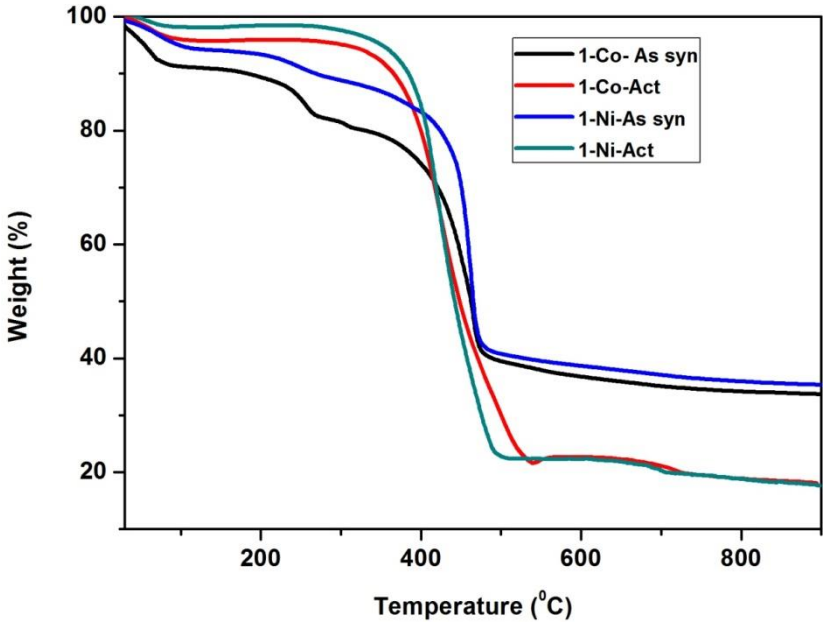

Fig. S5. TGA of as-synthesized and activated samples of **1-Co** and **1-Ni**.

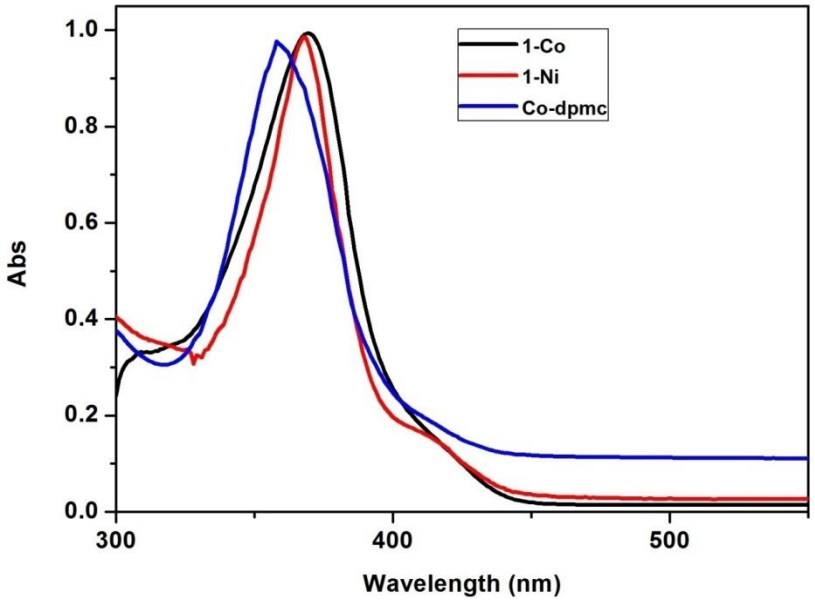

Fig. S6. UV-Visible absorption profiles of **1-Co**, **1-Ni**, and **Co-dpmc** in DMSO solution.

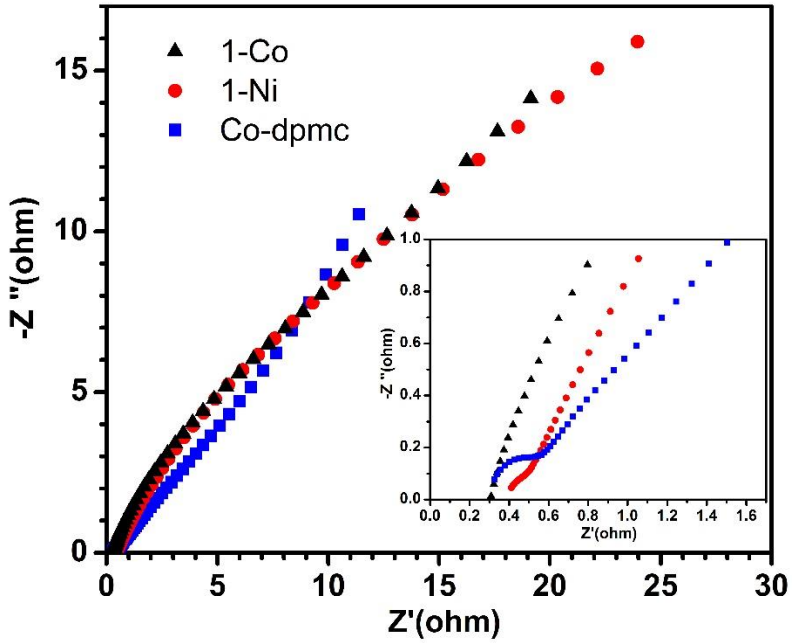

Fig. S7. Electrochemical impedance spectroscopy (EIS) Nyquist plots for **1-Co**, **1-Ni** and **Co-dpmc** electrodes. (Inset shows the magnified region).

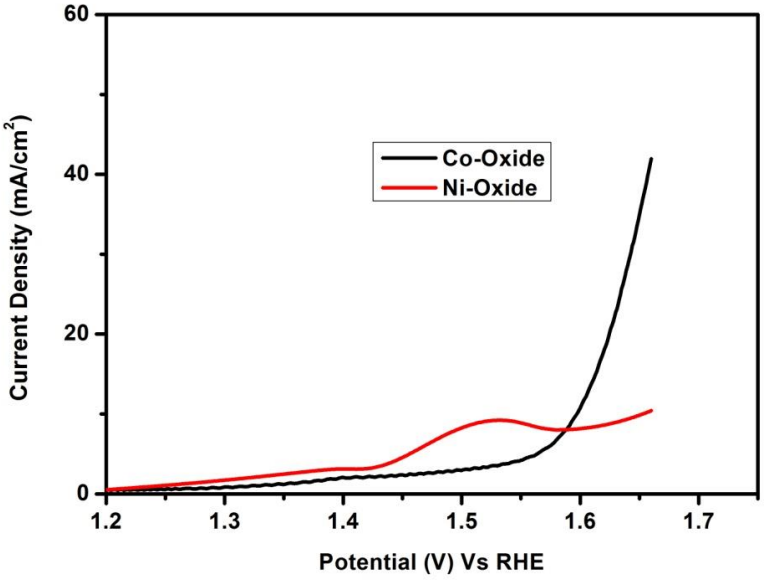

Fig. S8. Linear sweep voltammetry (LSV) curves of metal oxides in 1M KOH.

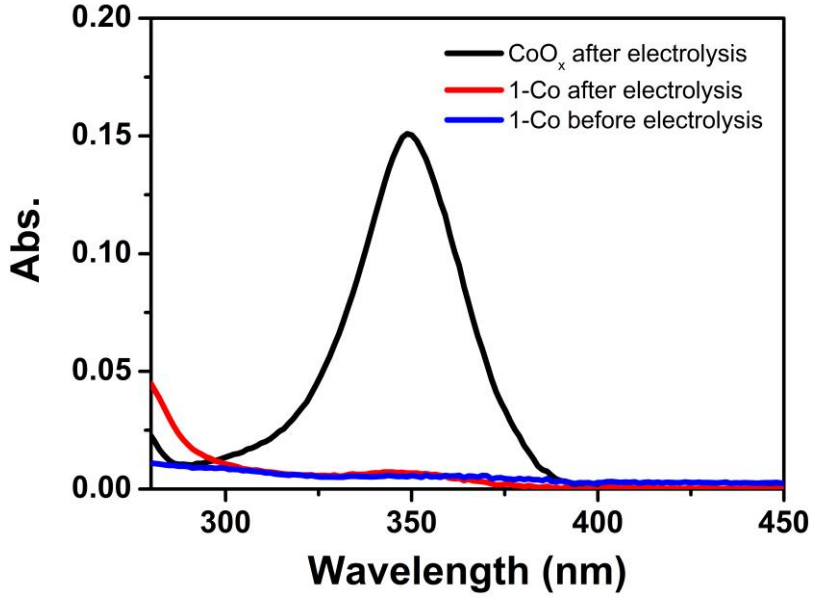

Fig. S9. UV-Visible absorption spectra of electrolyte solution before and after electrolysis by using **CoO_x** and **1-Co** as catalyst.

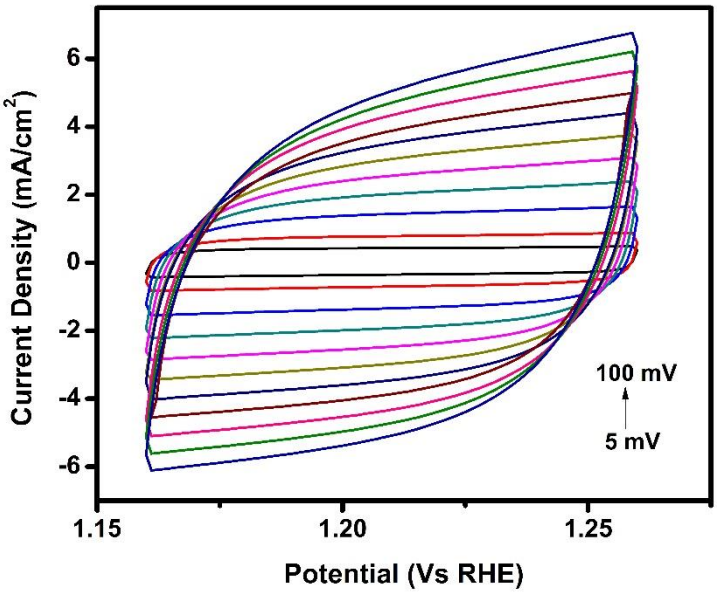

Fig. S10. CV curves of **1-Ni** from 5 to 100 mV/s scan rates in the range of 1.16 to 1.26 V vs. RHE.

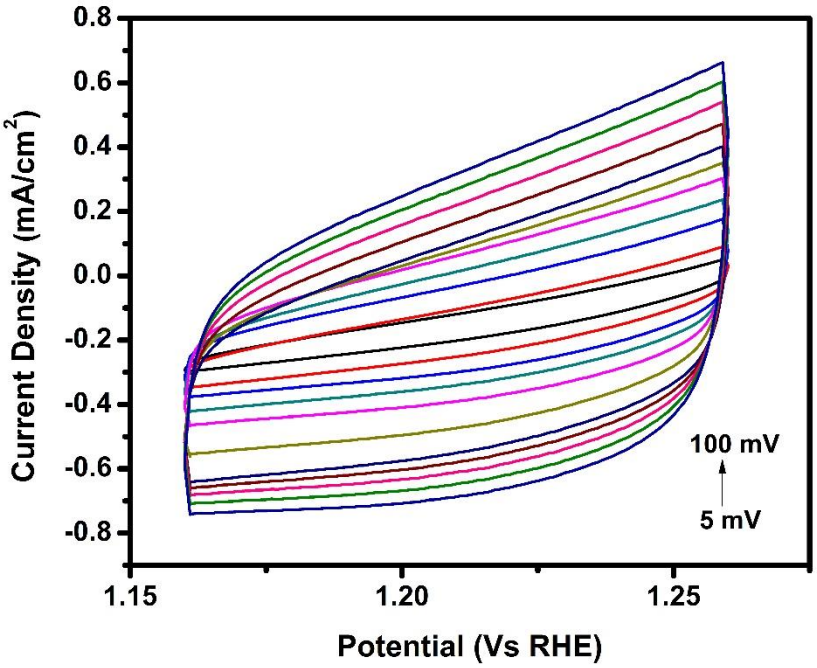

Fig. S11. CV curves of **Co-dpmc** from 5 to 100 mV/s scan rates in the range of 1.16 to 1.26 V vs. RHE.

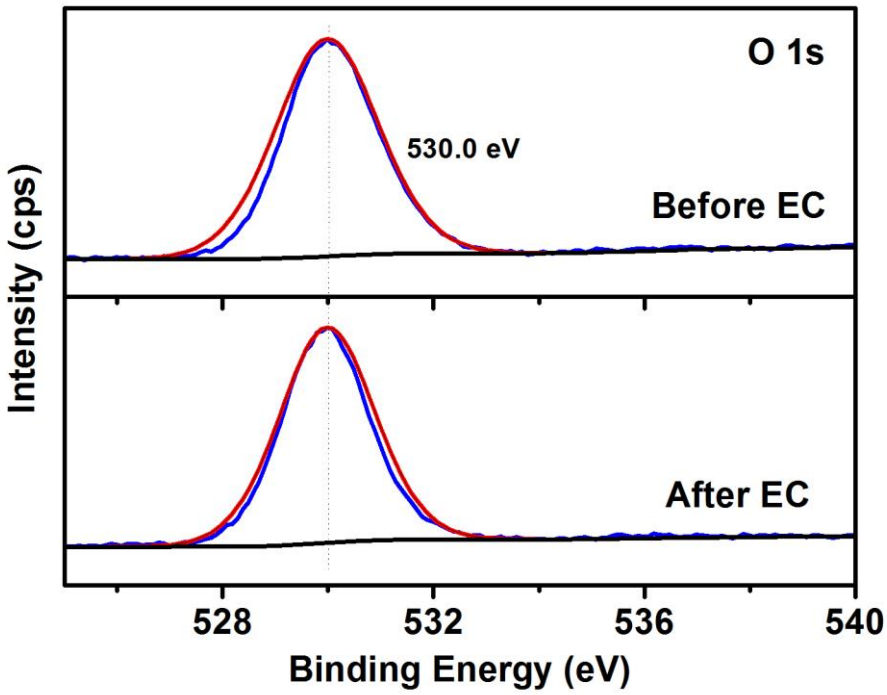

Fig. S12. O1s spectra of **1-Co** before and after electrolysis.

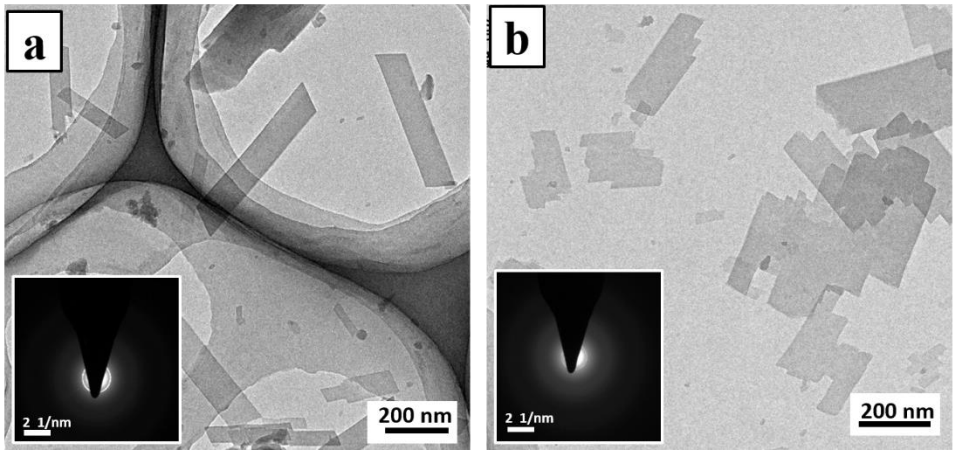

Fig. S13. TEM images of 1-Co (a) before and (b) after 1000 CV cycles.

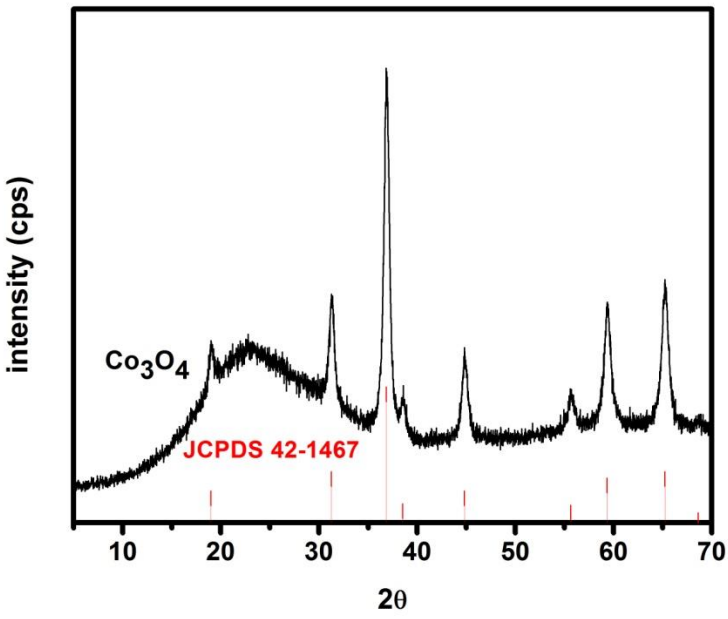

Fig. S14. PXRD Pattern of cobalt oxide.

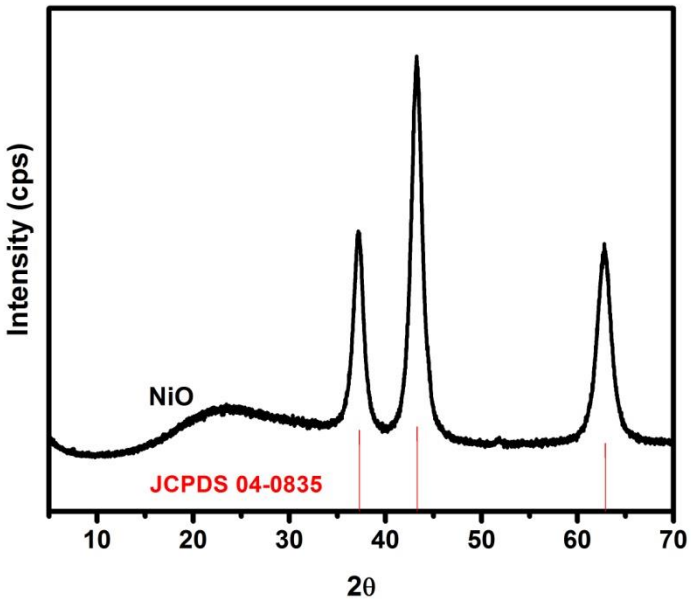

Fig. S15. PXRD Pattern of nickel oxide.

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