Electronic Supplementary Information

Two New Ni/Co-MOFs as Electrocatalysts for the Oxygen Evolution Reaction in Alkaline Electrolytes†

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Table S1 Selected bond lengths (Å) and bond angles (°) for **Ni-MOF** and **Co-MOF**

Ni-MOF			
Ni(1)-O(1)#1	2.1275(18)	O(2)-Ni(1)-O(1)#1	95.13(6)
Ni(1)-O(1)	2.1192(19)	O(2)#2-Ni(1)-O(1)#1	95.13(6)
Ni(1)-O(2)#2	2.0534(15)	O(2)-Ni(1)-O(1)	90.83(6)
Ni(1)-O(2)	2.0535(15)	O(2)#2-Ni(1)-O(1)	90.83(6)
Ni(1)-O(12)#2	2.0209(15)	O(2)#2-Ni(1)-O(2)	85.48(8)
Ni(1)-O(12)	2.0209(15)	O(12)-Ni(1)-O(1)	87.54(6)
O(1)-Ni(1)#3	2.1275(18)	O(12)-Ni(1)-O(1)#1	86.81(6)
O(1)-Ni(1)-O(1)#1	171.88(4)	O(12)-Ni(1)-O(2)#2	91.30(6)
O(12)#2-Ni(1)-O(1)#1	86.81(6)	O(12)-Ni(1)-O(2)	176.37(6)
O(12)#2-Ni(1)-O(1)	87.54(6)	O(12)#2-Ni(1)-O(2)	91.30(6)
O(12)#2-Ni(1)-O(2)#2	176.37(6)	O(12)-Ni(1)-O(12)#2	91.87(9)
Symmetrical codes: #1 x-1/2, y, -z+5/2; #2 x, -y-1/2, z; #3 x+1/2, y, -z+5/2.			
Co-MOF			
Co(1)-O(1)#1	2.1842(15)	O(2)-Co(1)-O(1)#1	94.45(5)
Co(1)-O(1)	2.1505(15)	O(2)-Co(1)-O(1)	91.42(5)
Co(1)-O(2)	2.0819(12)	O(2)-Co(1)-O(2)#2	85.04(7)
Co(1)-O(2)#2	2.0819(12)	O(7)#2-Co(1)-O(1)	88.16(5)
Co(1)-O(7)#2	2.0573(12)	O(7)#2-Co(1)-O(1)#1	86.33(5)
Co(1)-O(7)	2.0573(12)	O(7)-Co(1)-O(1)	88.16(5)
O(1)-Co(1)#3	2.1842(15)	O(7)-Co(1)-O(1)#1	86.33(5)
O(1)-Co(1)-O(1)#1	172.03(3)	O(7)#2-Co(1)-O(2)	91.22(5)
O(2)#2-Co(1)-O(1)	91.42(5)	O(7)#2-Co(1)-O(2)#2	176.22(5)
O(2)#2-Co(1)-O(1)#1	94.45(5)	O(7)-Co(1)-O(2)	176.22(5)
O(7)-Co(1)-O(2)#2	91.22(5)	O(7)-Co(1)-O(7)#2	92.52(7)
Symmetrical codes: #1 x+1/2, y, -z+1/2; #2 x, -y+1/2, z; #3 x-1/2, y, -z+1/2.			

Fig. S1. The coordination modes of H_2L^{2-} with Ni(II) ion in **Ni-MOF** and **Co-MOF**.

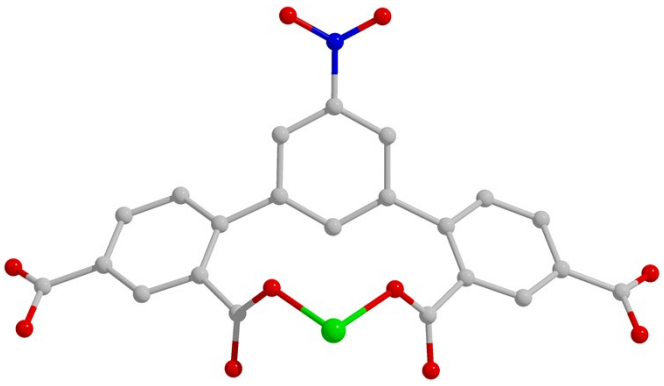
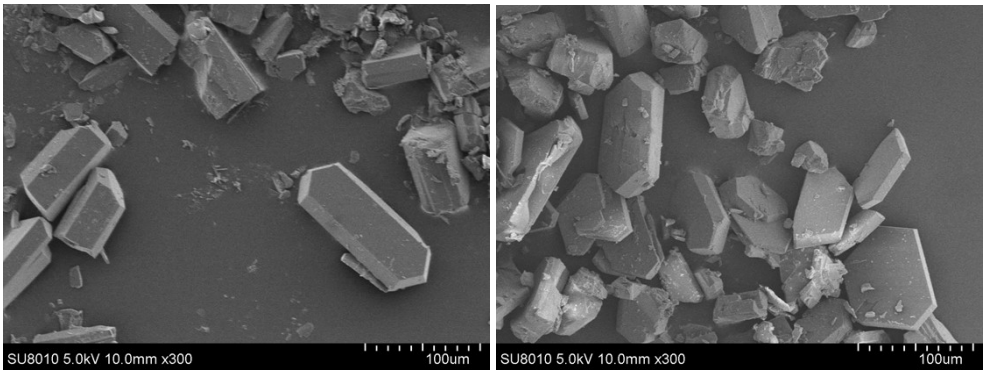
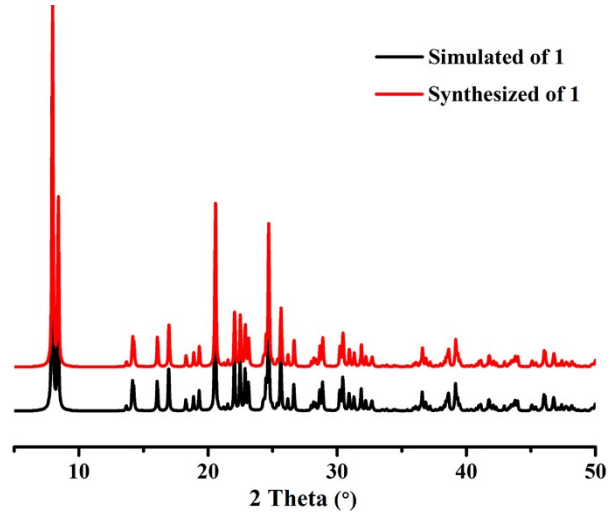


Fig.S2. SEM images of (a) **Ni-MOF** and (b) **Co-MOF**.

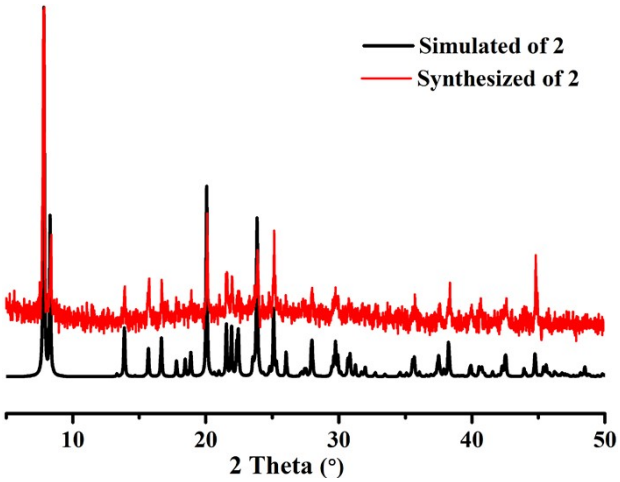


(a) **(b)**

Fig. S3. PXRD patterns of **Ni-MOF** and **Co-MOF** in (a-b) simulated from the X-ray single-crystal structure and experimental samples.



(a)



(b)

Fig. S4. TGA curves for **Ni-MOF** and **Co-MOF** (**1**-**2**).

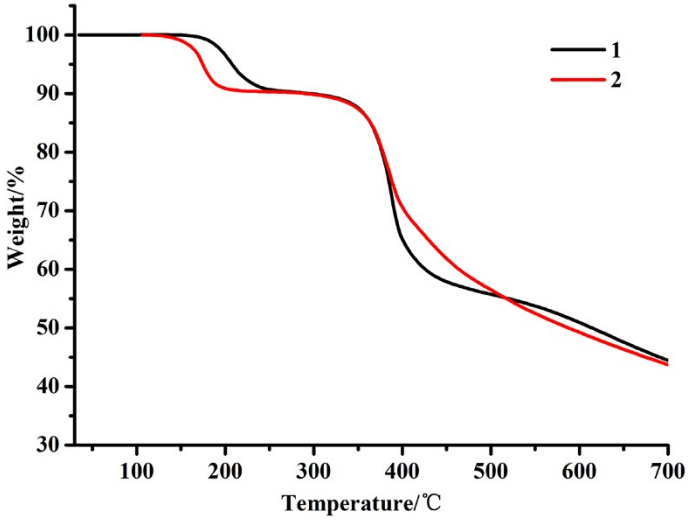
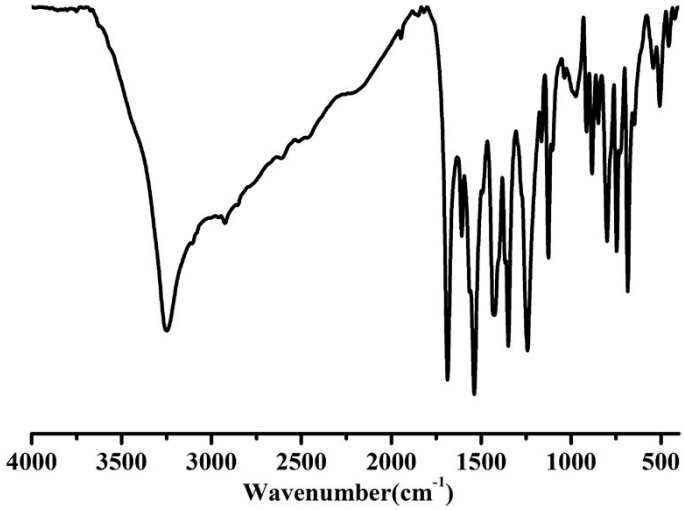
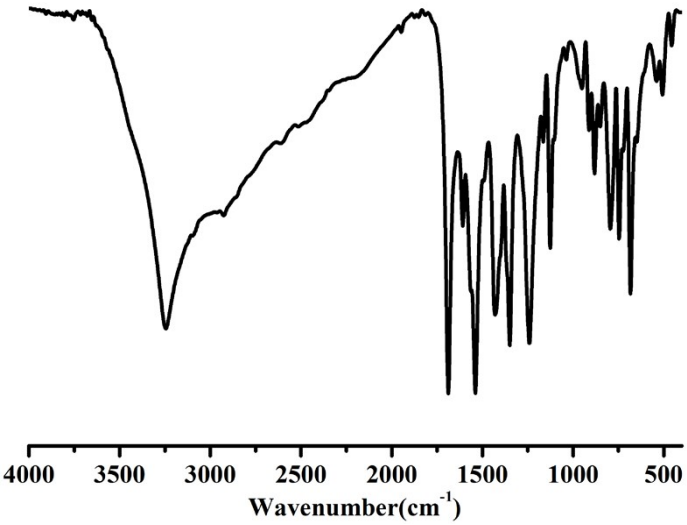


Fig. S5. IR spectra of the as-synthesized **Ni-MOF** and **Co-MOF** in (a-b).

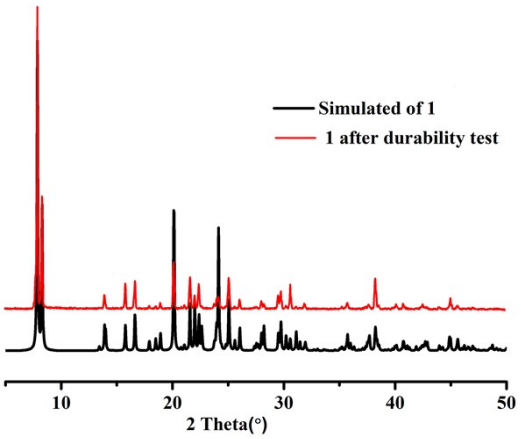


(a)

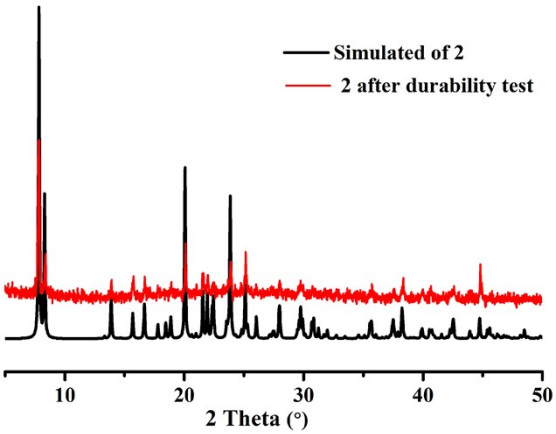


(b)

Fig. S6. PXRD patterns of **Ni-MOF** and **Co-MOF** in (a-b) simulated from the X-ray single-crystal structure and after durability test.



(a)



(b)

Turnover Frequency Calculation

The turnover frequency (TOF) was calculated through the equation below:

$$\mathrm{TOF} = \frac{j \times \mathrm{A_{geo}}}{4 \times \mathrm{F} \times \mathrm{n}}$$

Where F is the Faraday constant (96, 485C mol^{-1}), and n stands for moles of the total active sites in the targeted materials. In this work, the active sites are assumed to be Co or Ni atoms in the samples. The moles of the Co were estimated through thermos gravimetric analysis.

The Tafel slope was calculated from the Tafel equation (derived from Butler-Volmer equation under high anodic overpotential conditions) in a logarithm form:

$$\eta = b \log(j / \mathrm{j_0})$$

Where η, b, j_0 are overpotential, Tafel slope and overall current density at equilibrium, respectively.

Table S2. Comparison of OER performance for electrocatalysts in this work and some recently reported active electrocatalysts.

Catalyst	J (mA cm^{-2})	η (mV)	Electrolyte	Ref.
Ni-MOF	10	355	1.0 M KOH	This work
Co-MOF	10	394	1.0 M KOH	This work
LiNiCo-OH	10	340	1.0 M KOH	1
$NiCo_{2.7}OH$	10	350	1.0 M KOH	2
NNU-23	10	365	0.1 M KOH	3
FeCo-MNS	10	298	0.1 M KOH	4
NiCo-UMOFNs	10	250	1.0 M KOH	5
$CoxFe_{1-x}$-MOF-74	10	280	1.0 M KOH	6
NiFe-MOF/OM-NFH	10	270	1.0 M KOH	7
Co-MOF/NF	10	311	1.0 M KOH	8
CoO_x-ZIF	10	400	1.0 M KOH	9
NCNTFs	10	370	1.0 M KOH	10
$Fe1Co_2$–P/C	10	360	1.0 M KOH	11
$A_{2.7}B$-MOF-$FeCo_{1.6}$	10	288	1.0 M KOH	12
Fe–Ni MOF	10	285	1.0 M KOH	13
CTGU-14	10	376	1.0 M KOH	14

Supplementary References

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