

Supporting Information

**Iron-doped novel Co-based metal-organic frameworks for
preparation of bifunctional catalysts with amorphous
structure for OER/HER in alkaline solution**

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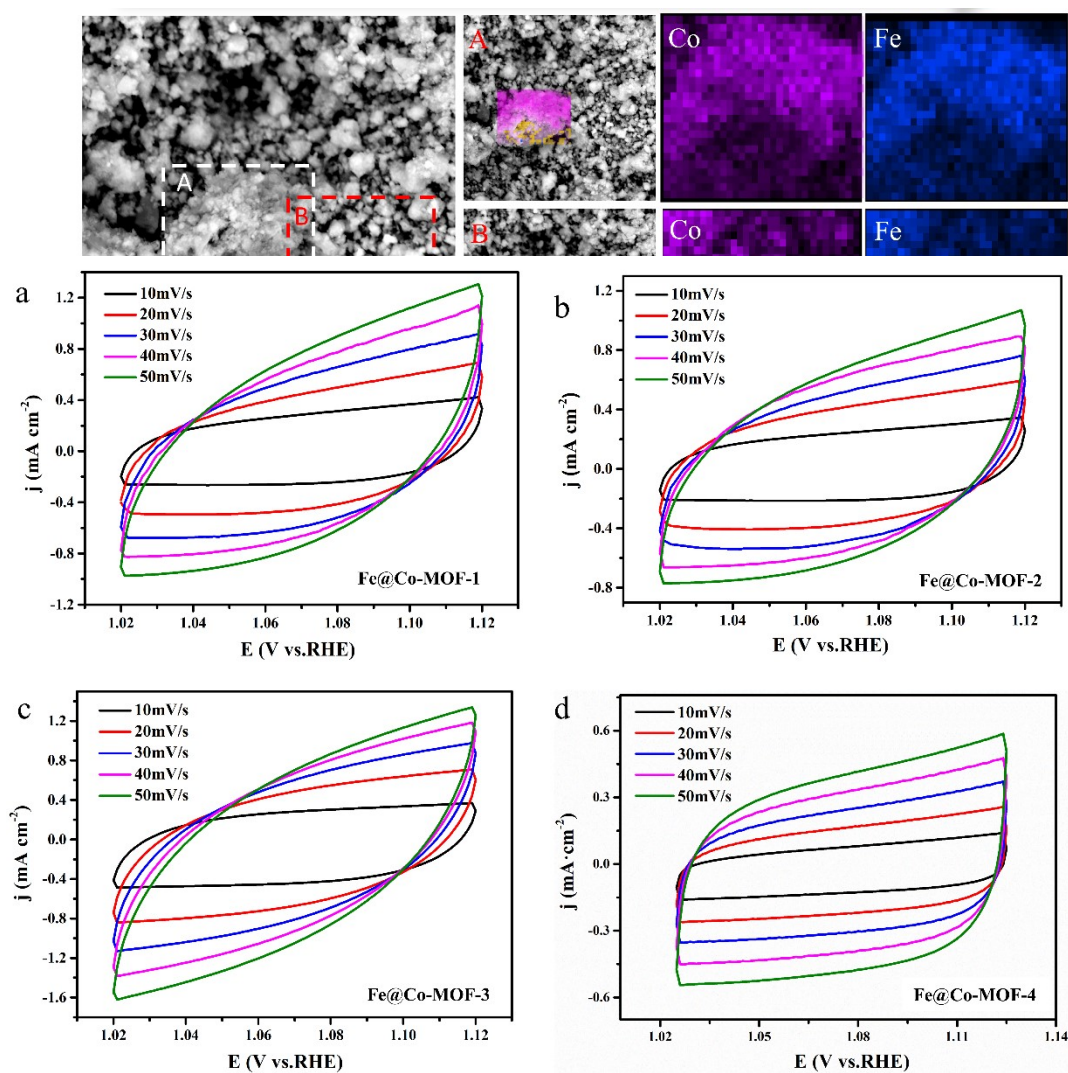


Figure S8. Cyclic voltammograms (CV) of **a)** Fe@Co-MOF-1. **b)** Fe@Co-MOF-2. **c)** Fe@Co-MOF-3. **d)** Fe@Co-MOF-4.

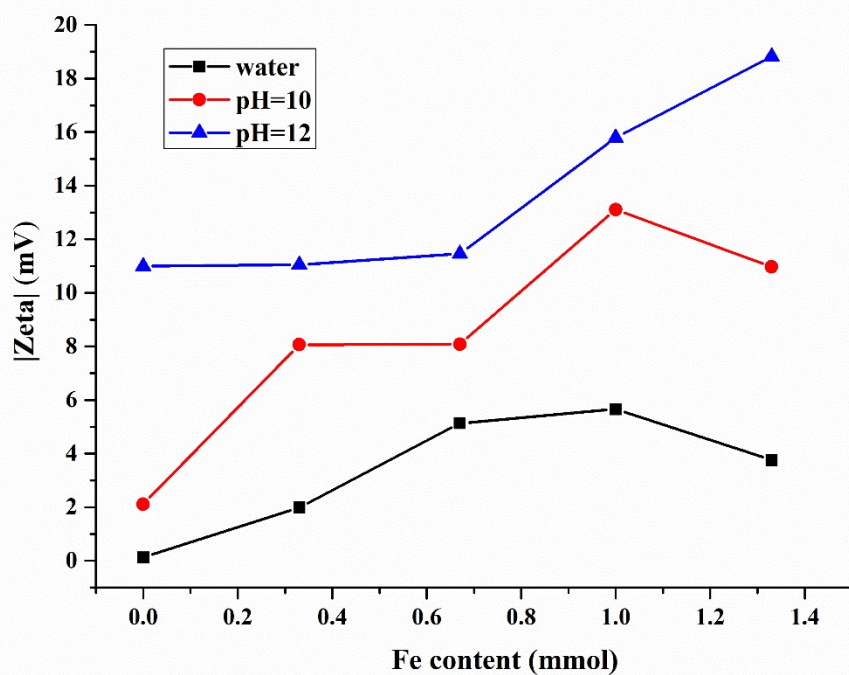


Figure S9. Zeta potential measurement data for Co-MOF, Fe@Co-MOF-1, Fe@Co-MOF-2, Fe@Co-MOF-3 and Fe@Co-MOF-4.

Table S1. List of ingredients for different catalysts.

	Co-MOF	FeSO ₄ •7H ₂ O
Co-MOF	0.1 mmol	0
Fe@Co-MOF-1	0.1 mmol	0.033 mmol
Fe@Co-MOF-2	0.1 mmol	0.066 mmol
Fe@Co-MOF-3	0.1 mmol	0.1 mmol
Fe@Co-MOF-4	0.1 mmol	0.133 mmol

Table S2. Crystallographic data and structural refinements for Co-MOF.

Compound	Co
chemical formula	C ₂₆ H ₁₆ CoN ₆ O ₅
formula weight	697.57
crystal size (mm)	0.11
temperature (K)	273(2)
radiation	0.71073
crystal system	Monoclinic
space group	P2 ₁ /c
Unit cell dimensions	<i>a</i> =13.942(2) (Å) <i>b</i> =13.1857(19) (Å)

	$c=18.636(3)$ (Å)
	$\alpha=90.00^\circ$
	$\beta=111.414(3)^\circ$
	$\gamma=90.00^\circ$
Volume/ $V(\text{Å}^3)$	3189.5(8)
Z	4
$\rho(\text{calc})$ (g/cm ³)	1.453
F (000)	1444.0
μ (mm ⁻¹)	0.600
θ range (deg)	1.569 to 25.008
Independent reflections	15957 ($R_{\text{int}}=0.0666$, $R_{\text{sigma}}=0.0852$)
Data/restraints/parameters	5615/ 231/ 485
GOF	0.991
R_1/wR_2 [$I > 2\sigma(I)$]	0.0548/ 0.1224
R_1/wR_2 (all data)	0.1098/ 0.1534
large peak and hole(e/Å ³)	0.379/ -0.443

Table S3. Selected Bond lengths (Å) and Angles (°) for Co-MOF.

Parameter	Value	Parameter	Value
Co(1)-O(4)#3	2.156(3)	Co(1)-O(5)#3	2.192(3)
Co(1)-O(1)	2.033(3)	Co(1)-O(2)#2	2.019(3)
Co(1)-N(6)#1	2.181(3)	Co(1)-N(1)	2.151(3)
O(4)#3-Co(1)-N(6)#1	90.31(12)	O(2)#2-Co(1)-O(1)	116.88(11)
O(4)#3-Co(1)-O(5)#3	60.04(11)	O(2)#2-Co(1)-N(6)#1	87.65(13)
O(1)-Co(1)-O(4)#3	150.30(12)	O(2)#2-Co(1)-O(5)#3	152.38(12)
O(1)-Co(1)-N(6)#1	87.03(12)	O(2)#2-Co(1)-N(1)	92.11(13)
O(1)-Co(1)-O(5)#3	90.33(11)	N(1)-Co(1)-O(4)#3	92.58(12)
O(1)-Co(1)-N(1)	90.51(12)	N(1)-Co(1)-N(6)#1	177.11(12)
N(6)#1-Co(1)-O(5)#3	89.21(12)	N(1)-Co(1)-O(5)#3	92.33(12)
O(2)#2-Co(1)-O(4)#3	92.53(12)		

Complex 1 Symmetry code: #1= x, 1+y, z; #2= -x, -y, -z; #3= 1+x, 1/2-y, 1/2+z.

Table S4. Hydrogen-bonding Geometry of Co-MOF. (Å and °)

D-H...A	D-H	H...A	[D...A]	\angle D-H...A
C10-H10...O4#1	0.93(5)	2.6(3)	3.497(4)	162.3(2)
C17-H17...O5#2	0.929(5)	2.559(3)	3.386(7)	148.4 (2)

Symmetry code: #1= -1-x, -1/2+y, -1/2-z; #2= -1-x, -y, -z

Table S5. The OER performance of recently reported most active MOFs-based catalysts in alkaline media.

Number	Catalyst	Electrolyte	Overpotential (mV)	Ref.
1	Fe@Co-MOF-3	1 M KOH	247 mV@50mA·cm⁻²	<i>This work</i>
2	Co-MOF	1 M KOH	315 mV@10mA·cm⁻²	<i>This work</i>
3	ZIF-FeCo/C	1 M KOH	250 mV@10mA·cm ⁻²	1
4	ZIF-67/CoNiAl-LDH/NF	1 M KOH	303 mV@10mA·cm ⁻²	2
5	CoP-InNC@CNT	1 M KOH	270 mV@10mA·cm ⁻²	3
7	FeCo-MNS-1.0	0.1 M KOH	367 mV@150mA·cm ⁻²	4
8	CoP/NF	1 M KOH	317 mV@50mA·cm ⁻²	5
9	FCO-Vo@NC	1 M KOH	318 mV@10mA·cm ⁻²	6
10	CoCu-MOF NBs	1 M KOH	271 mV@10mA·cm ⁻²	7
11	Fe ₂ Ni MIL-88B	1 M KOH	264 mV@10 mA·cm ⁻²	8
13	CoNi MOF-mCNTs	1 M KOH	306 mV@10mA·cm ⁻²	9
14	Co ₃ S ₄ /EC-MOF	1 M KOH	336 mV@100mA·cm ⁻²	10
15	CoNiFe LTHs	1 M KOH	262 mV@10mA·cm ⁻²	11
16	3DGS-Co _{3.0} Cu _{1.0} -MOF	0.1 M KOH	460 mV@10mA·cm ⁻²	12
17	CuCo-MOF	1 M KOH	340 mV@10mA·cm ⁻²	13
16	Ni _{0.75} Fe _{0.25} BDC	1 M KOH	310 mV@10mA·cm ⁻²	14
15	aCo(OH) ₂ -ZIF-L/NF-40	0.1 M KOH	290 mV@100mA·cm ⁻²	15

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