Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Cobalt Metal Organic Framework (Co-MOF): A bi-functional Electro active material for Oxygen Evolution and Reduction Reaction

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Calculation of mass activity and Turnover frequency (TOF)

The mass activity (A/g) of all the samples were calculated by dividing the observed current density (at η=370 mV) by the mass of electrocatalyst loaded onto the working electrode surface as per the following equation, [1]

$$MA = \frac{j}{m}$$

Further the number of moles of active site are determined by dividing the molecular mass of the sample to the mass of material loaded (0.25 mg/cm^2) onto the electrode surface. The values of TOF were evaluated by assuming all the metal ions as the active catalytic centers as per the following equation,

$$TOF = \frac{j \times S}{4 \times F \times n}$$

Here, j, S, F and n are the observed current density, geometrical surface area of the working electrode (0.19 cm^2), faraday constant (96485.3 C mol^{-1}) and number of moles of active sites present in the catalyst taken. Since four electrons are needed to evolve one mole of O_2, so the term ¼ is used.

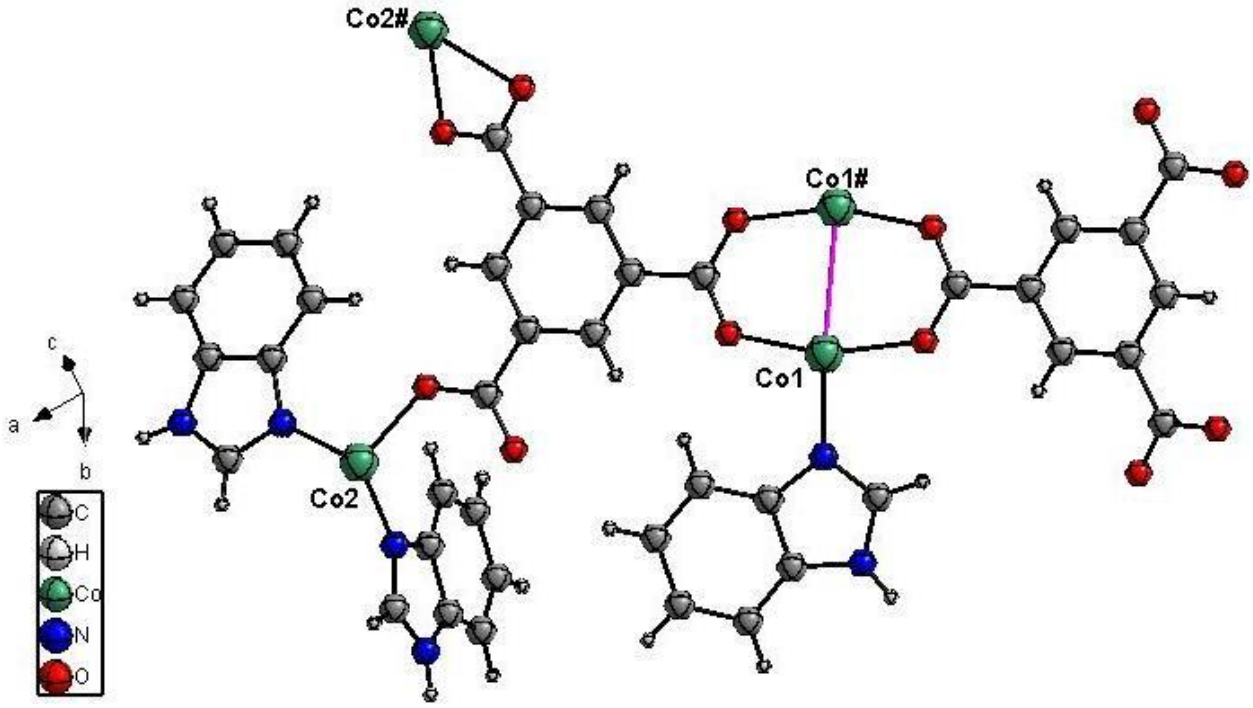

Figure S 1 Asymmetric unit of $[Co_4(BTC)_3\ (BIM)_6]$ [solvent]

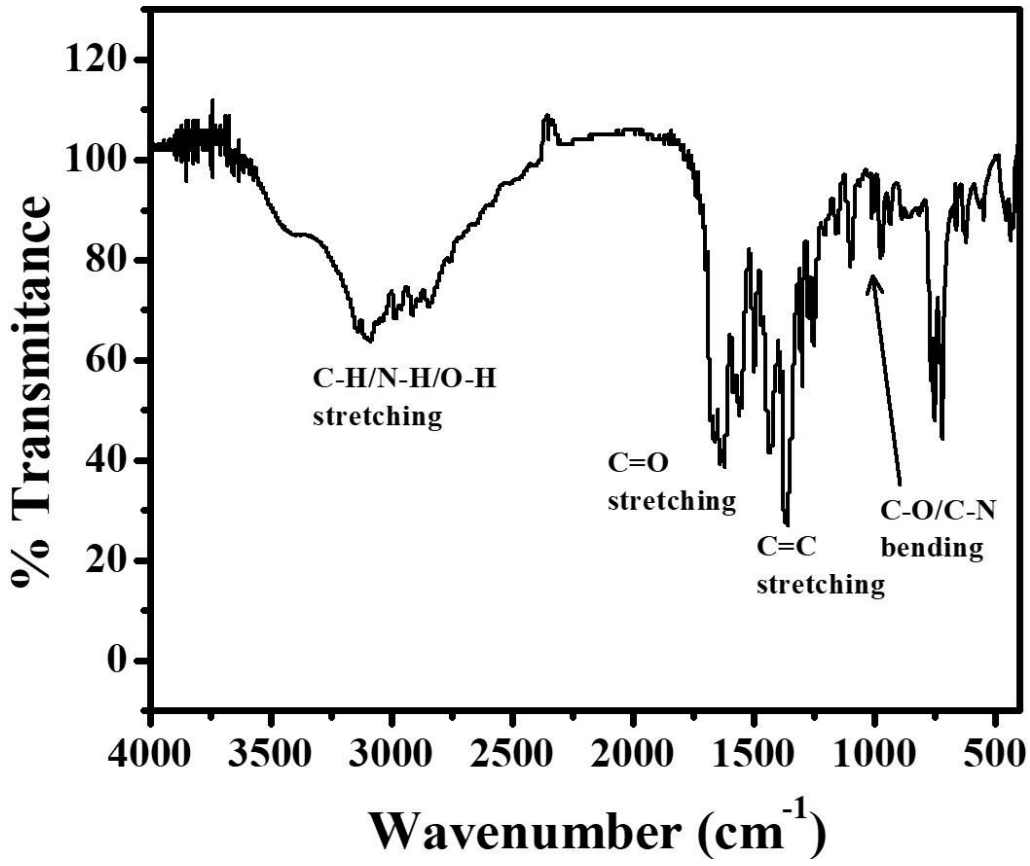

Figure S 2 FTIR spectrum of Co-MOF

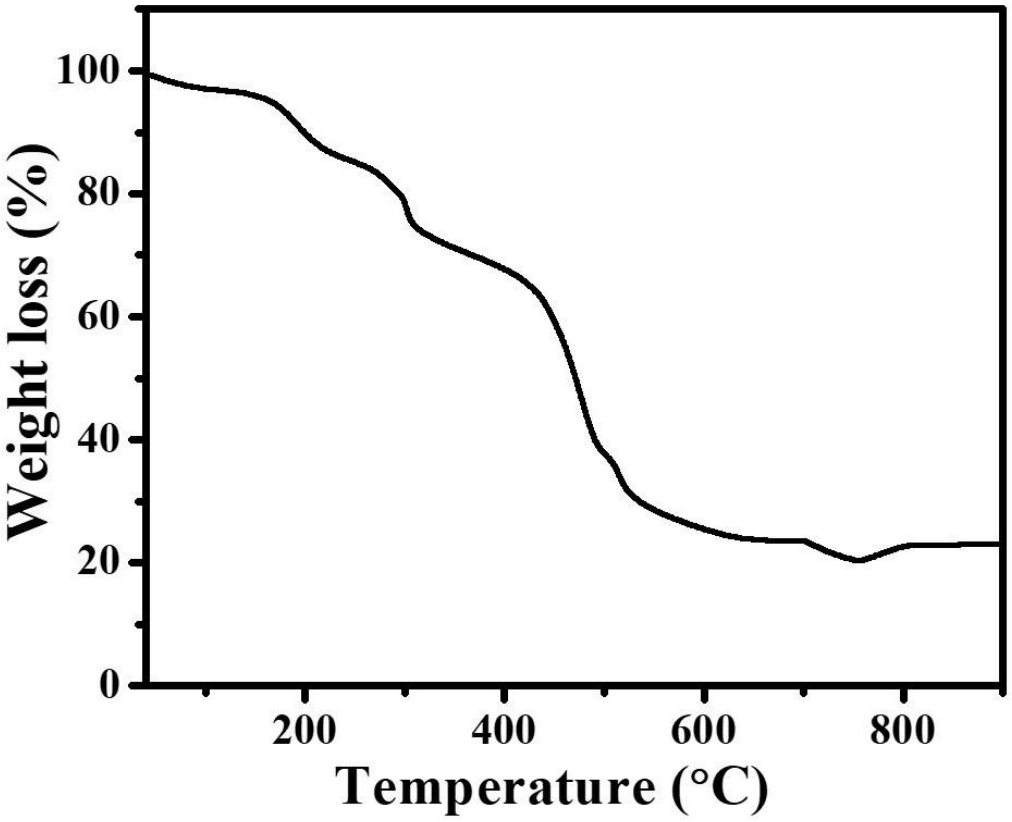

Figure S 3 Thermo gravimetric analysis of the Co-MOF

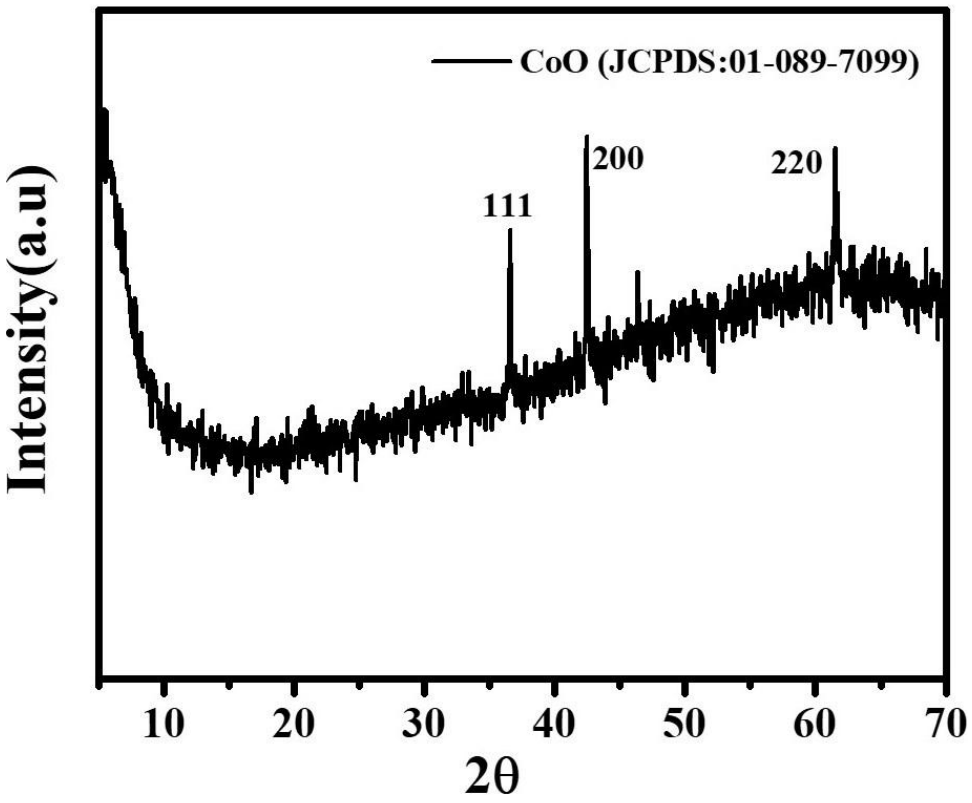

Figure S 4 X-ray diffraction pattern of Co-MOF after the thermo gravimetric analysis.

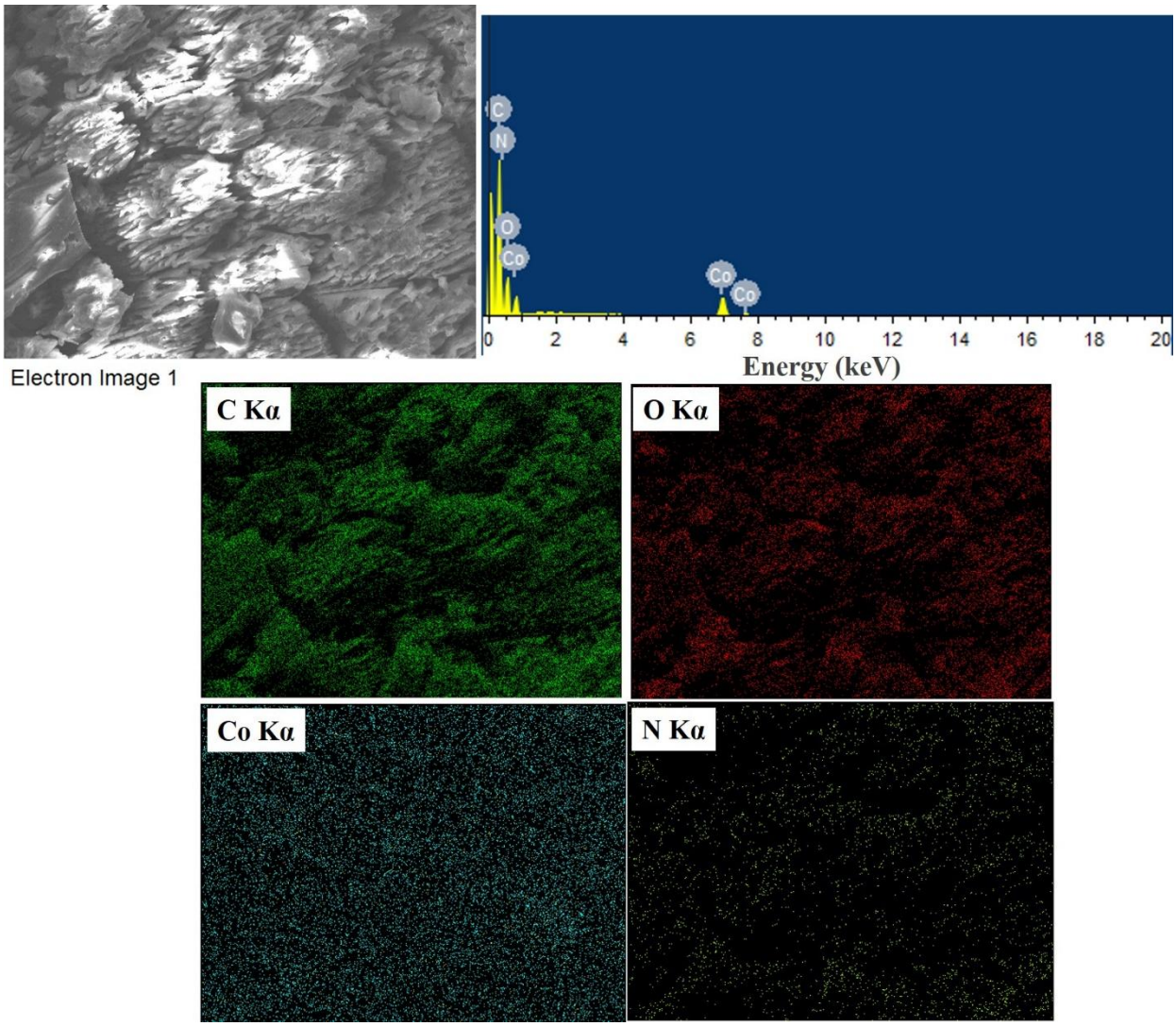

Figure S 5 EDS spectrum and corresponding elemental mapping of Co-MOF.

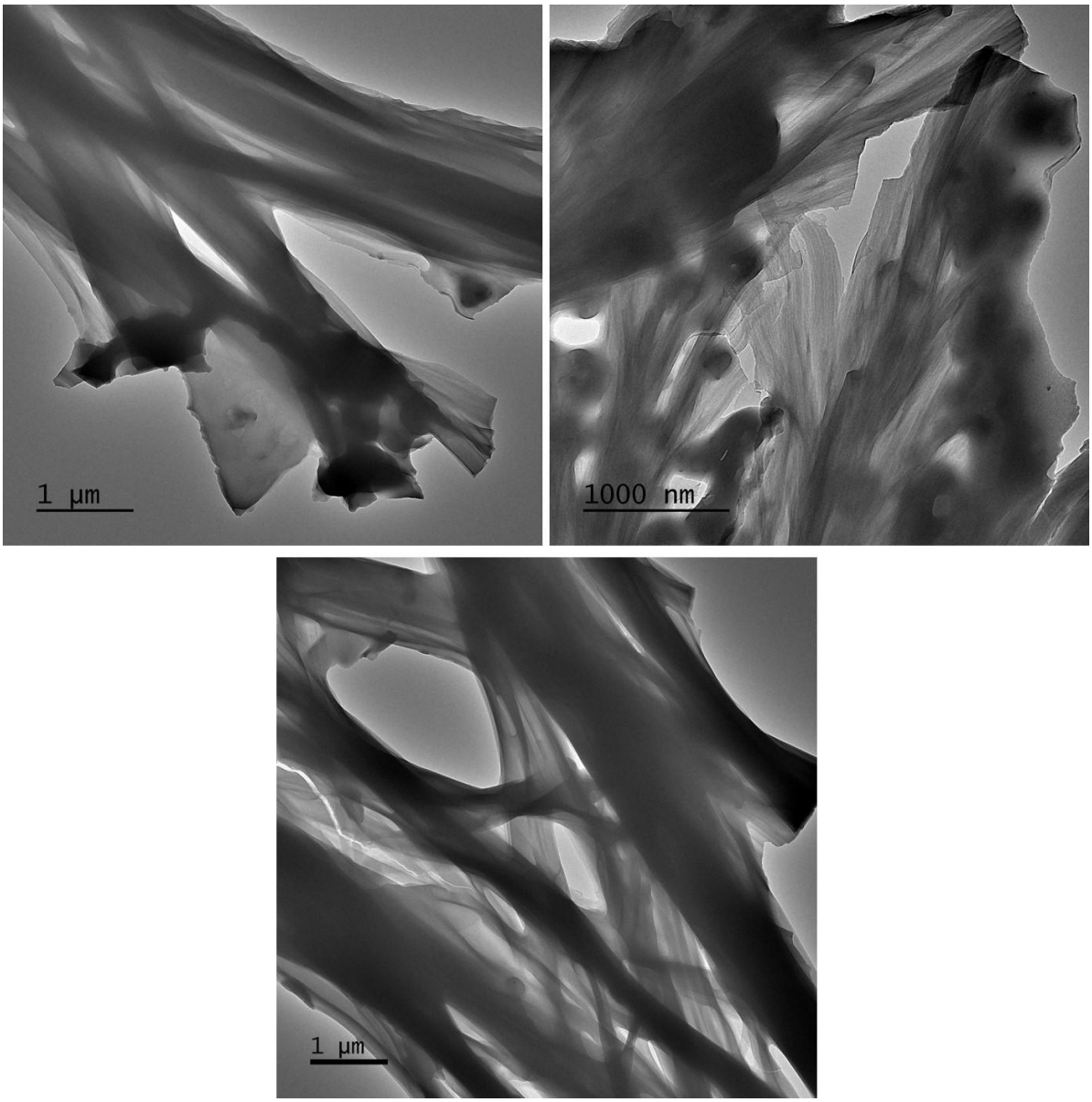

Figure S 6 Transmission electron microscopic images of Co-MOF.

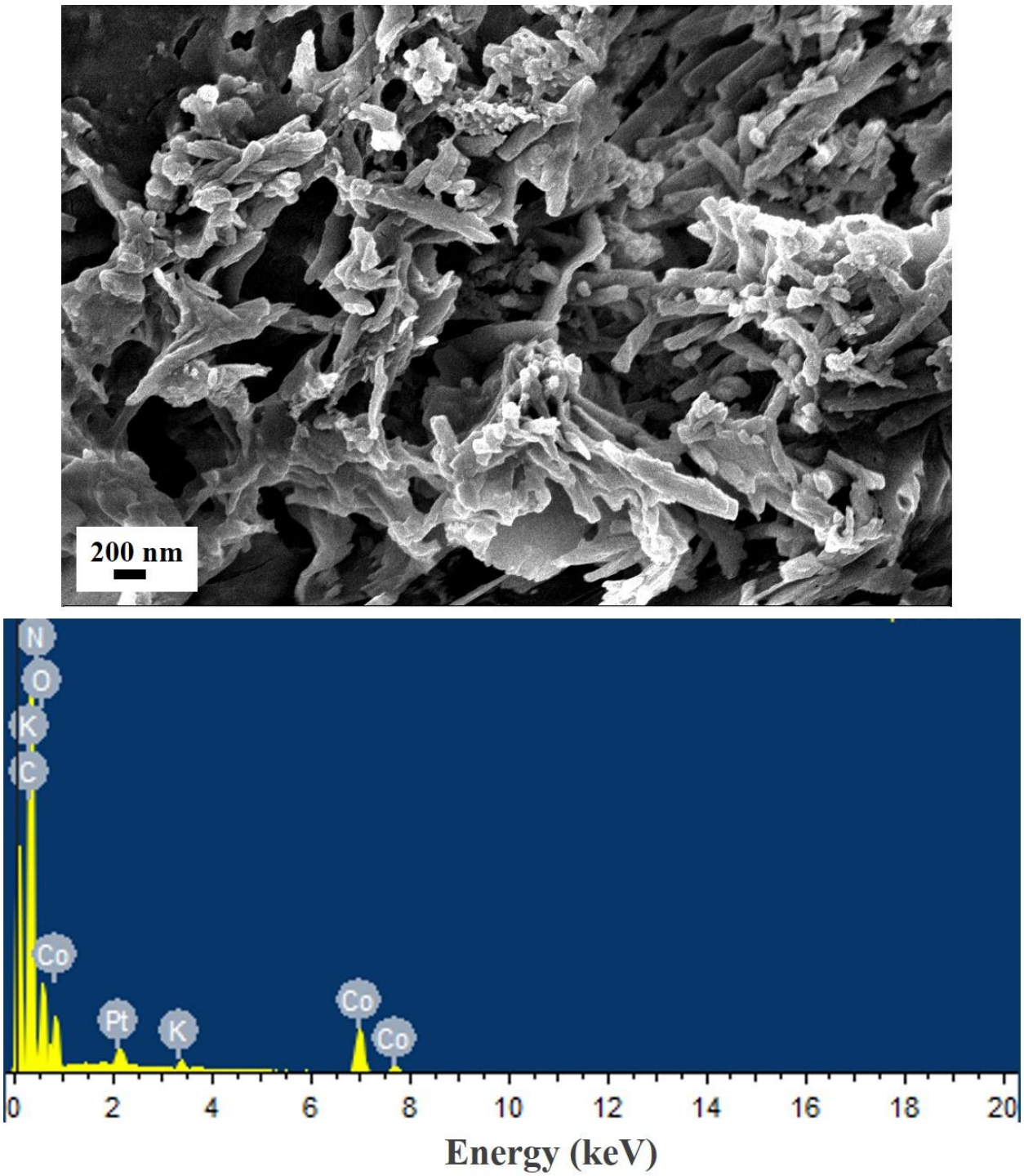

Figure S 7 FESEM, EDS and XRD pattern of Co-MOF after the ORR stability measurement.

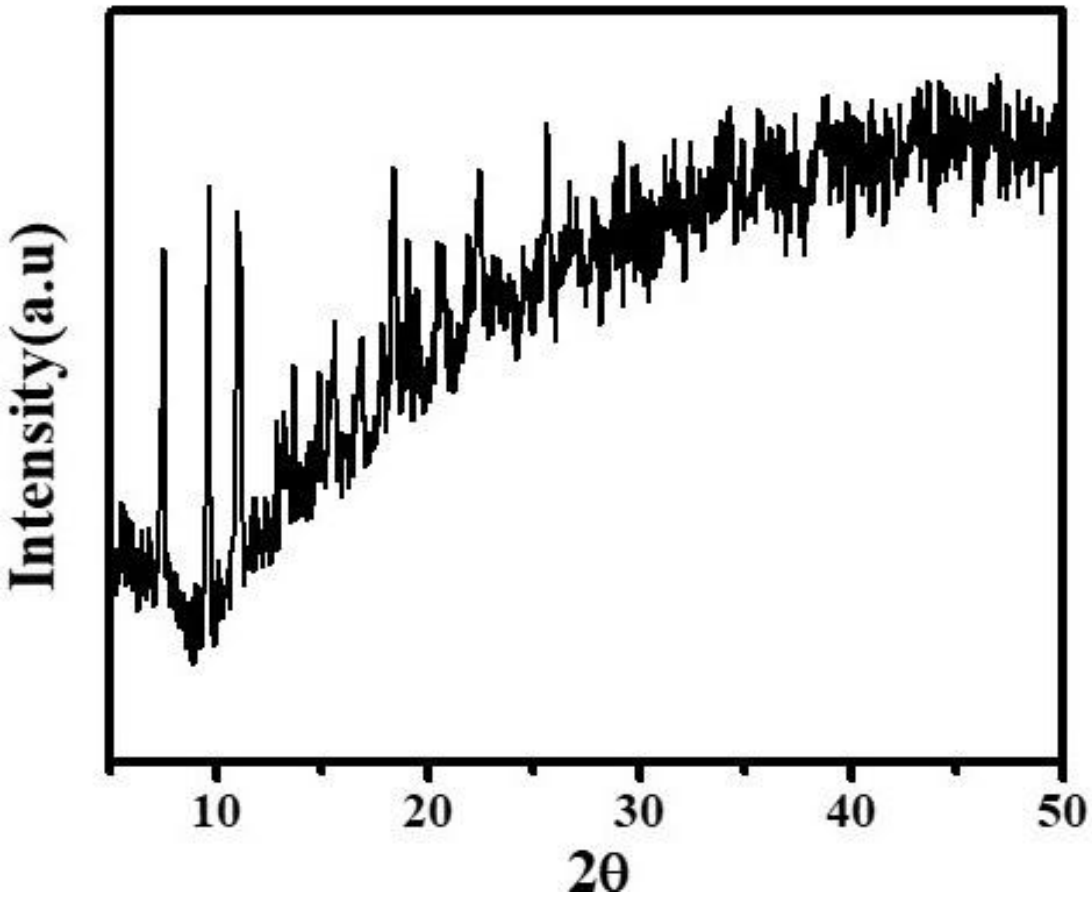

Figure S 8 X-ray diffraction pattern for Co-MOF after ORR stability test

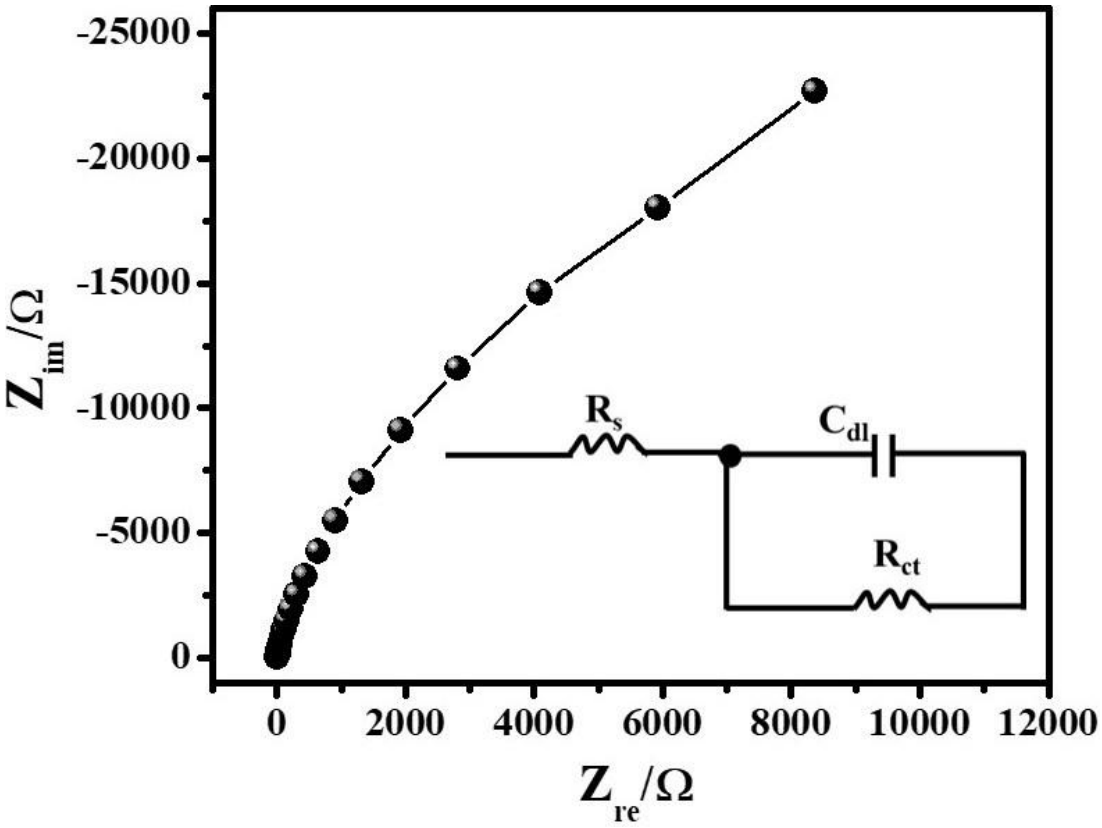

Figure S 9 Nyquist impedance spectrum of Co-MOF. Inset is the fitted circuit diagram.

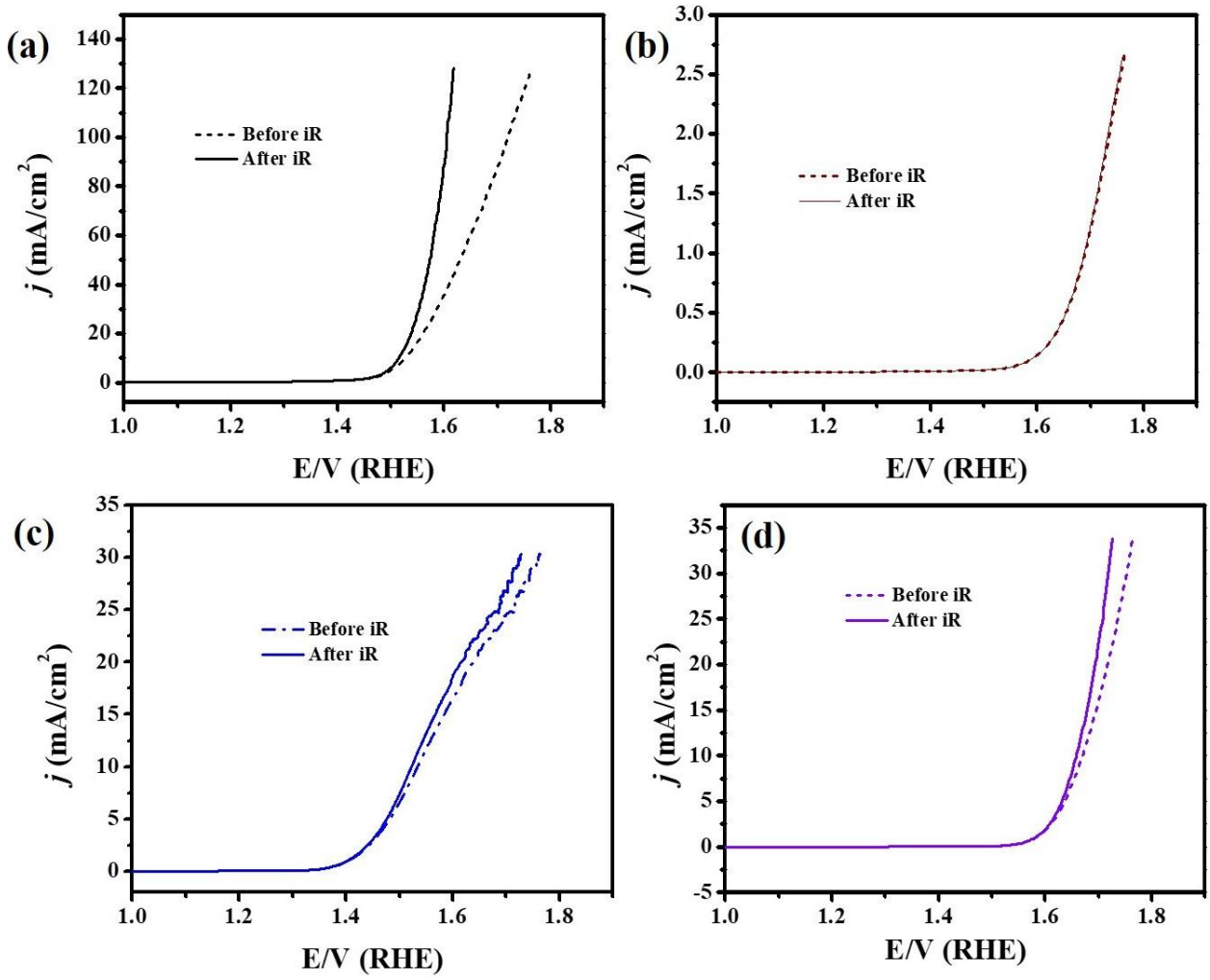

Figure S 10 Linear sweep voltammograms for Co-MOF (a), AB (b), commercial RuO_2 (c) and CoO after TGA (d) for OER before and after the iR-compensation in 1 M KOH electrolyte at a sweep rate of 5 mV/s.

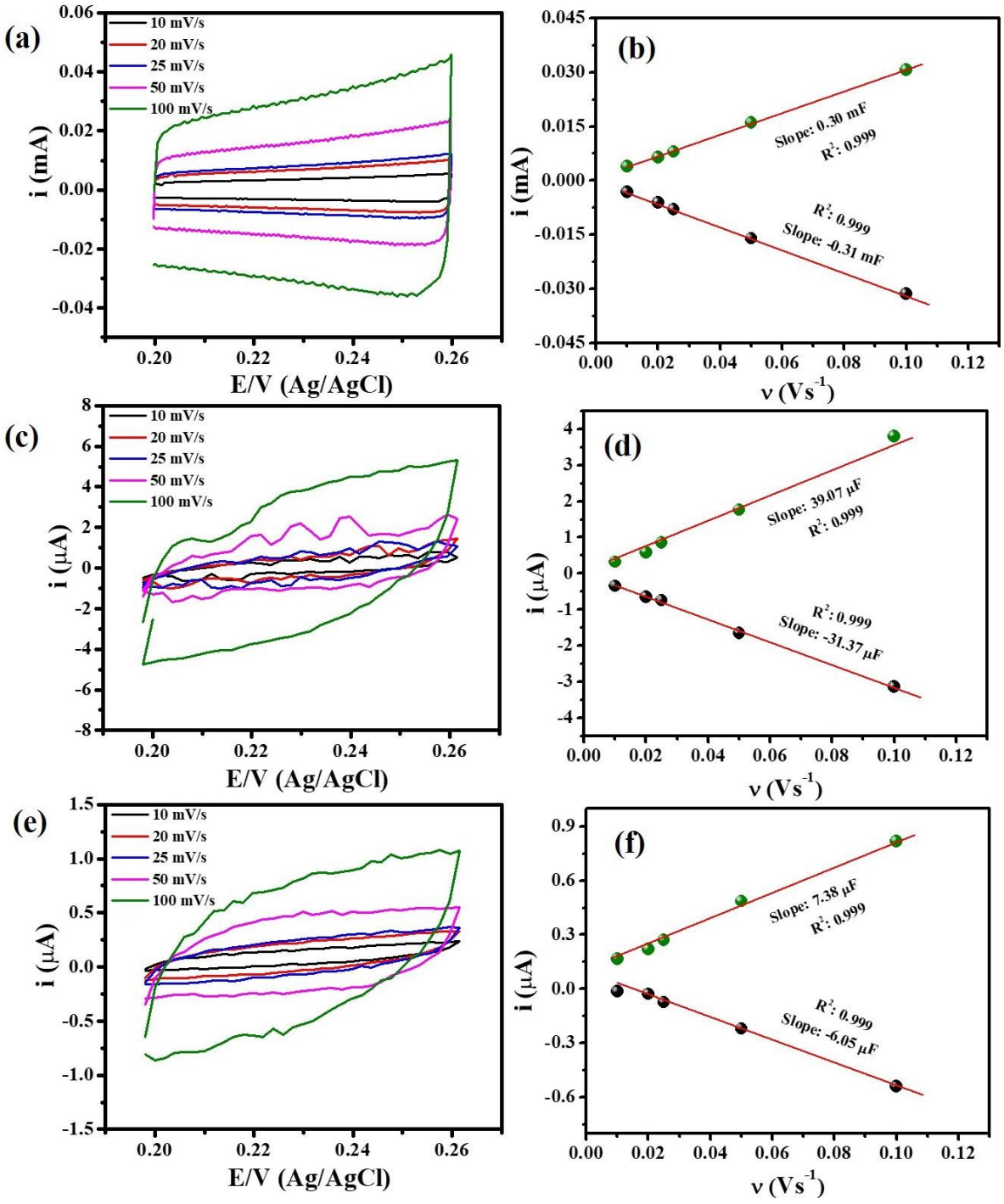

Figure S 11 Cyclic voltammogram at different sweep rates and plot of current density at 0.23 V vs. Ag/AgCl to the sweep rate to determine the double layer capacitance by commercial RuO_2 (a, b), Co3O4 (c, d) and AB (e, f) modified GCE in 1 M KOH electrolyte.

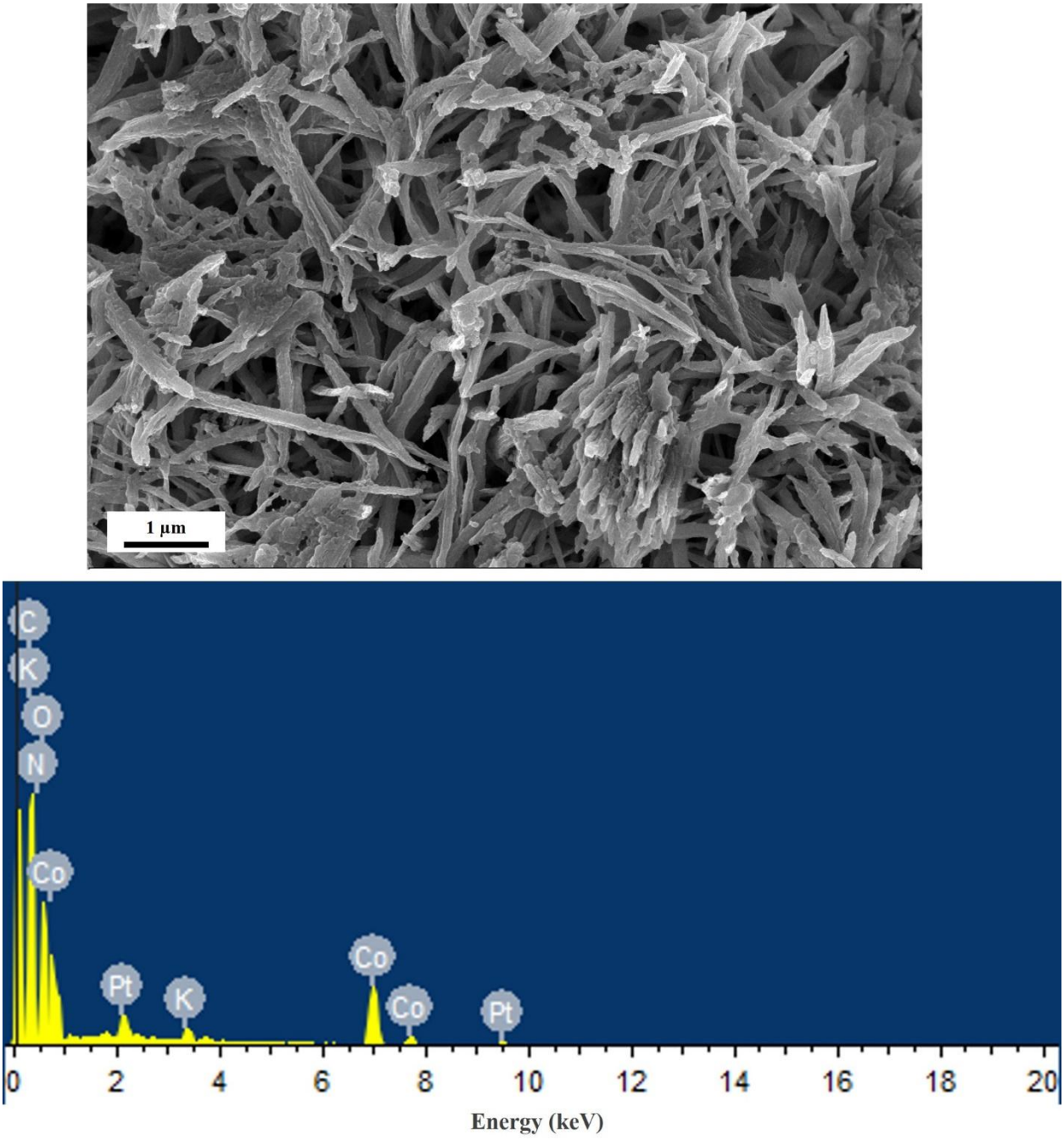

Figure S 12 FESEM, EDS and XRD pattern of Co-MOF after the OER stability measurement.

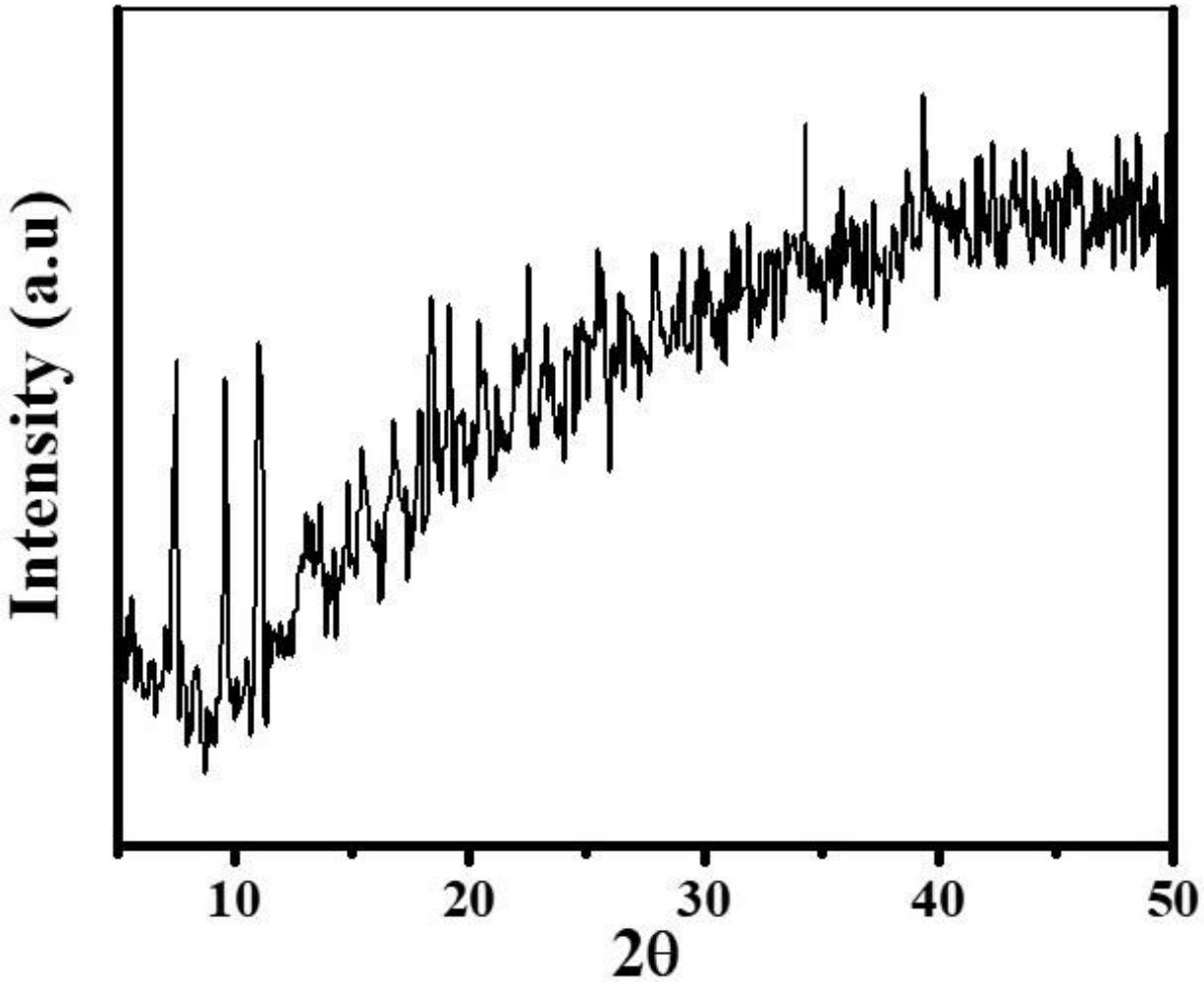

Figure S 13 X-ray diffraction pattern for Co-MOF after OER stability test

Sl. No	Catalysts	Electrolyte (Conc.)	Overpotential (mV)	Tafel Slope (mV/dec)	Reference
1	NiCo-UMOFNs	1 M KOH	250@10 mA cm^{-2}	142	Nat. Energy, 2016, 1, 16181.
2	$[Co(C_{12}H_6O_4)(H_2O)_4]$	0.1 M KOH	520@10 mA cm^{-2}	42	J. Am. Chem. Soc. 2014, 136, 13925
3	Fe_3-Co_2	0.1 M KOH	GC:283@10 mA·cm-2 Cu Foam:237@10 mA cm^{-2}	43 79	J. Am. Chem. Soc. 2017, 139, 1778
4	Co-WOC-1	0.1 M KOH	390@1 mA cm^{-2}	128	Angew. Chem. Int. Ed. 2016, 55, 2425.
5	Cu-MOF	0.5 M H_2SO_4	310@2 mA cm^{-2}	65	Adv. Funct. Mater. 2013, 23, 5363.
6	Co-TpBpy	pH = 7	400@1 mA cm^{-2}	59	Chem. Mater. 2016, 28, 4375.
7	CoOx-ZIF	1M KOH	318@10 mA cm^{-2}	70.3	Adv. Funct. Mater. 2017, 1702546.
9	NiFe LDH/NF	1M KOH	240@10 mAcm^{-2}	----	Science 2014, 345, 1593
10	MAF-X27-OH	1M KOH	387@10 mA cm^{-2}	----	J. Am. Chem. Soc. 2016, 138, 8336-8339
11	Co-ZIF-9	pH = 13.4	510@10 mA cm^{-2}	----	Nanoscale 2014, 6, 9930-9934.
12	FeTPyP-Co	0.1M NaOH	330@10 mA cm^{-2}	----	J. Am. Chem. Soc. 2016, 138, 3623-3626
13	CoTPyP	0.1M NaOH	400@10 mAcm^{-2}	----	J. Am. Chem. Soc. 2016, 138, 3623-3626
14	FeTPyP	0.1 M NaOH	400@10 mA cm^{-2}	----	J. Am. Chem. Soc. 2016, 138, 3623-3626
15	NU-1000	pH = 11	566@10 mA cm^{-2}	----	ACS Appl. Mater. Interfaces 2015, 7, 28223-28230.
16	Fe–CoS_2 Nanosheets	1.0 M KOH	302@10 mA cm^{-2}	128	Chem. Commun., 2019,55, 2469-2472.
17	CoS_2 hollow Nano sphere	1.0 M KOH	290@10 mA cm^{-2}	57	Nanoscale, 2018,10, 4816-4824.
18	$NiCo_2O_4$ nanoparticles	1.0 M KOH	350@10 mA cm^{-2}	43	Chem Cat Chem, 2019, 11, 412 – 416.
19	N, S–codoped graphene supported CoS_2		393@10 mA cm^{-2}	81	J. Power Source, 2018, 389, 178-187.
20	Co-MOF	1 M KOH	280@10 mA cm^{-2}	51	This work
21	Commercial RuO_2	1 M KOH	330@10 mA cm^{-2}	72	

22	Co_3O_4 (post TGA)	1 M KOH	430@10 mA cm^{-2}	71	

Table S1. Table showing the comparison of activity of the Co-MOF of the present work with the reported metal organic frameworks for oxygen evolution reaction.

References

1. Min-Rui Gao, Xuan Cao, Qiang Gao, Yun-Fei Xu, Ya-Rong Zheng, Jun Jiang, and Shu-Hong Yu, Nitrogen-Doped Graphene Supported $CoSe_2$ Nanobelt Composite Catalyst for Efficient Water Oxidation, *ACS Nano* 2014 *8* (4), 3970-3978.