Fabricating bimetallic cobalt-iron MOF nano/microcrystalline particles: strong bifunctional electrocatalytic activity and overall water splitting

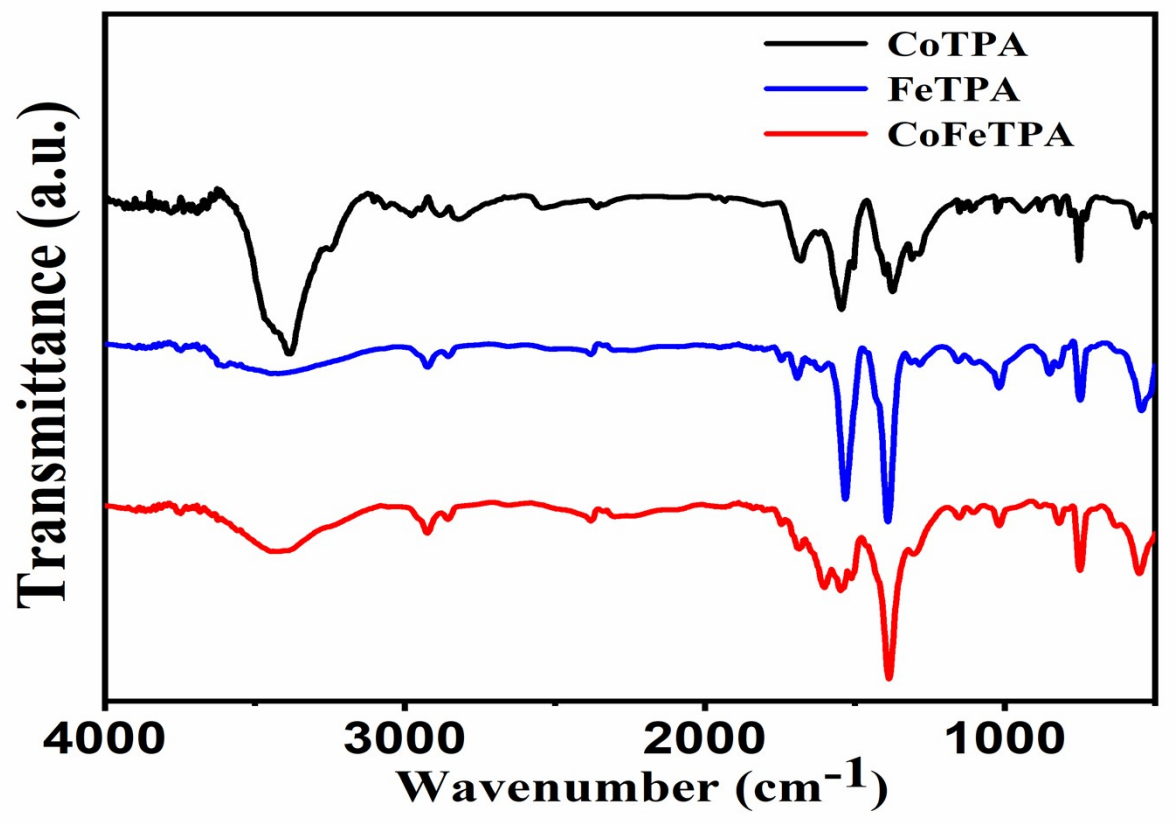

Figure S1. FTIR spectra of CoTPA, FeTPA and CoFeTPA 11.

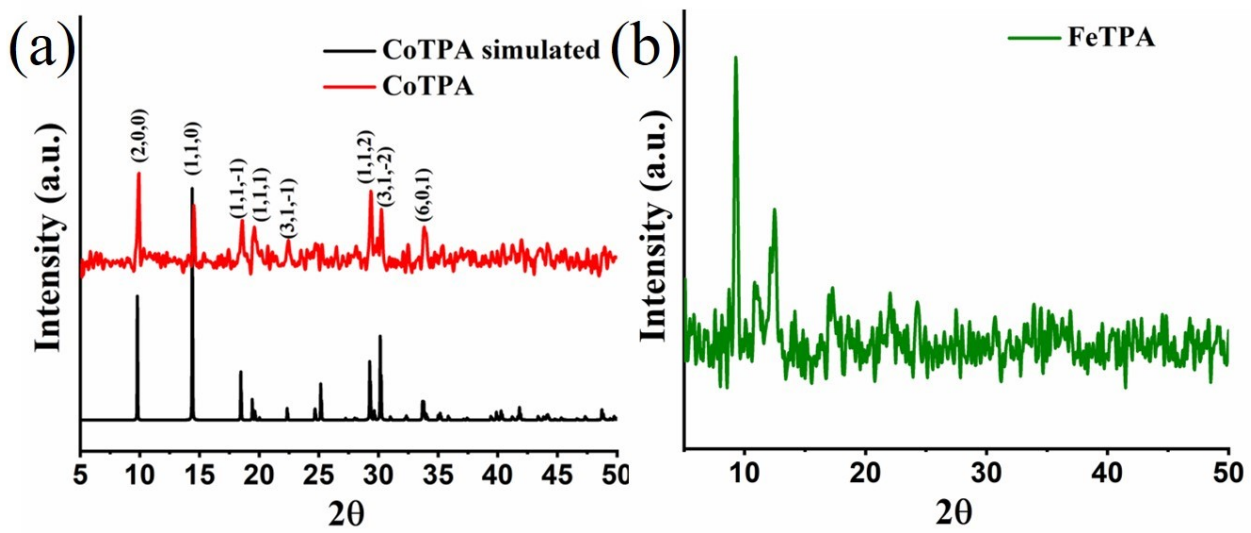

Figure S2. Comparison of simulated PXRD of CoTPA and FeTPA with the corresponding experimental PXRD pattern.

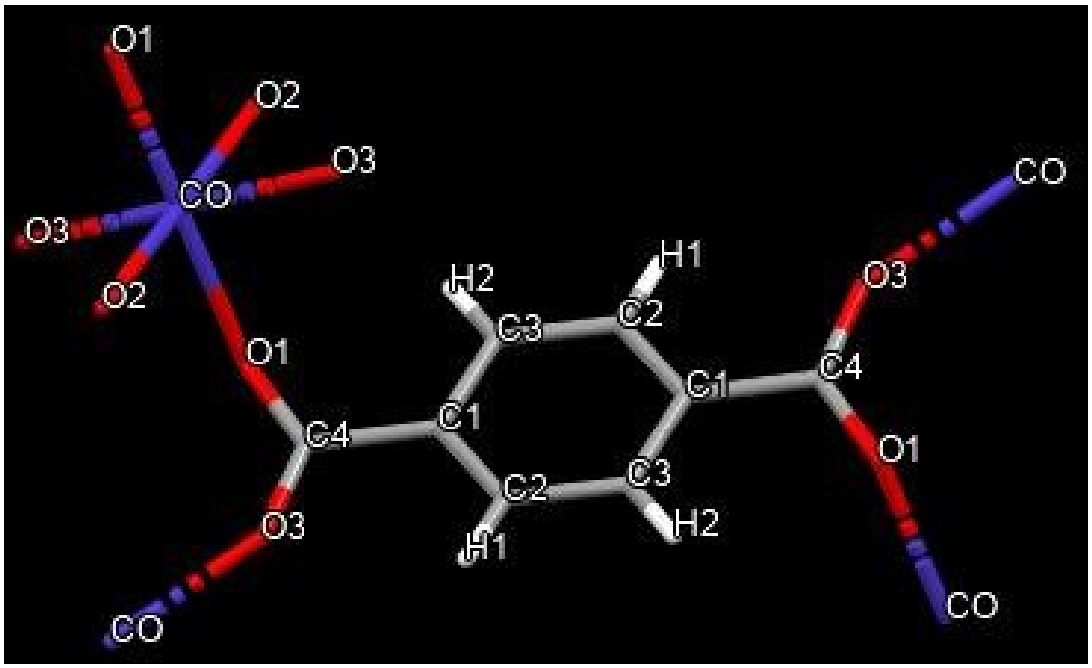

Figure S3. CoTPA structure in the crystal lattice (CCDC No. 163139). O1 and O3 are terephthalic acid carboxylate oxygen and O2 is a water molecule oxygen.

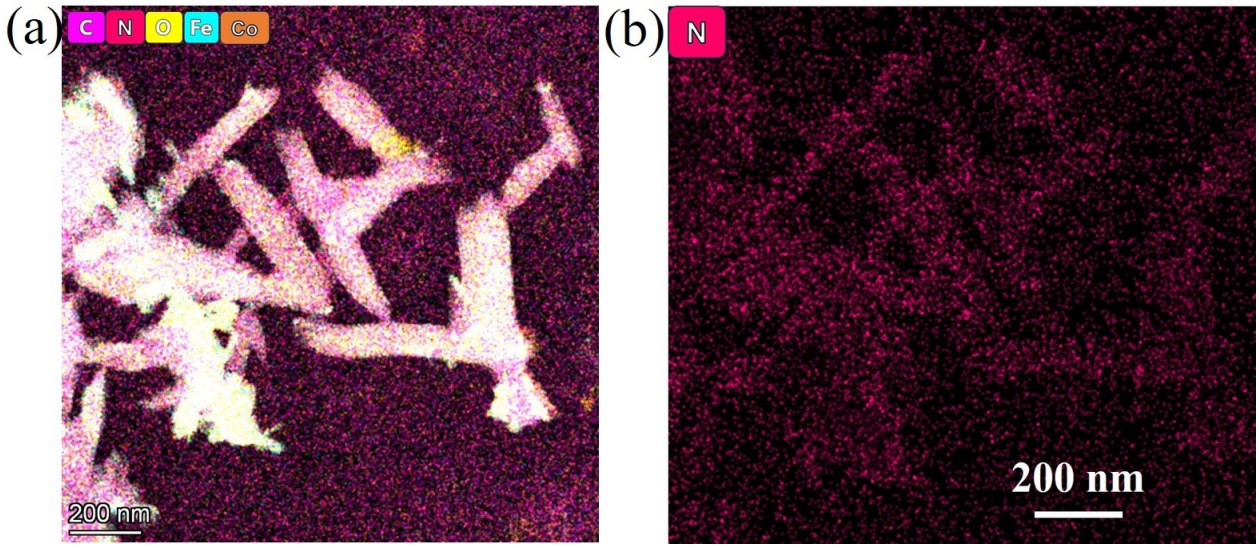

Figure S4. HAADF-STEM elemental mapping CoFeTPA nanorods (a) mapping with all elements and (b) N.

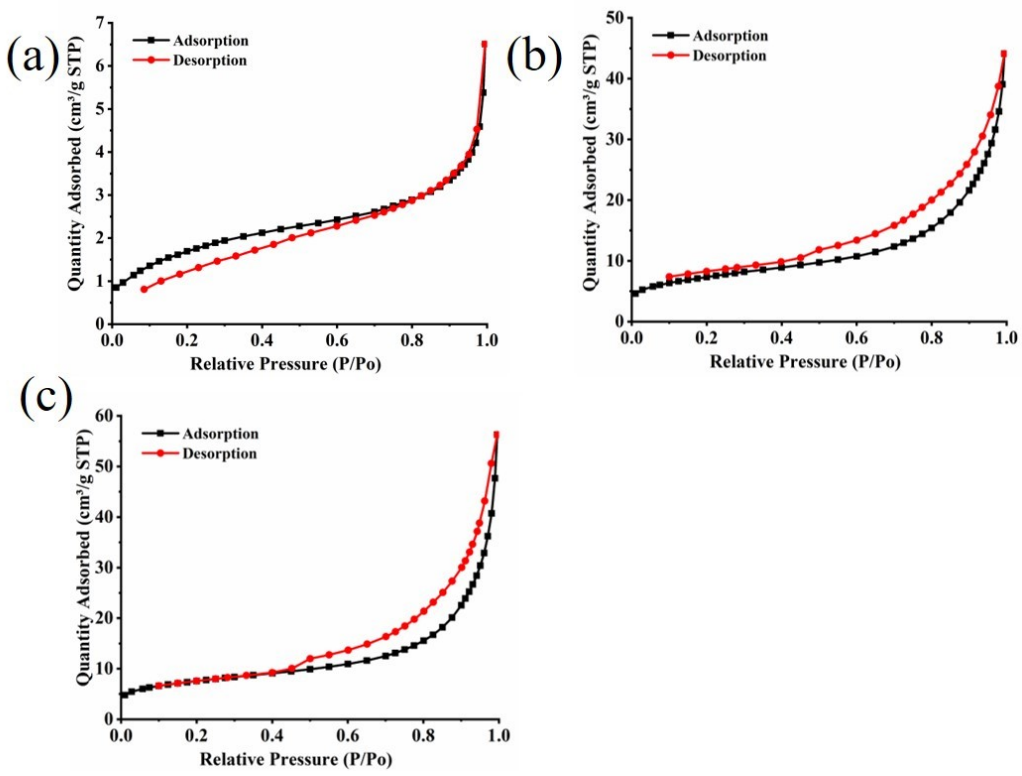

Figure S5. BET graphs of (a) CoTPA, (b) FeTPA and (c) CoFeTPA.

Table S1. BET data of CoTPA, FeTPA and CoFeTPA.

	Surface area	Pore volume BJH	Average Pore diameter
FeTPA	21.2259 m^2/g	0.064078 cm^3/g	12.0754 nm
CoFeTPA	25.1197 m^2/g	0.085577 cm^3/g	13.6271 nm
CoTPA	4.5993 m^2/g	0.009566 cm^3/g	8.3193 nm

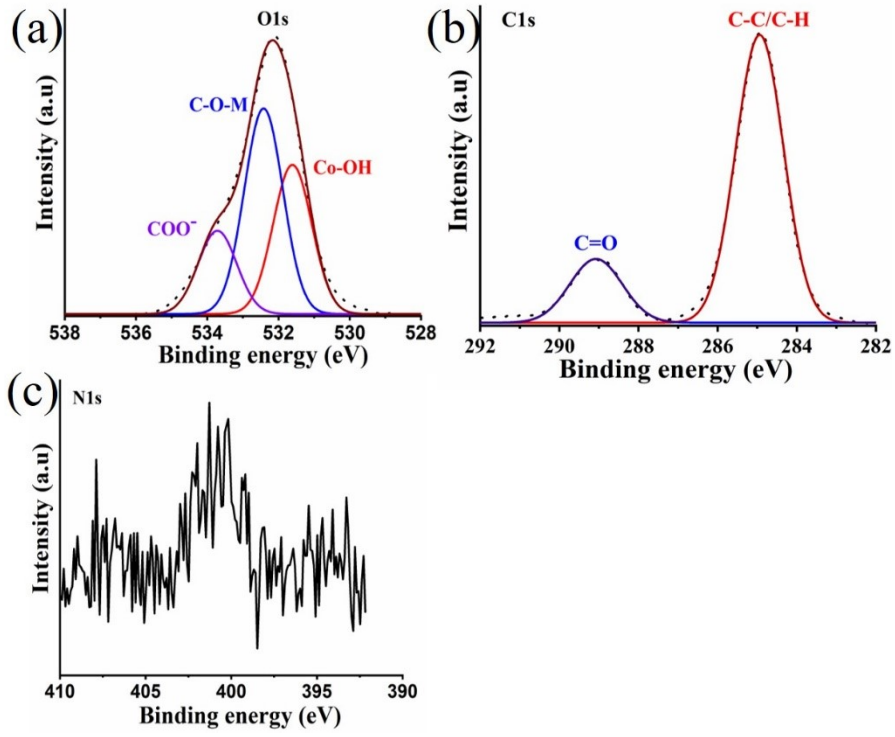

Figure S6. High resolution XPS spectra of (a) O1s, (b) C1s and (c) N1s of CoTPA.

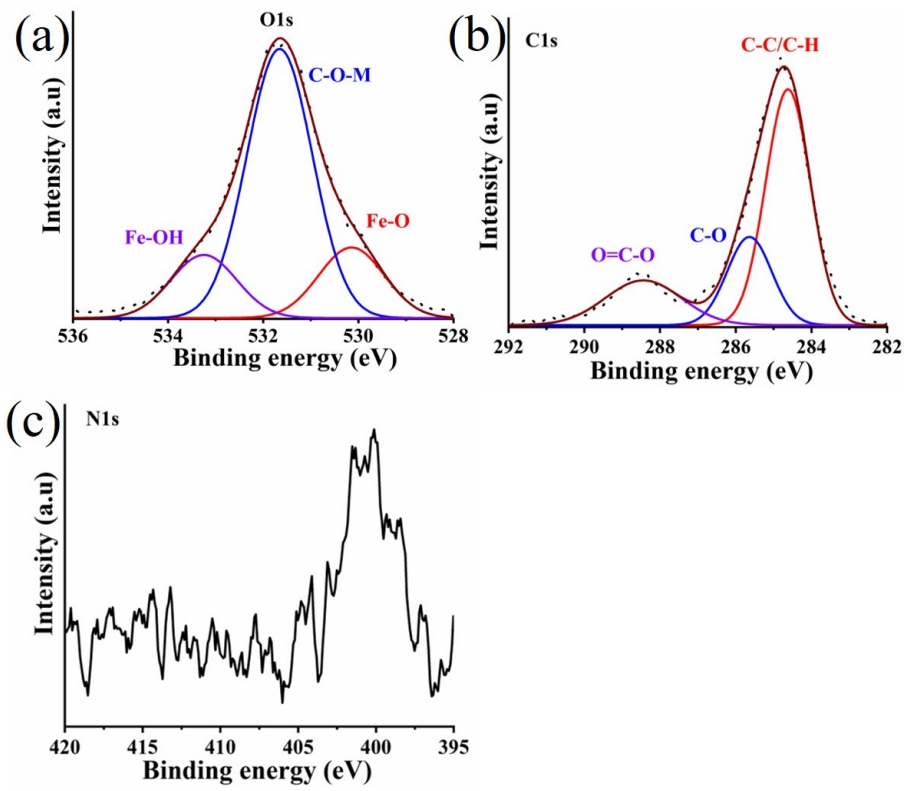

Figure S7. High resolution XPS spectra of (a) O1s, (b) C1s and (c) N1s of FeTPA.

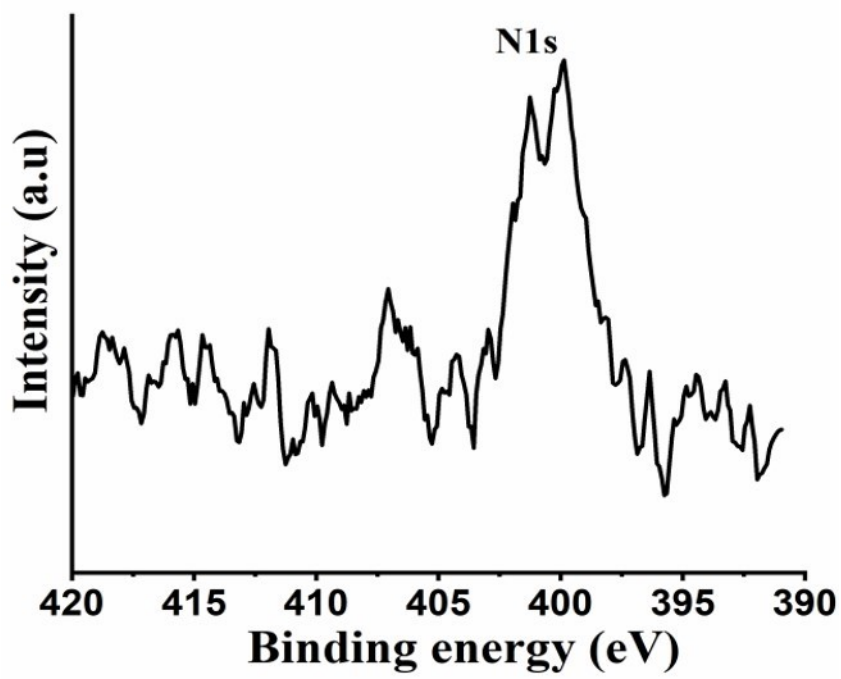

Figure S8. High resolution N1s XPS spectrum of CoFeTPA11.

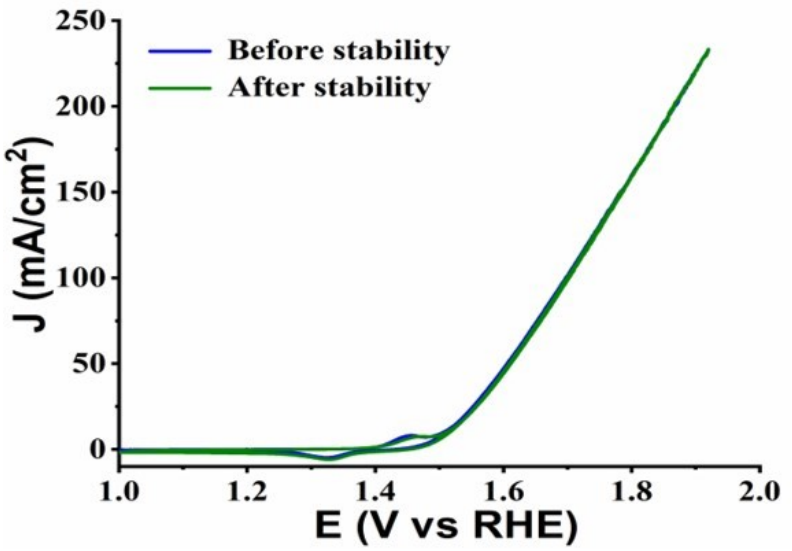

Figure S9. OER LSV polarization curve of bimetallic CoFeTPA MOF before and after stability studies.

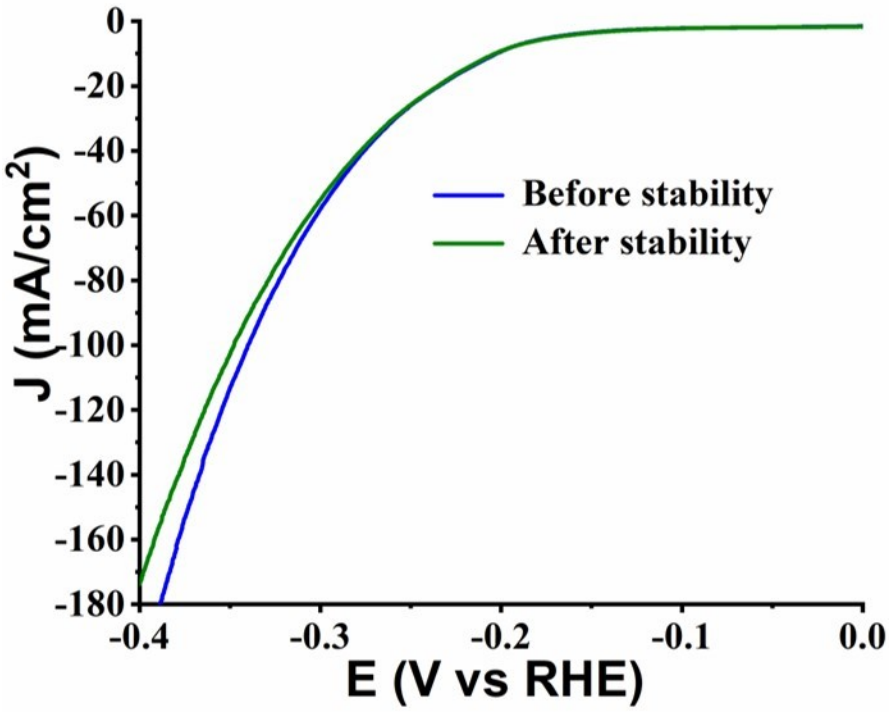

Figure S10. HER LSV polarization curve of bimetallic CoFeTPA MOF before and after stability studies.

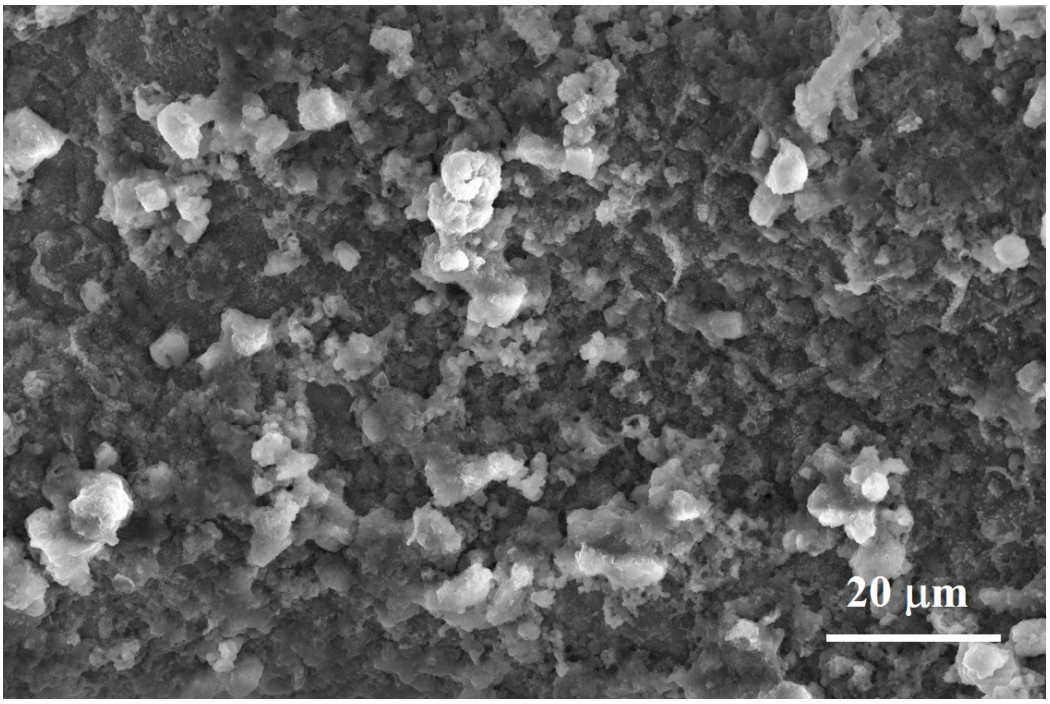

Figure S11. HR-SEM image of CoFeTPA11 after catalysis.

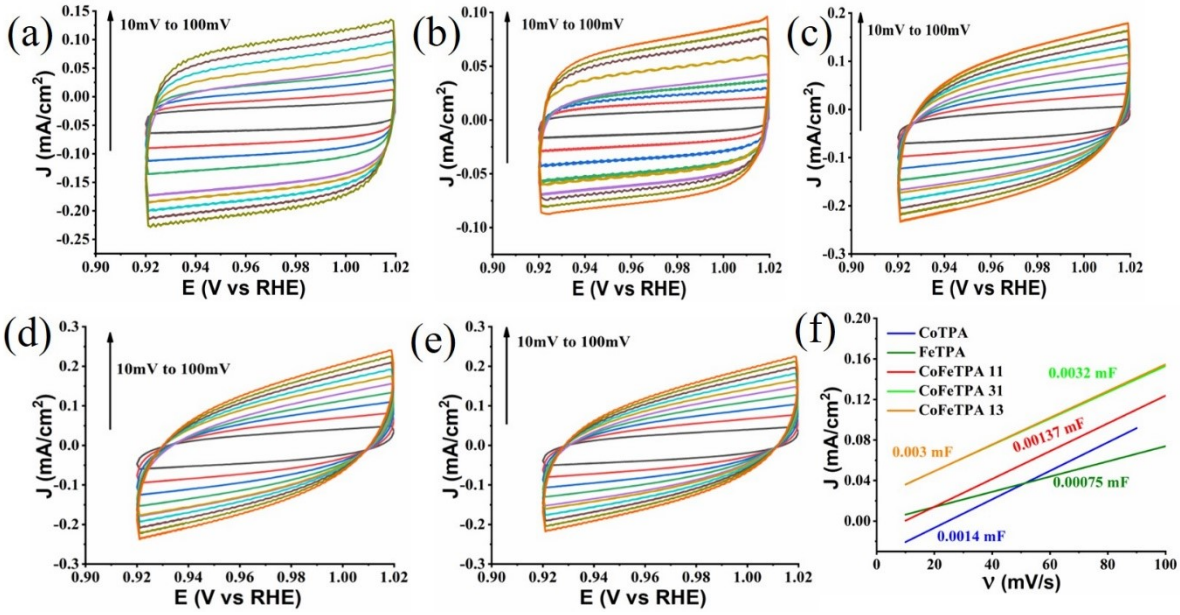

Figure S12. Double layer capacitance of (a) CoTPA, (b) FeTPA, (c) CoFeTPA11, (d) CoFeTPA31 and (e) CoFeTPA13 and (d) capacitive currents as a functional of scan rate.

Table S2. Turnover Frequency (TOF) of CoTPA, FeTPA and bimetallic CoFeTPA MOFs.

The catalysts turnover frequency (TOF) was calculated using the formula TOF= jA/4nF. Where A represents the geometrical surface area of the working electrode (0.5), j represents the current density ($mAcm^{-2}$), F represents the Faraday's constant (96485.3C mol^{-1}), n indicates the number of metal atoms present on the metal surface in moles, and 4 represents the electron count for molecular oxygen. We calculated the current density at the overpotential of 270mV for OER and 300mV for HER respectively.

	Turnover frequency at 270 mV OER (S^{-1})	Turnover frequency at 300mV HER (S^{-1})
CoTPA	0.57	1.63
FeTPA	5.52	0.67
CoFeTPA 11	2.38	2.98
CoFeTPA 31	1.89	0.57
CoFeTPA 13	1.63	1.09

After determining the molar average Co/Fe atomic mass, we calculated moles by taking a ratio of the mass of the catalyst to the average atomic mass. The value was substituted in the formula TOF= jA/4nF.

	The ratio of cobalt Co^{2+} (58.93 u)	Ratio of Fe^{3+} (55.84)	Net metal concentration
CoTPA	1	0	58.93
FeTPA	0	1	55.84
CoFeTPA 11	0.5 (0.5 ×58.93= 29.46)	0.5 (0.5 ×55.84= 27.92)	57.38
CoFeTPA 31	0.75 (0.75 ×58.93= 44.19)	0.25 (0.25 ×55.84= 13.96)	58.15
CoFeTPA 13	0.25 (0.25 ×58.93= 14.73)	0.75 (0.75 ×55.84= 41.88)	56.61

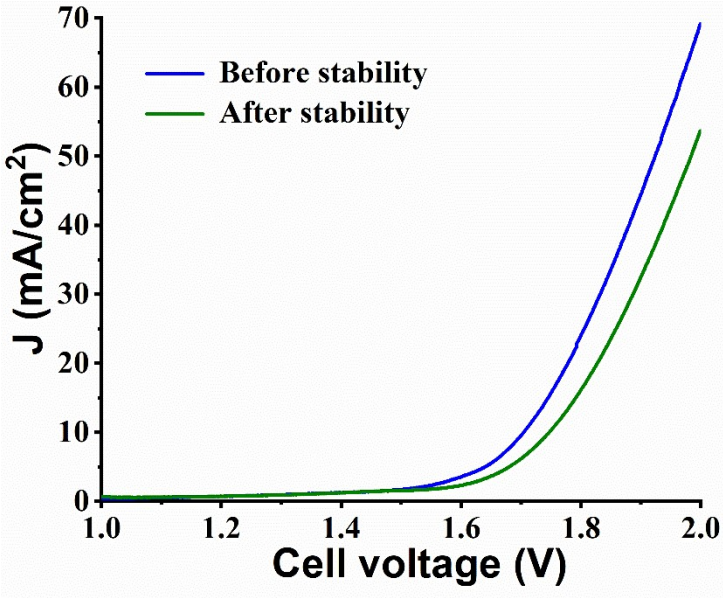

Figure S13. Overall water splitting polarization curve of bimetallic CoFeTPA11 before and after stability studies.

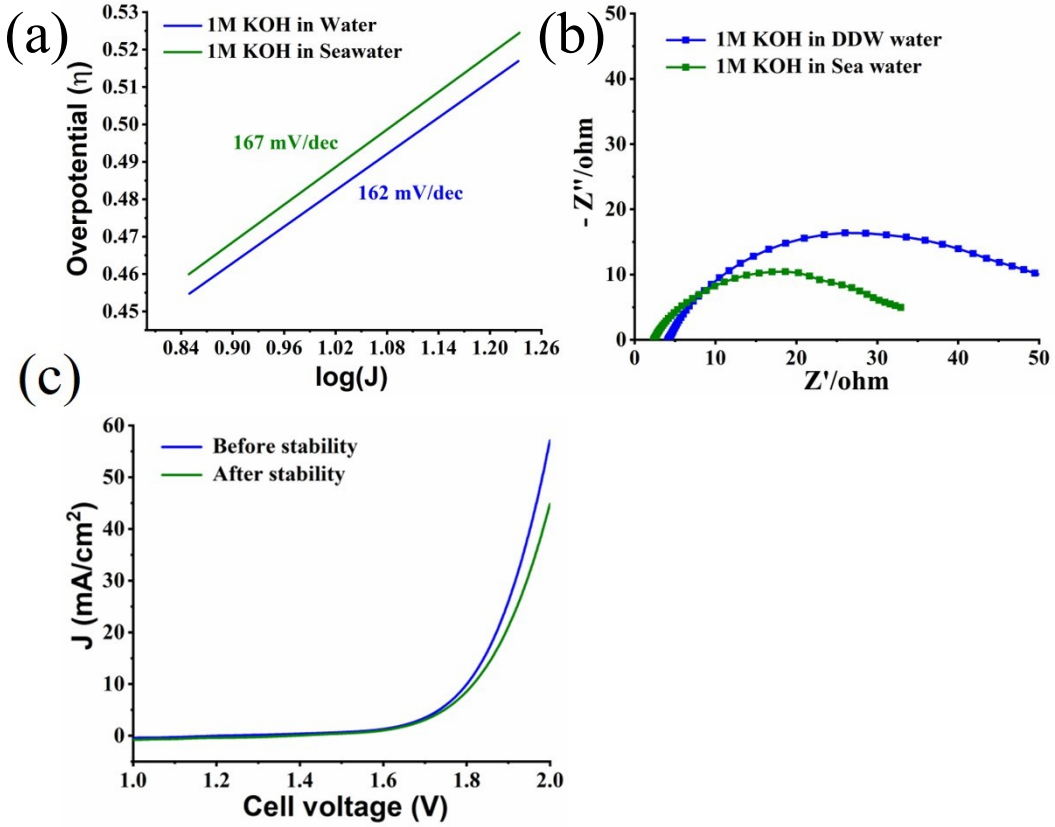

Figure S14. (a) Tafel plot, (b) electrochemical impedance spectra and (c) overall water splitting polarization curve before and after stability studies of CoFeTPA11 in sea water.