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SUPPORTING INFORMATION

Synthesis of Diverse Stable MOFs and Their Electro Catalytic Capabilities towards Desulfurization, Water Splitting and various Nitrophenol Reduction

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Figure S1. EDAX images of a) Al-C MOF, b) Co-C MOF c) Ni-C MOF.

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Al-C MOF

Co-C MOF

Ni-C MOF

1

2

3

S.No.	Catalyst	Element	Element weight (%)					
		Al	Co	Ni	С	Ν	0	

-

-

10.28

-

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10.58

4.72

8.37

8.55

39.57

25.74

22.57

45.02

55.62

58.29

Table S1. The synthetic composite weight percentage obtained from EDAX.

Table S2. The N_2 adsorption-desorption isotherms were employed to obtain the BET surface area $(m^2 g^{-1})$ and pore volume $(cm^3 g^{-1})$ of Co-C MOF, Ni-C MOF and Al-C MOF.

S.No.	Catalyst	BET surface area (m ² g ⁻¹)	pore volume (cm ³ g ⁻¹)
1	Co-C MOF	164	1.83
2	Ni-C MOF	147	1.4
3	Al-C MOF	123	0.3



Fig. S2 (a-c) HR-TEM images of as-synthesized catalysts Al-C MOF, and Ni-C MOF.



Figure S3. XPS spectrum of Al-C MOF: (a) full survey, (b) C 1s, (c) N 1s, (d) O 1s and (e) Al 2p.

Figure S3 (a) shows full XPS survey of synthesized Al-C MOF. Figure S3 (b-d) displays the deconvoluted spectra of C 1s, O 1s and Al 2p. The C 1s peak was deconvoluted into its several components and the fitted curves with peaks that correspond to C=C (sp^2)

:284.89 eV) and C-C (sp² :288.91 eV) are displayed in **Figure S3 (b)**. **Figure S3 (c)** depicts the N1s deconvoluted peaks and the sample revealed three peaks for pyridinic-N (399.89 eV), pyrrolic-N (399.97 eV) and graphitic-N (401.66 eV) respectively. **Figure S3 (d)** shows the deconvoluted O 1s spectrum of the sample. The spectrum confirmed the presence of carbon bonds with oxygen such as CO and C-O-C at binding energies of 532.12 and 533.40 eV respectively. **Figure S3 (c)** displays the deconvoluted Al 2p spectrum of the sample and the peaks observed at 74.69, 74.49 and 75.29 eV indicate the Al 2p oxide, Al 2p3/2 and Al 2p1/2 respectively. The peaks that appear at 532.90 and 534.07 eV in the O 1s spectrum indicates the presence of C-O bonding and the C-O-H bonding respectively.



Figure S4. XPS spectrum of Ni-C MOF: (a) full survey, (b) C 1s, (c) N 1s, (d) O 1s and (e) Ni 2p.

Similarly, a full XPS survey of synthesized Co-C MOF is shown in **Figure S4 (a)** which indicates the presents of C 1s, N1s, O1s and Ni 2p. **Figure S4 (b)** shows the fitted curves with peaks for C=C (sp²: 284.89 eV) and C-C (sp²: 288.91 eV) which correspond to the deconvoluted C 1s peaks. **Figure S4 (c)** shows the N 1s deconvoluted peaks at 397.43, 397.49

and 398.20 eV which correspond to pyridinic-N, pyrrolic-N and graphitic-N respectively. **Figure S4 (d)** shows the deconvoluted O 1s spectrum which confirms the presence of carbon bonds with oxygen such as CO and C-O-C at binding energies of 532.12 and 533.40 eV respectively. **Figure S4 (e)** shows two spin-orbit doublets (853.77 eV and 872.71 eV), two shake up satellites (859.95 eV and 877.80 eV) that are all indicative of the Ni²⁺ valence state are well-fitted into the Ni 2p spectrum. The Ni²⁺ valence state is strongly represented in Ni 2p spectrum by the energies of 856.71 eV and 870.90 eV two spin-orbit doublets (853.77 eV and 872.71 eV) and shake up satellites (859.95 eV and 870.90 eV two spin-orbit doublets (853.77 eV and 872.71 eV) and shake up satellites (859.95 eV and 877.80 eV). Nickel peaks with three distinct chemical conditions represent the Ni 2p_{3/2}.



Figure S5. (a) Co-C MOF II Ni-C MOF LSV curves of overall water splitting (b) CA measured at the applied voltage of 1.67 V at 20 mA/cm² for 72 h.

S.No.	Electrode	ТР			ВТР		DBT			
	materials	Onset potential (V)	Tafel slope (mV / dec)	R _{ct} values (Ω)	Onset potential (V)	Tafel slope (mV / dec)	R _{ct} values (Ω)	Onset potential (V)	Tafel slope (mV / dec)	\mathbf{R}_{ct} values (Ω)
1	Ni-C-MOF	1.82	178	18927	1.73	217	14619	1.72	324	12787
2	Al-C-MOF	1.62	94	8519	1.61	176	11135	1.63	207	8962
3	Co-C-MOF	1.54	69	4238	1.52	126	4864	1.55	126	6327
4	Pt/C	1.49	39	547	1.36	53	650	1.35	57	1287

Table. S3 Electrochemical parameters obtained from LSV and EIS on the electrooxidation of TP, BT and DBT.

S.No.	Electrode	HER			OER		
	materials	Over potential (mV)	Tafel slope (mV / dec)	R _{ct} values (Ω)	oOver potential (mV)	Tafel slope (mV / dec)	R _{ct} values (Ω)
1	Ni-C-MOF	225	114	130	440	199	274
2	Al-C-MOF	622	276	363	350	182	206
3	Co-C-MOF	510	183	242	220	169	149
4	Pt/C	137	39	47	-	-	-
5	RuO ₂	-	-	-	130	43	56

 Table S4. Electrochemical parameters towards water splitting reactions

Reduction of *p*-NP, DNP and TNP using Al-C MOF

The catalytic activity of the synthesized Al-C MOF in the reduction of *p*-NP, DNP and TNP was observed using a UV-Visible spectrophotometer. *p*-NP, DNP and TNP typically absorb in the UV-vis absorption range at 400, 389 and 392 nm. The production of an intermediate nitrophenolate ion and the colour changes from light yellow to dark yellow and the peak appeared at 400, 351 and 388 nm confirm the formation of 2-diaminophenol, 2,4-diaminophenol and 2,4,6-triaminophenol. The enhanced catalytic activity of the synthesized Al-C MOF took 48, 60 and 72 mins for reduction of *p*-NP, 4-NP and 4-AP respectively. Based on the kinetic graphs displayed in **Figure S6**, the rate constant values for the *p*-NP, DNP and TNP synthesized Al-C MOF with first-order kinetics are 34.70×10^{-2} , 25.00×10^{-2} and 24.00×10^{-2} min⁻¹ respectively.



Figure S6. UV absorption spectra and kinetic plots for the reduction of (**a & d**) p-Nitrophenol (*p*-NP), (**b & e**) dinitrophenol (DNP) and (**c & f**) trinitrophenol (TNP) by using Al-C MOF.

Reduction of p-NP, DNP and TNP using Co-C MOF

Similarly, using a UV-Visible spectrophotometer, the catalytic activity of the synthesized Co-C MOF in the reduction of *p*-NP, DNP and TNP was detected. At 400, 389 and 392 nm the *p*-NP, DNP and TNP normally absorb in the UV-vis absorption range. The formation of a nitrophenolate intermediate ion, a shift in colour from light to dark yellow and the appearance of peaks at 400, 354 and 388 nm indicates of the formation of 2-diaminophenol, 2,4-diaminophenol and 2,4,6-triaminophenol. The synthesised Co-C MOF reduced *p*-NP, 4-NP and 4-AP in 32, 40 and 48 mins respectively which indicates the increased catalytic activity of the compound. According to the kinetic graphs shown in **Figure S7**, the rate constant values with first-order kinetics for the *p*-NP, DNP and TNP synthesized Al-C MOF are 87.00×10^{-2} , 26.00×10^{-2} and 29.00×10^{-2} min⁻¹ respectively.



Figure S7. UV absorption spectra and kinetic plots for the reduction of (**a** & **d**) p-Nitrophenol (*p*-NP), (**b** & **e**) dinitrophenol (DNP) and (**c** & **f**) trinitrophenol (TNP) by using Co-C MOF.

S.No.	Electrode materials	<i>p</i> -NP to pAP (mins)	DNP to DAP (mins)	TNP to TAP (mins)
1	Ni-C MOF	10	16	24
2	Al-C MOF	48	60	72
3	Co-C MOF	32	40	48



Figure S8 (a-c) CVs recorded in non-faradic region at different scan rates for the determination of ECSA for Al, Co and Ni- C MOFs respectively (d-f) the corresponding C_{dl} plot of Al, Co and Ni- C MOFs.



Figure S9 FE-SEM images of (a) Co and (b) Ni- C MOFs after carrying out long-time stability for OER and HER in 1 M KOH for 48 hours.



Figure S10 XRD patterns of Co and Ni- C MOFs after carrying out long-time stability for OER and HER in 1 M KOH for 48 hours.