Layered sql-Type Cobalt Triazine–Carboxylate MOF for Enhanced Pseudocapacitance and Visible-Light Hydrogen Evolution

Manish Kukreja[a], Saman Shaheen[b] , Tokeer Ahmad[b], Musheer Ahmad[c], Nohyun Lee[d], Anil Kumar Astakala[d], Nazrul Haq[e], Na'il Saleh[f*] Kafeel Ahmad Siddiqui[a]

[a]Department of Chemistry, National Institute of Technology Raipur, G. E. Road Raipur – 492010, Chhattisgarh, India

[b]Nanochemistry Laboratory, Department of Chemistry, Jamia Millia Islamia, New Delhi, Delhi (India) – 110025

[c]Department of Applied Chemistry, Faculty of Engineering and Technology, ZHCET, Aligarh Muslim University, Aligarh, UP (India) – 202002

[d]School of Advanced Materials Engineering, Kookmin University, Seoul 02707, South Korea

[e]Department of Pharmaceutics, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia.

[f]Department of Chemistry, College of Science, United Arab Emirates University, POBox 15551, Al Ain, United Arab Emirates.

[a] e-mail: kasiddiqui.chy@nitrr.ac.in

Table S1. Crystallographic and refinement data for the Co-MOF.

Identification code	Co-MOF
Empirical formula	$C_{24}H_{40}Co_3N_6O_{26}$
Formula weight	1005.41
Temperature/K	293(2)
Crystal system	monoclinic

Space group	$P2_1/n$
a/Å	11.88510(17)
b/Å	7.94529(11)
c/Å	21.6352(3)
α/°	90
β/°	93.4735(13)
γ/°	90
Volume/Å^3	2039.27(5)
Z	2
ρ_{calc}g/cm^3	1.6372
μ/mm^{-1}	1.304
F(000)	1032.8
Crystal size/mm^3	0.33 × 0.21 × 0.17
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.78 to 54.78
Index ranges	$-14 \leq h \leq 15$, $-10 \leq k \leq 10$, $-26 \leq l \leq 27$
Reflections collected	30888
Independent reflections	4410 [R_{int} = 0.0315, R_{sigma} = 0.0212]
Data/restraints/parameters	4410/2/301

Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0275, wR_2 = 0.0706
Final R indexes [all data]	R_1 = 0.0323, wR_2 = 0.0734
Largest diff. peak/hole / e $Å^{-3}$	0.52/-0.47
CCDC number	2524495

Table S2. Selected bond length between the atoms of **{[$Co_3(Tci)_2(\mu_2\text{-}H_2O)_2(H_2O)_4]\cdot 2H_2O\}_n$.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Co1	O2	1.9798(12)		O7	C11	1.270(2)
Co1	O2[1]	1.9798(12)		O8	C11	1.227(3)
Co1	O10	2.1410(13)		O9	C12	1.212(2)
Co1	O10[1]	2.1410(13)		N1	C3	1.469(2)
Co1	O11	2.1689(12)		N1	C4	1.375(2)
Co1	O11[1]	2.1689(12)		N1	C12	1.375(2)
Co2	O1	2.0541(13)		N2	C4	1.380(2)
Co2	O5[2]	2.0621(13)		N2	C5	1.471(2)
Co2	O10	2.1749(14)		N2	C8	1.377(2)
Co2	O11[1]	2.1825(13)		N3	C8	1.379(2)
Co2	O12	2.0592(15)		N3	C9	1.473(2)
Co2	O13	2.0930(15)		N3	C12	1.383(2)
O1	C1	1.253(2)		C1	C2	1.505(2)
O2	C1	1.257(2)		C2	C3	1.510(3)
O3	C4	1.211(2)		C5	C6	1.511(3)
O4	C7	1.257(2)		C6	C7	1.504(3)
O5	C7	1.258(2)		C9	C10	1.510(3)
O6	C8	1.211(2)		C10	C11	1.501(3)

[1]2-X,1-Y,1-Z; [2]1/2+X,3/2-Y,-1/2+Z; [3]-1/2+X,3/2-Y,1/2+Z

Table S3. Selected bond angels between the atoms of **{[$Co_3(Tci)_2(\mu_2\text{-}H_2O)_2(H_2O)_4]\cdot 2H_2O\}_n$.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O2[1]	Co1	O2	180.0		Co2[1]	O11	Co1[1]	95.28(5)
O10[1]	Co1	O2	88.61(6)		C4	N1	C3	117.11(14)
O10	Co1	O2	91.39(6)		C12	N1	C3	118.82(15)
O10	Co1	O2[1]	88.61(6)		C12	N1	C4	124.04(15)
O10[1]	Co1	O2[1]	91.39(6)		C5	N2	C4	116.83(14)
O10[1]	Co1	O10	180.0		C8	N2	C4	124.44(15)
O11	Co1	O2[1]	90.37(5)		C8	N2	C5	118.65(14)
O11	Co1	O2	89.63(5)		C9	N3	C8	118.20(14)
O11[1]	Co1	O2[1]	89.63(5)		C12	N3	C8	124.30(14)
O11[1]	Co1	O2	90.37(5)		C12	N3	C9	117.48(14)
O11[1]	Co1	O10	80.12(5)		O2	C1	O1	125.60(17)
O11	Co1	O10	99.88(5)		C2	C1	O1	118.26(17)
O11	Co1	O10[1]	80.12(5)		C2	C1	O2	116.14(16)
O11[1]	Co1	O10[1]	99.88(5)		C3	C2	C1	112.00(16)
O11[1]	Co1	O11	180.0		C2	C3	N1	111.96(15)
O5[2]	Co2	O1	178.28(5)		N1	C4	O3	122.05(17)
O10	Co2	O1	90.33(6)		N2	C4	O3	122.01(17)
O10	Co2	O5[2]	91.09(5)		N2	C4	N1	115.94(15)

O11[1]	Co2	O1	90.75(5)	C6	C5	N2	110.87(15)
O11[1]	Co2	O5[2]	88.56(5)	C7	C6	C5	112.74(16)
O11[1]	Co2	O10	79.08(5)	O5	C7	O4	124.37(16)
O12	Co2	O1	89.35(7)	C6	C7	O4	117.90(16)
O12	Co2	O5[2]	89.16(7)	C6	C7	O5	117.73(16)
O12	Co2	O10	175.59(6)	N2	C8	O6	122.34(16)
O12	Co2	O11[1]	96.53(6)	N3	C8	O6	122.33(16)
O13	Co2	O1	89.88(7)	N3	C8	N2	115.33(15)
O13	Co2	O5[2]	91.10(7)	C10	C9	N3	110.09(15)
O13	Co2	O10	90.05(6)	C11	C10	C9	112.78(16)
O13	Co2	O11[1]	169.11(6)	O8	C11	O7	124.81(19)
O13	Co2	O12	94.35(6)	C10	C11	O7	116.80(18)
C1	O1	Co2	129.15(12)	C10	C11	O8	118.36(19)
C1	O2	Co1[1]	132.62(12)	N1	C12	O9	122.42(17)
C7	O5	Co2[3]	126.50(12)	N3	C12	O9	121.74(16)
Co2	O10	Co1[1]	96.32(5)	N3	C12	N1	115.84(15)

Table S4 Solvent masks information for Co-MOF.

Number	**X**	**Y**	**Z**	**Volume**	**Electron count**	**Content**
1	0.000	-0.321	0.000	66.3	20.7	?
2	0.250	-0.399	0.750	52.3	18.2	?
3	0.500	-0.855	0.500	66.3	20.7	?
4	0.750	-0.384	0.250	52.3	18.2	?

Table S5. Crystallographic parameters of Co-MOF, 2θ, FWHM,s (D_p), interplanar spacing (d), and estimated number of crystalline layers (D/d)

Planes (hkl)	2θ ( )	θ ( )	FWHM ( )	b (rad)	θ (rad)	D_p (nm)	d-spacing (Å)	d-spacing (nm)	Layers (D/d)
(002)	8.22	4.11	0.20	0.0034	0.071	40.65	10.71	1.07	37.99
(101)	8.70	4.35	0.10	0.0017	0.075	81.32	10.24	1.02	79.72
(011)	11.86	5.93	0.10	0.0017	0.10	81.52	7.53	0.75	108.69
(110)	13.40	6.70	0.11	0.0019	0.11	74.22	6.66	0.66	112.45
(013)	16.60	8.30	0.09	0.0015	0.14	91.05	5.35	0.53	171.79
(202)	17.48	8.74	0.10	0.0017	0.15	82.04	5.14	0.51	160.86

(113)	18.51	9.25	0.13	0.0022	0.16	63.20	4.83	0.48	131.66
(014)	19.85	9.9	0.12	0.0020	0.17	68.60	4.52	0.45	152.44
(114)	21.59	10.78	0.12	0.0020	0.18	75.05	4.18	0.41	183.04
(312)	26.94	13.47	0.19	0.0033	0.23	43.89	3.33	0.33	133.00
(313)	28.66	14.33	0.14	0.0024	0.25	59.78	3.16	0.31	192.83
(404)	35.37	17.68	0.10	0.0017	0.30	85.11	2.51	0.25	340.44
Average crystalline size and Average no. of layers						**70.53**			**150.41**

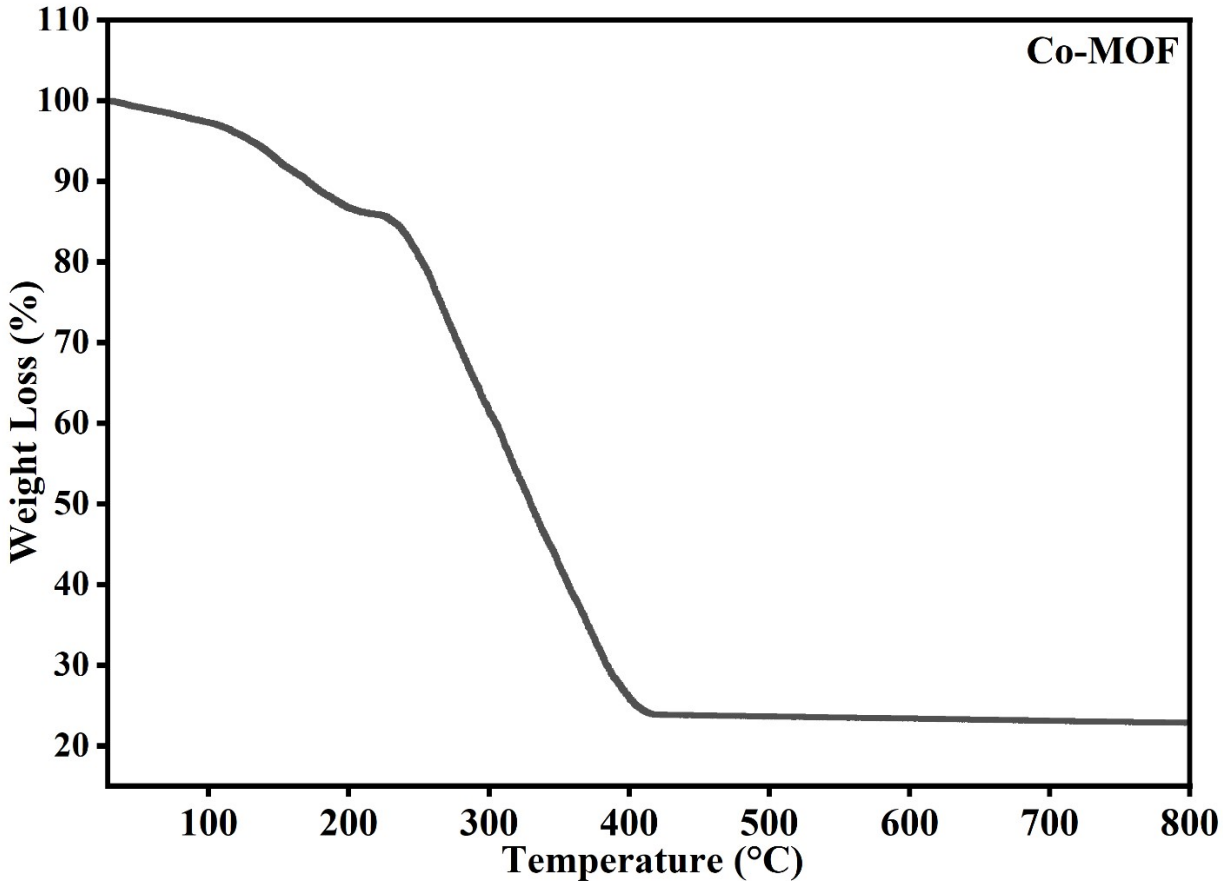

Fig. S1. Thermogravimetric curve of $\{[Co_3(Tci)_2(\mu_2\text{-}H_2O)_2(H_2O)_4]\cdot 2H_2O\}_n$, showing dehydration and subsequent ligand decomposition.

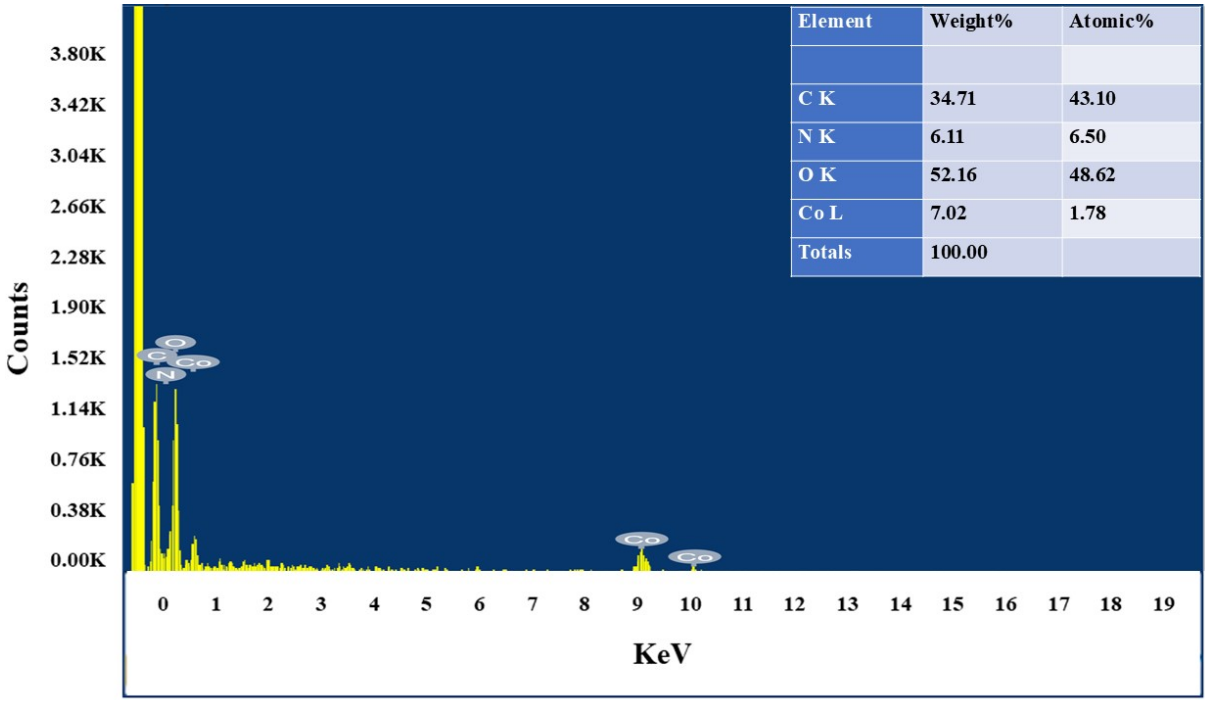

Fig. S2. The EDX spectrum of Co-MOF confirmed the presence and composition of C, N, O, and Co.

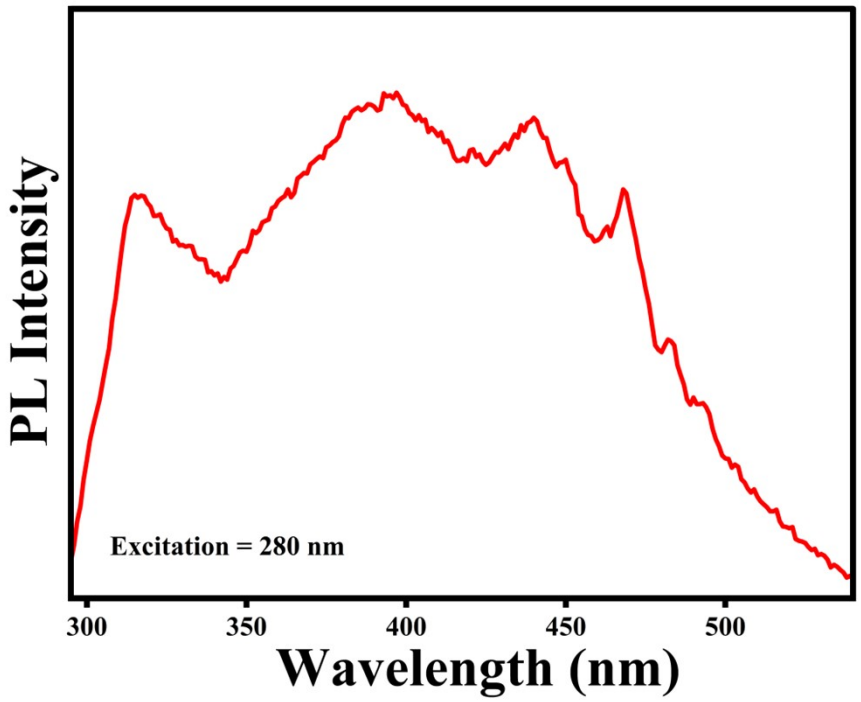

Fig.S3. Photoluminescence spectra of Co-MOF with excitation at 280 nm.

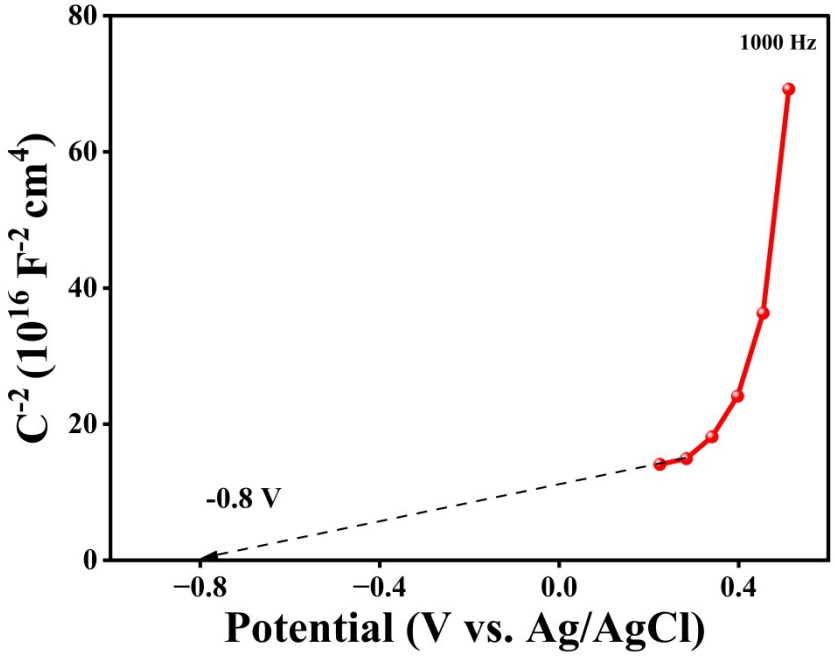

Fig. S4. Mott-Schottky curve of Co-MOF

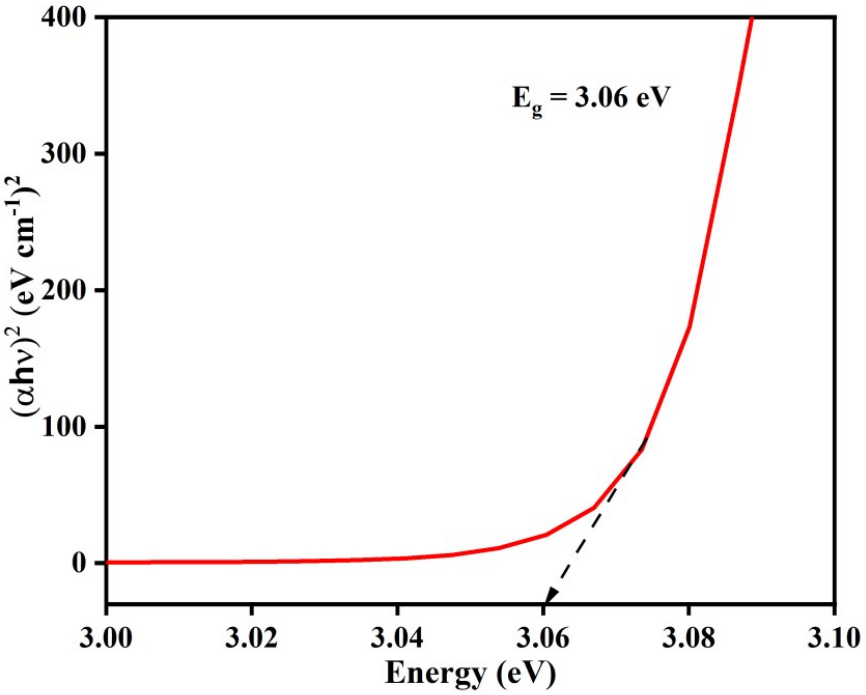

Fig. S5. UV-DRS spectra of Co-MOF

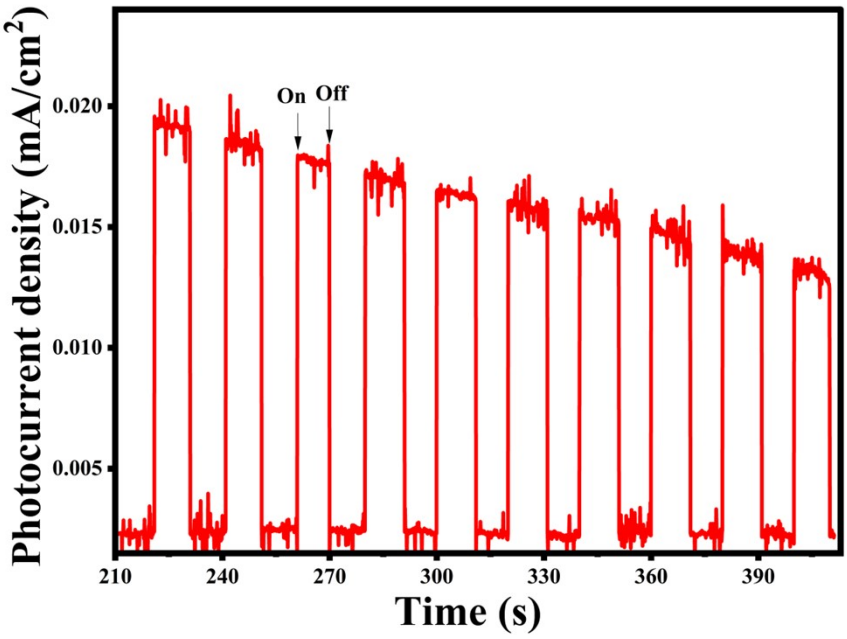

Fig. S6. Transient photocurrent response of Co-MOF

Table S6. Comparative analysis of as-synthesised catalysts.

Catalysts	Photocatalytic H_2 evolution	Light source	Tafel slope (mV/dec)		Ref.
			EC	**PEC**	
Co-MOF	6.03 mmol $h^{-1}g^{-1}$	200 W Xenon Lamp	107.5	86	This work
CIZS/Ni-MOF	2.64 mmol $h^{-1}g^{-1}$	300 W Xenon Lamp	-	-	1
$ZnIn_2S_4$@Ni-MOF-74	1.823 mmol $h^{-1}g^{-1}$	300 W Xenon Lamp	-	-	2
CuCoNi-	-	-	116.1	-	3

LTH/Cu-BTC/CF					
Co-MOF@Zn-800	-	-	146.6	-	4
Co/NC@PMDA	-	-	135.3	-	5

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