Bifunctional Cu(II)-based 2D Coordination Polymer and its Composite for High Performance Electrochemical Energy Storage Application

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Table S1. Crystal data and structure refinement for CP-1.	
CCDC NO.	**2165040**
Identification code	CP-1
Empirical formula	$C_9H_{11}ClCu_2O_{10}$
Formula weight	441.726
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	*Cmce*
a/Å	28.8070(12)
b/Å	28.1264(12)
c/Å	7.3819(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	5981.1(4)
Z	16
ρ_{calc}g/cm^3	1.962

μ/mm^{-1}	3.069
F(000)	3535.9
Crystal size/mm^3	0.53 × 0.27 × 0.19
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.66 to 56.58
Index ranges	-38 ≤ h ≤ 38, -37 ≤ k ≤ 37, -9 ≤ l ≤ 9
Reflections collected	44702
Independent reflections	3789 [R_{int} = 0.0560, R_{sigma} = 0.0229]
Data/restraints/parameters	3789/0/204
Goodness-of-fit on F^2	1.090
Final R indexes [I>=2σ (I)]	R_1 = 0.0555, wR_2 = 0.1406
Final R indexes [all data]	R_1 = 0.0692, wR_2 = 0.1534
Largest diff. peak/hole / e Å^{-3}	1.40/-1.23

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for CP-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	6780.8(3)	661.5(3)	2718.0(10)	12.3(2)
Cu2	5721.8(2)	3160.2(2)	2899.3(9)	8.8(2)
Cl1	7500	45.7(7)	2500	11.8(4)
Cl2	5000	2547.7(7)	2885(3)	8.3(4)
O1	7130.0(16)	1255.0(16)	2981(8)	24.4(11)
O2	6263.0(13)	2721.2(14)	2847(6)	9.3(8)
O3	6615.3(15)	3426.0(15)	2797(6)	14.0(9)
O4	6742.0(18)	648.1(18)	5403(7)	24.5(11)
O5	6789.9(18)	687.8(19)	13(8)	29.1(12)
O6	5742.1(18)	3158.8(18)	5593(6)	24.1(10)
O7	5736.1(18)	3172.0(19)	188(7)	26.6(11)
O8	5385.3(17)	3766.0(16)	2948(8)	25.6(12)
O9	6239.8(15)	5227.2(15)	2428(6)	13.2(9)
O10	5885.9(15)	5930.2(15)	2201(6)	13.6(9)
C1	7500	1450(3)	2500	10.3(16)
C2	7500	1984(3)	2500	7.7(15)
C3	7086(2)	2229(2)	2664(7)	7.5(11)
C4	7081.8(19)	2725.1(19)	2656(7)	7.3(10)
C5	7500	2976(3)	2500	6.7(8)
C6	6628(2)	2984(2)	2792(8)	10.6(11)
C7	5000	3956(3)	2850(10)	7.7(14)
C8	5000	4487(3)	2697(10)	6.7(8)

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for CP-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C9	5416.3(19)	4736(2)	2606(7)	9.4(10)
C10	5419(2)	5233(2)	2428(7)	7.3(11)
C11	5875(2)	5489(2)	2335(8)	11.4(11)
C12	5000	5476(3)	2340(10)	6.7(8)

Table S3. Anisotropic Displacement Parameters (Å^2×10^3) for CP-1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu1	7.5(3)	7.3(4)	22.1(4)	-1.5(3)	1.4(3)	1.5(3)
Cu2	6.3(3)	6.1(3)	14.0(4)	1.6(3)	-0.2(2)	0.5(2)
Cl1	9.8(9)	9.5(9)	16.1(10)	-0	0.8(7)	0
Cl2	7.1(8)	7.2(8)	10.5(8)	-0	-0	-1.1(6)
O1	13(2)	7(2)	52(3)	-4.8(18)	11(2)	-3(2)
O2	4.5(18)	7.7(19)	16(2)	0.6(15)	2.8(14)	-3.0(15)
O3	11(2)	8(2)	23(2)	3.7(16)	-0.9(17)	-0.4(16)
O4	26(3)	21(2)	27(3)	-1(2)	0(2)	-2(2)
O5	25(3)	22(3)	41(3)	3(2)	4(2)	6(2)
O6	28(3)	22(2)	23(2)	-2(2)	2(2)	-3.1(19)
O7	26(3)	26(3)	28(3)	-8(2)	-8(2)	6(2)
O8	14(2)	7(2)	56(4)	2.2(18)	-1(2)	2(2)
O9	9(2)	10(2)	21(2)	-1.6(17)	1.1(16)	0.8(16)
O10	12(2)	6(2)	22(2)	0.4(17)	-1.0(17)	0.6(16)
C1	15(4)	4(4)	12(4)	-0	0(3)	0
C2	7(4)	6(4)	10(4)	-0	1(3)	0
C3	6(3)	9(3)	8(2)	-1(2)	0.7(19)	-1.5(19)
C4	7(2)	10(3)	5(2)	1(2)	1.3(18)	-0.7(18)
C5	11.2(19)	5.8(18)	3.1(19)	-0	1(3)	0
C6	9(3)	7(3)	16(3)	3(2)	3(2)	-1(2)
C7	8(4)	7(3)	8(3)	-0	-0	0(3)
C8	11.2(19)	5.8(18)	3.1(19)	-0	1(3)	0
C9	8(2)	13(3)	6(2)	3(2)	-0.8(18)	-0.1(19)
C10	6(3)	9(3)	8(2)	-3(2)	0.5(18)	-1.1(19)
C11	6(3)	11(3)	18(3)	-2(2)	3(2)	-1(2)
C12	11.2(19)	5.8(18)	3.1(19)	-0	1(3)	0

Table S4. Bond Lengths for CP-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	Cl1[1]	2.7053(15)	O9	C11	1.283(7)
Cu1	O1	1.959(5)	O10	C11	1.246(7)
Cu1	O4	1.985(5)	C1	C2	1.500(11)
Cu1	O5	1.998(6)	C2	C3	1.382(7)
Cu1	O9[2]	1.983(4)	C2	C3[1]	1.382(7)
Cu2	Cl2[3]	2.7004(14)	C3	C4	1.397(7)
Cu2	O2	1.989(4)	C4	C5[1]	1.401(7)
Cu2	O6	1.989(5)	C4	C6	1.499(7)
Cu2	O7	2.002(5)	C7	C8	1.498(10)
Cu2	O8	1.960(5)	C8	C9[3]	1.390(7)
O1	C1[1]	1.251(6)	C8	C9	1.390(7)
O2	C6	1.287(7)	C9	C10	1.403(8)
O3	C6	1.244(7)	C10	C11	1.500(8)
O8	C7[3]	1.234(6)	C10	C12	1.389(7)

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

Table S5. Bond Angles for CP-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Cu1	Cl1[1]	99.10(15)	C2	C1	O1[1]	116.1(4)
O4	Cu1	Cl1[1]	95.18(15)	C2	C1	O1	116.1(4)
O4	Cu1	O1	86.9(2)	C3[1]	C2	C1	119.9(4)
O5	Cu1	Cl1[1]	87.37(15)	C3	C2	C1	119.9(4)
O5	Cu1	O1	93.5(2)	C3	C2	C3[1]	120.3(8)
O5	Cu1	O4	177.3(2)	C4	C3	C2[1]	120.3(6)
O9[2]	Cu1	Cl1[1]	101.79(13)	C5[1]	C4	C3	119.7(5)
O9[2]	Cu1	O1	159.07(19)	C6	C4	C3	119.6(5)
O9[2]	Cu1	O4	89.9(2)	C6	C4	C5[1]	120.7(5)
O9[2]	Cu1	O5	88.8(2)	C4	C5	C4[1]	119.6(7)
O2	Cu2	Cl2[3]	101.97(12)	O3	C6	O2	123.3(5)
O6	Cu2	Cl2[3]	91.45(15)	C4	C6	O2	115.8(5)
O6	Cu2	O2	89.7(2)	C4	C6	O3	120.8(5)
O7	Cu2	Cl2[3]	91.28(16)	O8	C7	O8[3]	128.1(8)
O7	Cu2	O2	88.6(2)	C8	C7	O8[3]	115.9(4)
O7	Cu2	O6	177.0(2)	C8	C7	O8	115.9(4)
O8	Cu2	Cl2[3]	100.00(15)	C9[3]	C8	C7	120.4(4)
O8	Cu2	O2	158.03(18)	C9	C8	C7	120.4(4)
O8	Cu2	O6	89.9(2)	C9	C8	C9[3]	119.2(7)

Table S5. Bond Angles for CP-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O8	Cu2	O7	90.8(2)	C10	C9	C8[3]	120.7(5)
Cu1	Cl1	Cu1[1]	100.38(7)	C11	C10	C9	119.1(5)
Cu2	Cl2	Cu2[3]	100.71(7)	C12	C10	C9	119.4(6)
C1[1]	O1	Cu1	141.7(5)	C12	C10	C11	121.5(5)
C6	O2	Cu2	106.6(3)	O10	C11	O9	123.7(6)
C7[3]	O8	Cu2	145.1(5)	C10	C11	O9	116.1(5)
C11	O9	Cu1[4]	106.7(4)	C10	C11	O10	120.2(5)
O1	C1	O1[1]	127.9(8)	C10[3]	C12	C10	120.7(7)

[1]3/2-X,+Y,1/2-Z; [2]+X,-1/2+Y,1/2-Z; [3]1-X,+Y,+Z; [4]+X,1/2+Y,1/2-Z

Table S6. Apparent rate constant (kapp), half-life time of reaction rate ($t_{1/2}$), and corresponding correlation factor (R^2) for degradation of MR dye over a CP-1 catalyst, an obtained value from the Langmuir Hinshelwood rate equation.

CP-1			
Parameters→ Catalyst amount↓	**k_{app}** (min^{-1})	**$t_{1/2}$** (min^{-1})	**R^2**
5 mg	0.03465	20	0.928
10 mg	0.03773	18.36	0.946
20 mg	0.06571	10.54	0.944

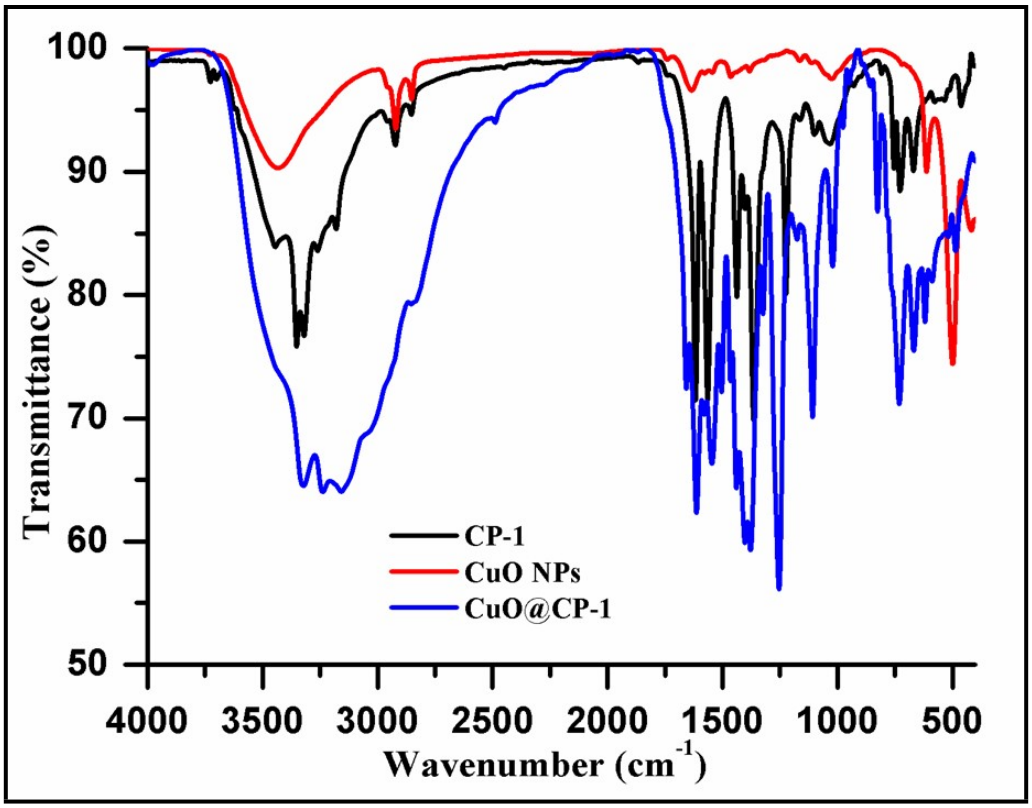
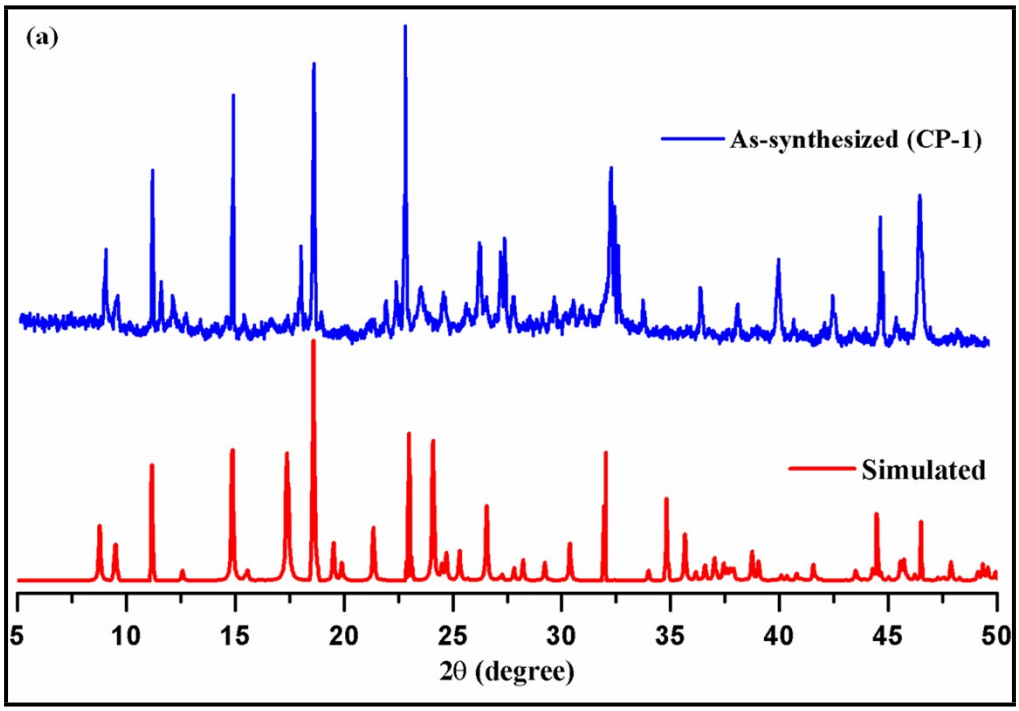


Figure S1. FTIR spectra of CP-**1**, CuO NPs and CuO@CP-**1**.



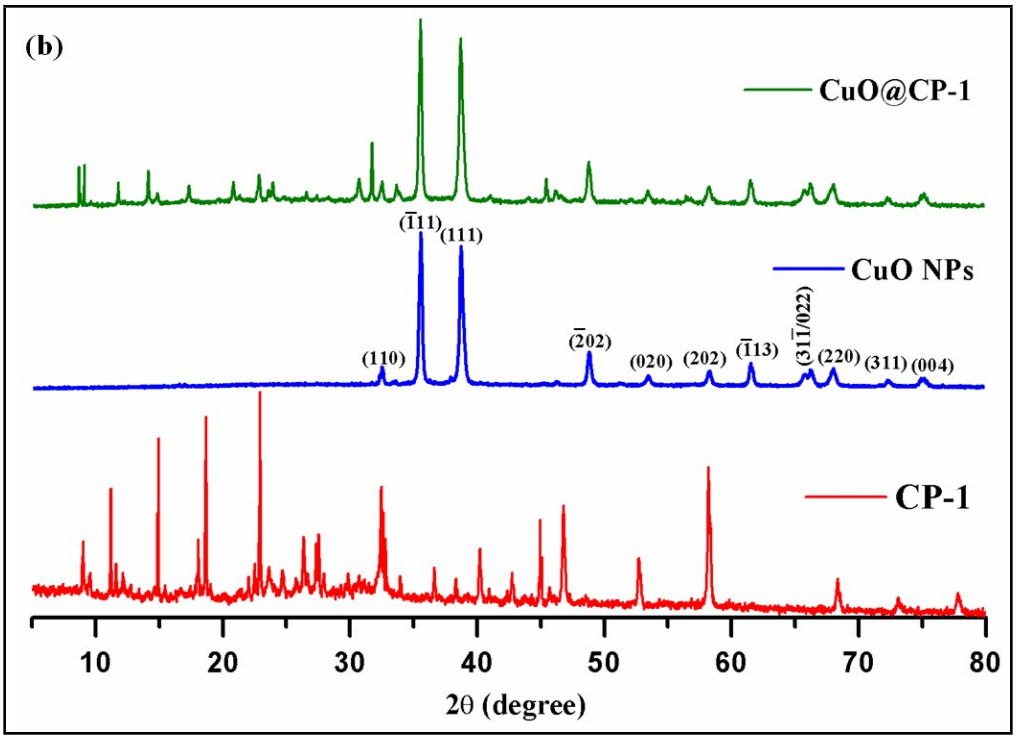


Figure S2. PXRD patterns (a) simulated of CP-**1**, as-synthesized CP-**1**, (b) As-synthesized CP-**1,** CuO NPs and CuO@CP-**1**.

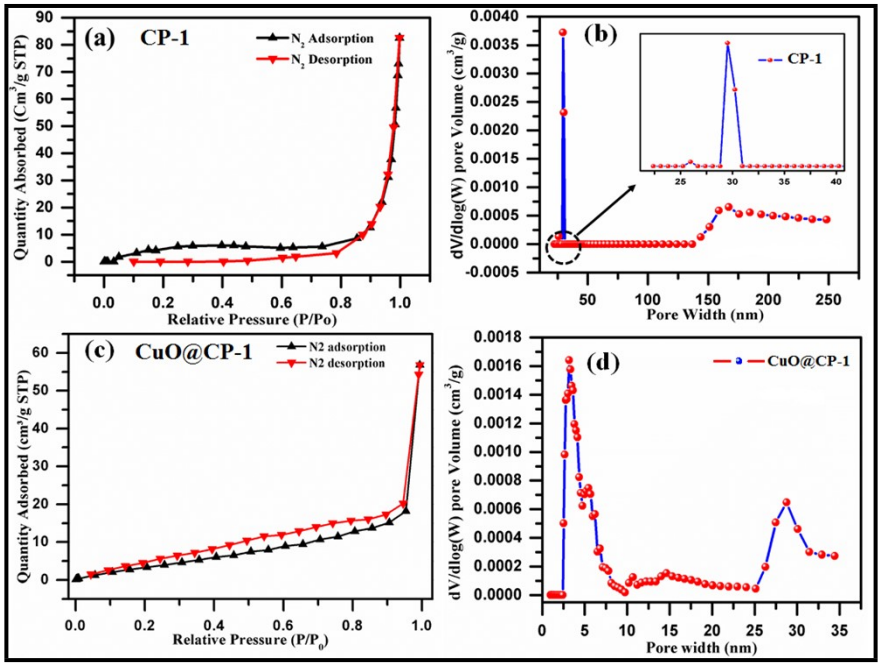


Figure S3. BET adsorption-desorption isotherm and BJH pore width distribution of N2 at 77k: (a, b) for CP-**1**, and (c, d) for CuO@CP-**1**.

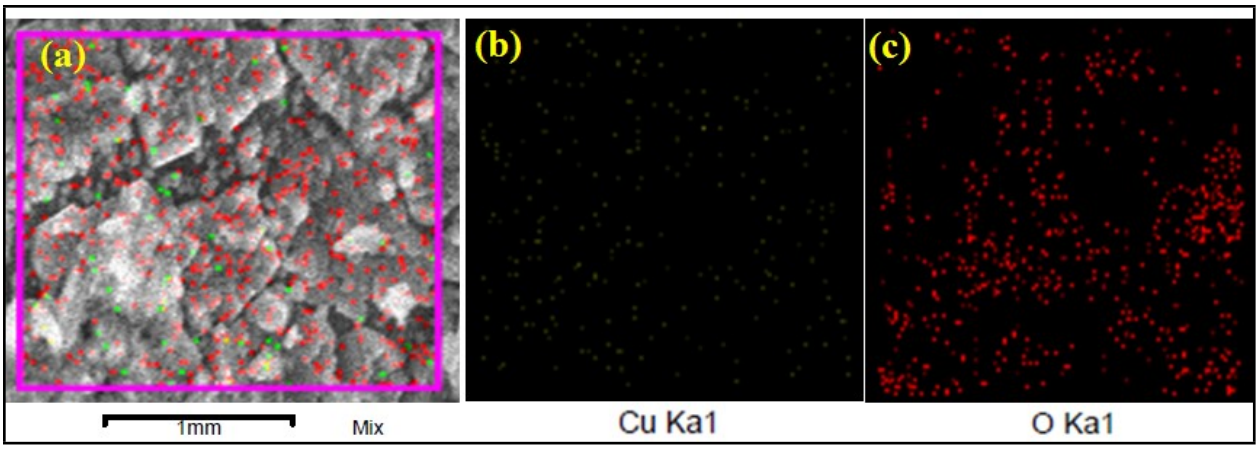


Figure S4. SEM images of CuO NPs on 1mm mixed selective area for elemental mapping (a-c).

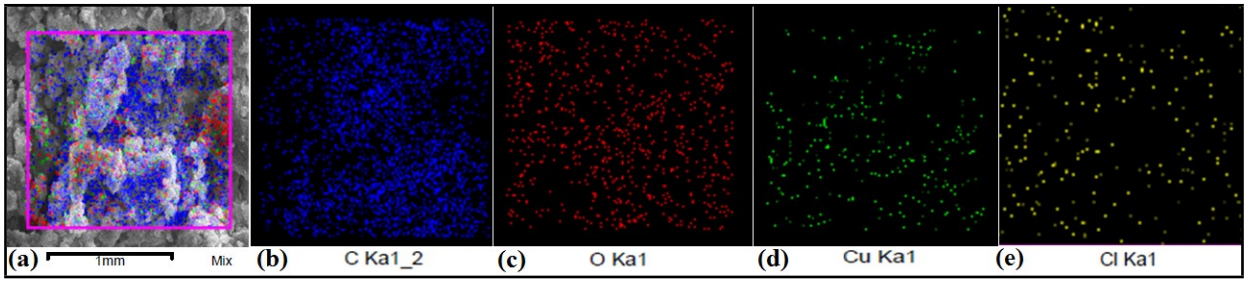


Figure S5. SEM images of CuO@CP-1 on 1mm mixed selective area for elemental mapping (a-e).

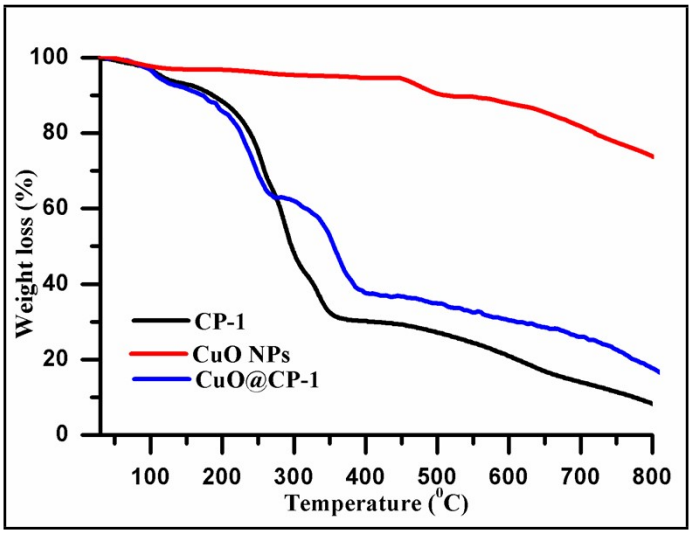


Figure S6. Thermogravimetric curves of as-synthesized coordination polymer (CP-**1**), nanoparticle (CuO) and composite (CuO@CP-**1**).

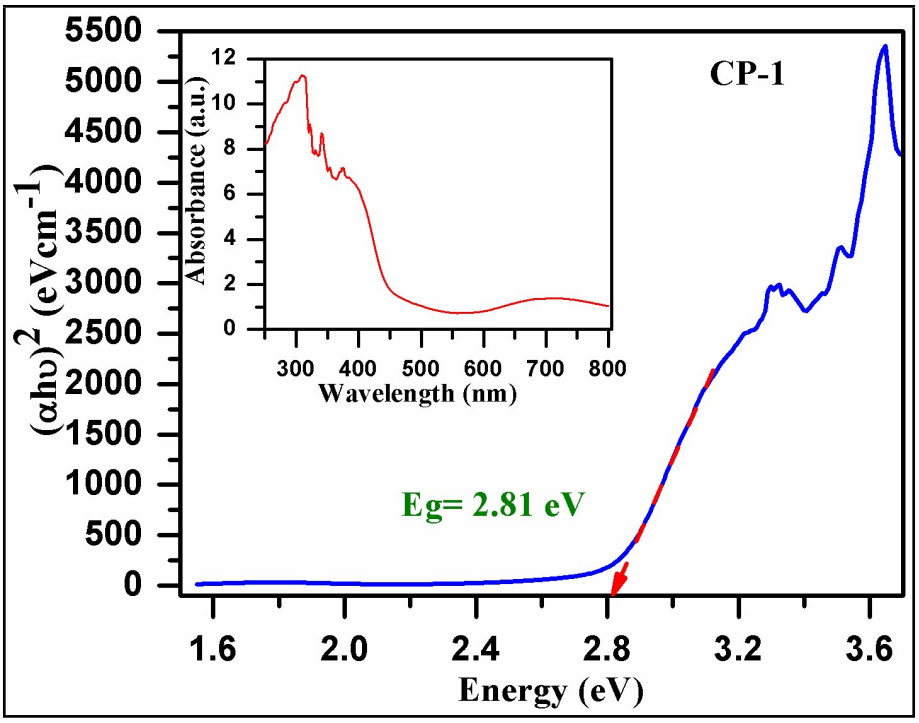


Figure S7. The experimental optical band gap of as-synthesized CP-**1**.

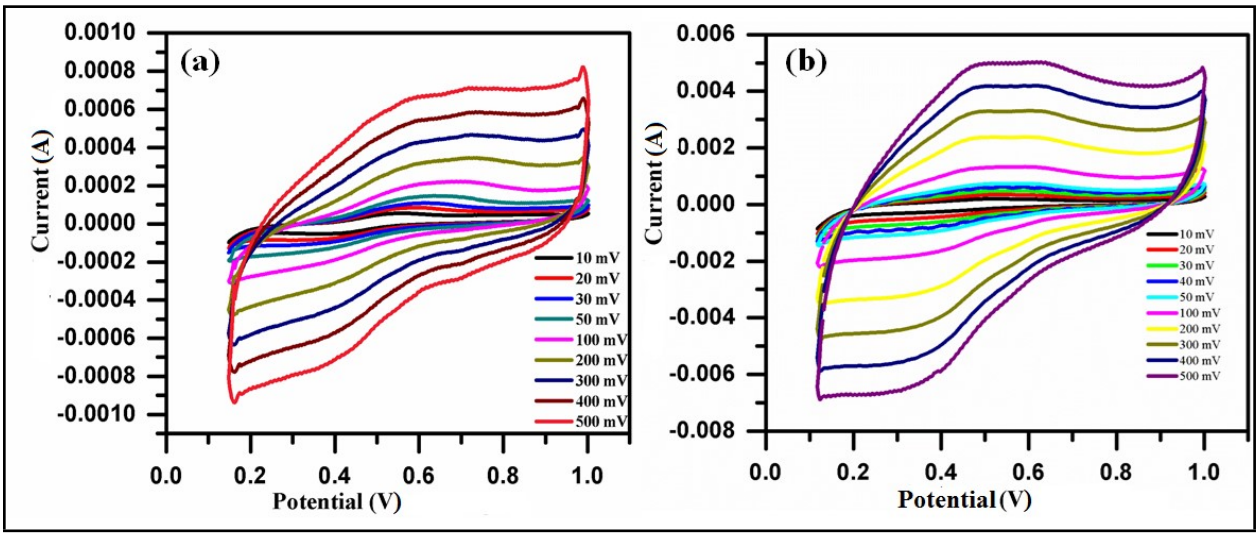


Figure S8. CV profiles of (a) CuO NPs, and (b) composite at different scan rates from 10-500 mVs^{-1}.

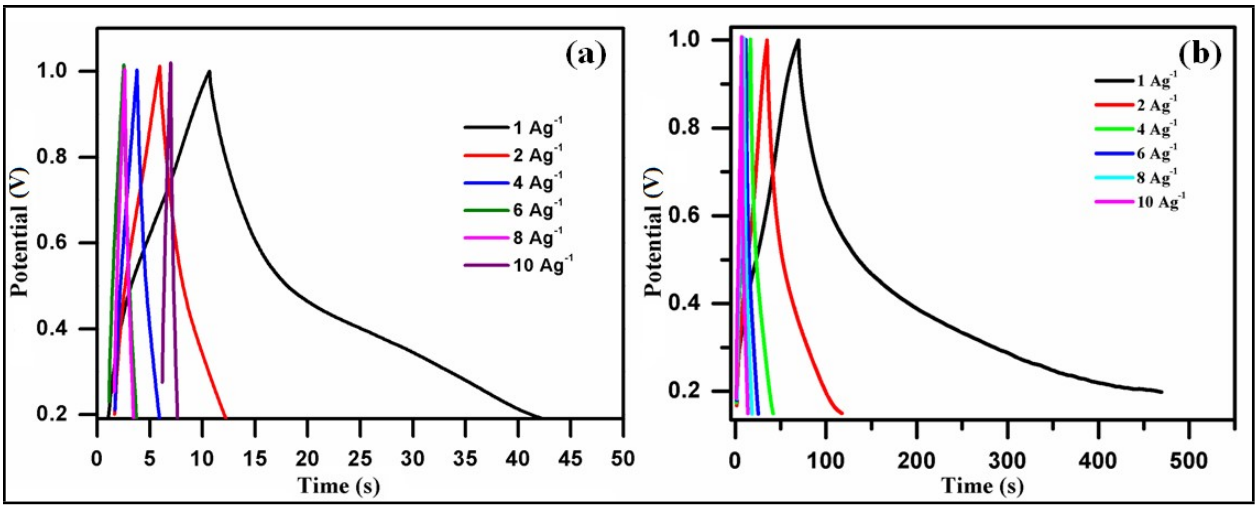


Figure S9. CD profiles of (a) CuO NPs, and (b) composite at different current density ranging from 1-10 A g^{-1}.

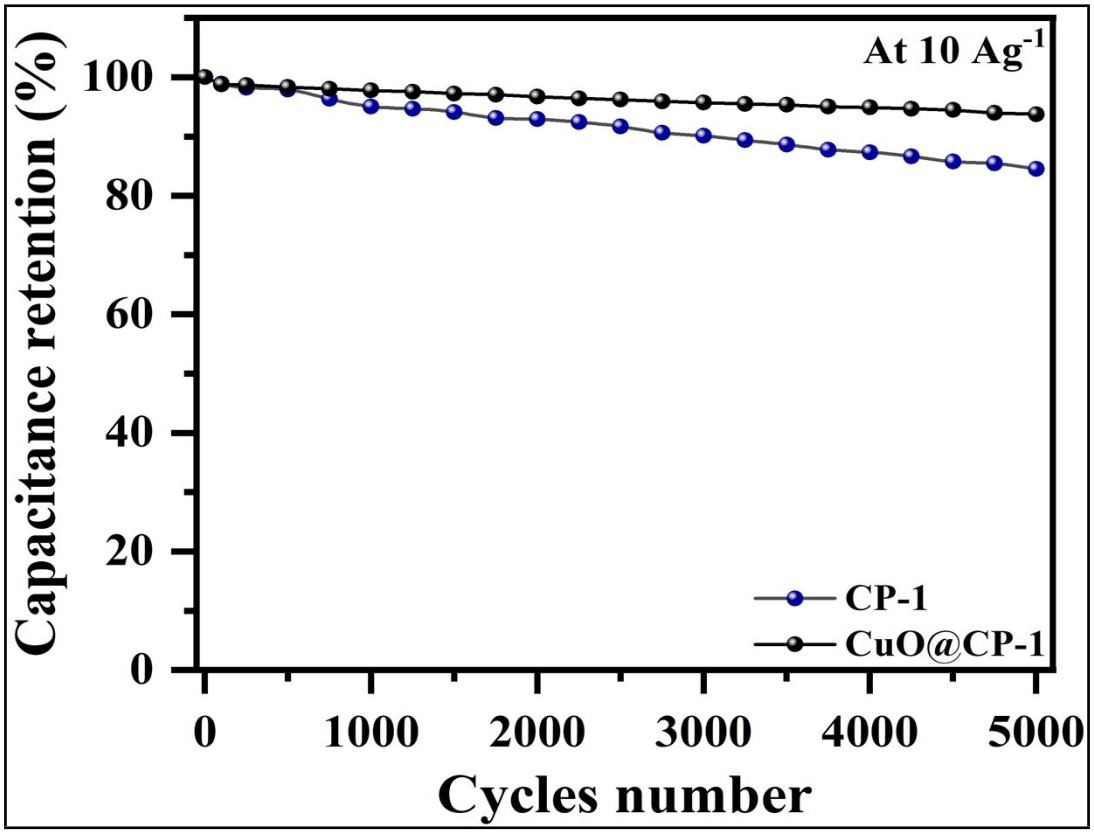


Figure S10. Cyclic stability of CP-**1**, CuO@CP-**1** up to 5000 charge-discharge cycles at 10 A g^{-1}.

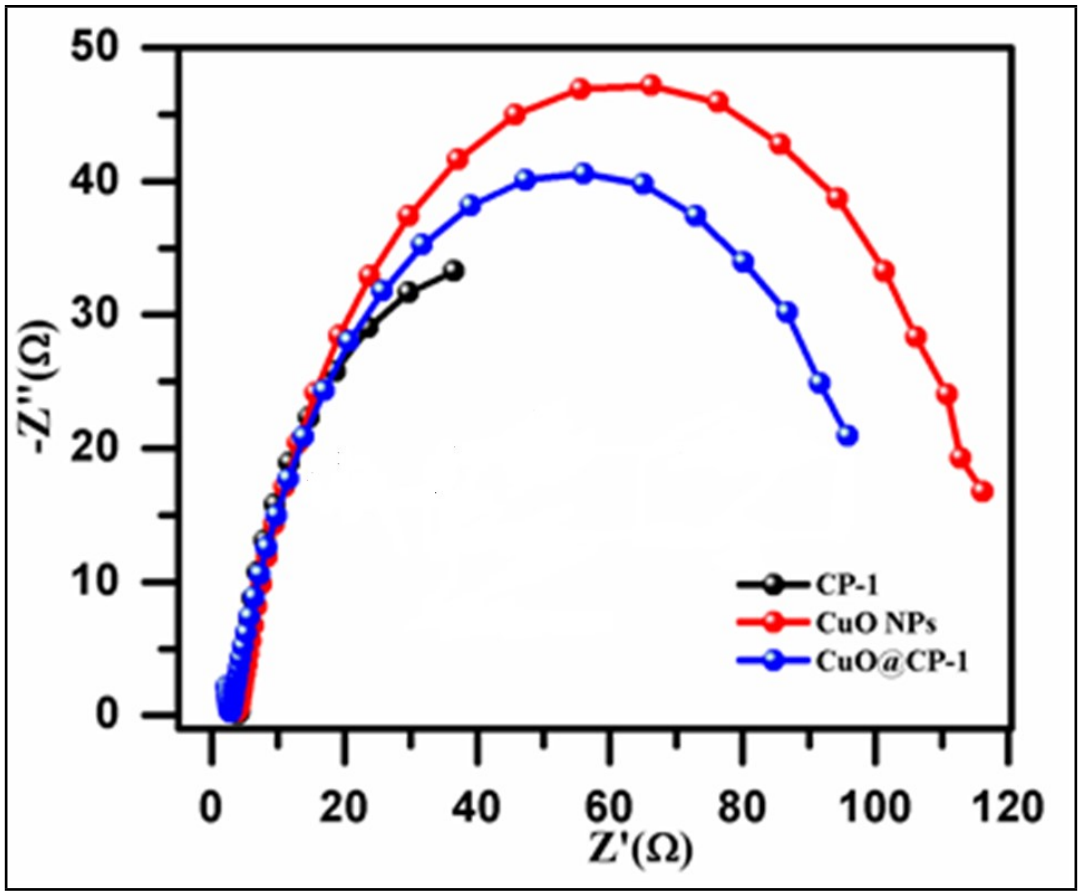


Figure S11. Nyquist plot of CP-**1**, CuO NPs and CuO@CP-**1** electrode materials.

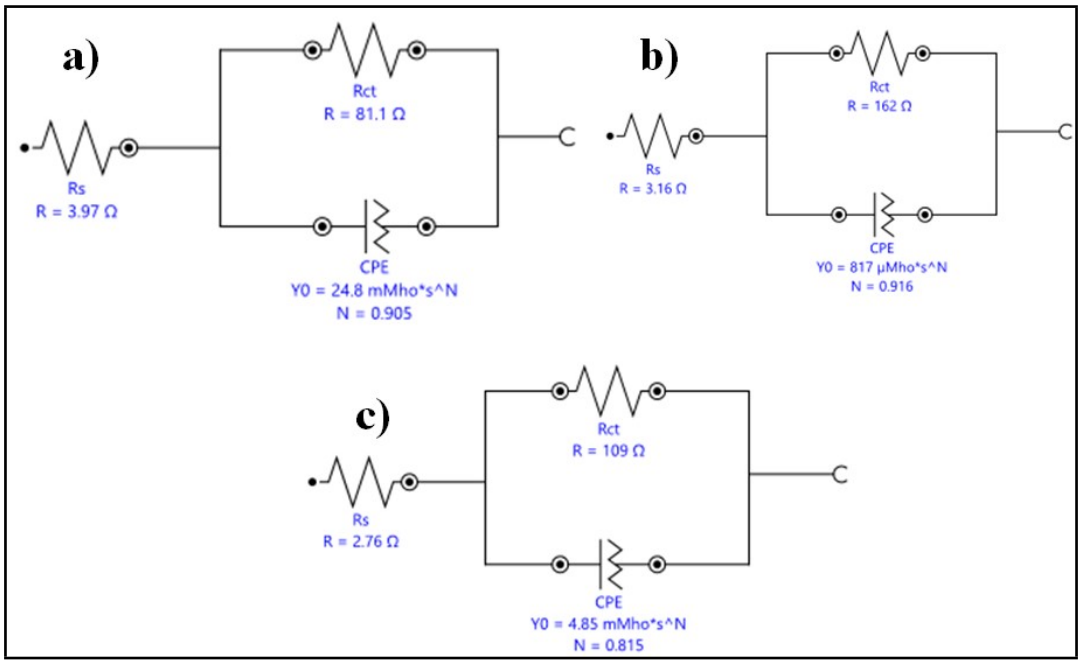


Figure S12: Equivalent circuits of the fabricated electrodes (a) CP-**1**, (b) CuO NPs (c) CuO@CP-1.

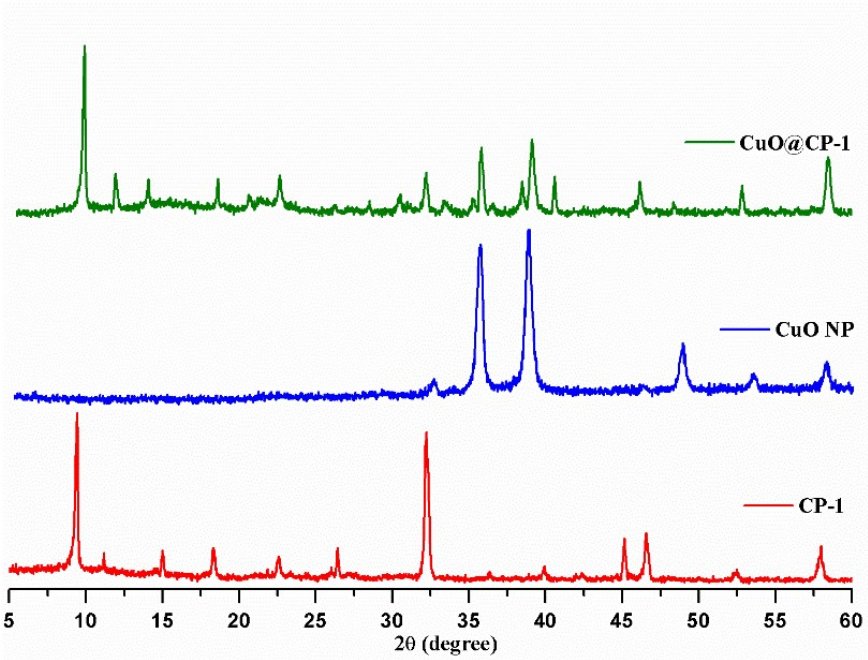


Figure S13: PXRD pattern (after electrochemical study) of CP-1, CuO NPs, and CuO@CP-1 electrode materials.

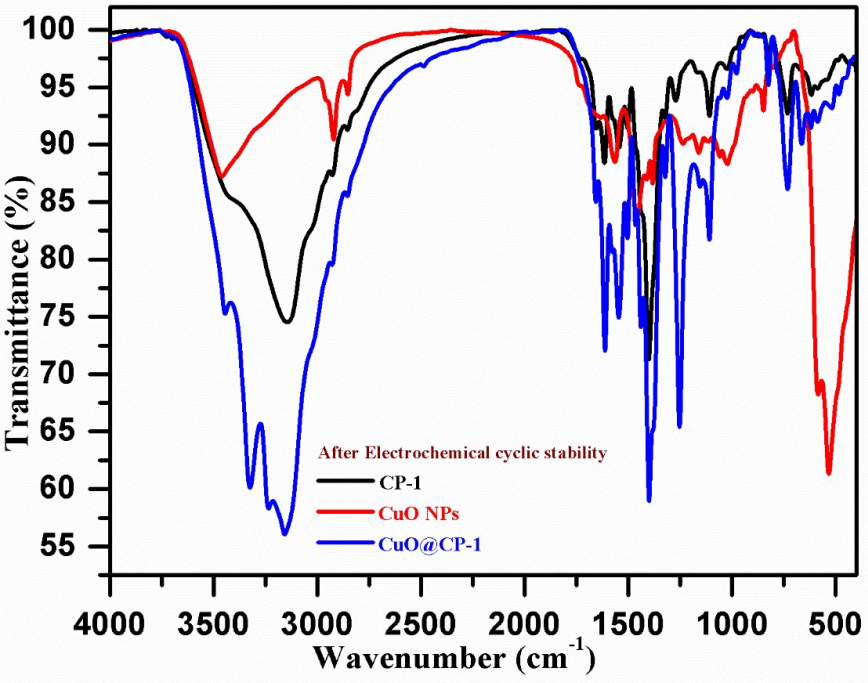


Figure S14: FTIR spectra (after electrochemical study) of CP-1, CuO NPs, and CuO@CP-1 electrode materials.