Dual Functional Cu(II)-CP and its rGO Composite for Selective Solvents Detection and High Performance Energy Storage

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Table S1. Crystal data and structure refinement for CP-1.

CCDC NO.	**2314704**
Identification code	CP-1
Empirical formula	$C_{78}H_{94}Cu_2N_{16}O_{17}$
Formula weight	1654.80
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.03413(11)
b/Å	10.81849(13)
c/Å	21.7385(2)
α/°	76.2238(10)
β/°	85.3859(9)
γ/°	63.0175(12)
Volume/Å^3	2041.39(5)
Z	1
ρ_{calc}g/cm^3	1.3460
μ/mm^{-1}	0.597
F(000)	869.1
Crystal size/mm^3	0.38 × 0.23 × 0.19
Radiation	Mo Kα (λ = 0.71073)

2Θ range for data collection/°	3.86 to 54.82
Index ranges	$-12 \leq h \leq 12$, $-13 \leq k \leq 13$, $-27 \leq l \leq 27$
Reflections collected	61154
Independent reflections	8854 [$R_{int} = 0.0351$, $R_{sigma} = 0.0280$]
Data/restraints/parameters	8854/0/541
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	$R_1 = 0.0541$, $wR_2 = 0.1722$
Final R indexes [all data]	$R_1 = 0.0718$, $wR_2 = 0.1890$
Largest diff. peak/hole / e $Å^{-3}$	0.73/-0.50

Table S2 Bond Lengths for CP-1

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O2	2.080(2)	C15	C16	1.380(4)
Cu1	O2[1]	2.080(2)	C16	C17	1.388(4)
Cu1	N1[1]	2.144(2)	C16	C19	1.507(4)
Cu1	N1	2.144(2)	C17	C18	1.377(4)
Cu1	N4	2.184(2)	C19	C20	1.525(4)
Cu1	N4[1]	2.184(2)	C20	C21	1.544(4)
Cu2	O1[2]	2.083(2)	C21	C22	1.507(4)
Cu2	O1	2.083(2)	C22	C23	1.376(4)
Cu2	N2	2.184(2)	C22	C26	1.375(4)
Cu2	N2[2]	2.184(2)	C23	C24	1.385(4)
Cu2	N3[2]	2.138(2)	C25	C26	1.373(4)
Cu2	N3	2.138(2)	O3	N7	1.214(6)
N1	C1	1.338(3)	O4	N7	1.172(5)
N1	C5	1.343(4)	O5	N7	1.191(5)
N2	C11	1.336(4)	O6	N8	1.200(4)
N2	C12	1.338(4)	O7	N8	1.214(4)
N3	C14	1.333(3)	O8	N8	1.236(5)
N3	C18	1.341(3)	N5	C27	1.339(5)
N4	C24	1.330(4)	N5	C31	1.315(5)
N4	C25	1.340(4)	N6	C37	1.324(5)
C1	C2	1.384(4)	N6	C38	1.326(5)
C2	C3	1.391(5)	C27	C28	1.382(5)
C3	C4	1.378(4)	C28	C29	1.372(5)
C3	C6	1.499(4)	C29	C30	1.385(5)
C4	C5	1.377(4)	C29	C32	1.501(4)
C6	C7	1.512(4)	C30	C31	1.402(5)
C7	C8	1.547(4)	C32	C33	1.527(5)

C8	C9	1.508(4)	C33	C34	1.529(5)
C9	C10	1.376(4)	C34	C35	1.497(4)
C9	C13	1.385(4)	C35	C36	1.382(4)
C10	C11	1.377(4)	C35	C39	1.387(4)
C12	C13	1.371(4)	C36	C37	1.384(5)
C14	C15	1.388(4)	C38	C39	1.366(5)

[1]1-X,1-Y,-Z; [2]-X,1-Y,1-Z

Table S3 Bond Angles for CP-1

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2[1]	Cu1	O2	180.0	C9	C8	C7	111.1(2)
N1[1]	Cu1	O2	87.24(10)	C10	C9	C8	122.5(3)
N1	Cu1	O2	92.76(10)	C13	C9	C8	121.2(3)
N1	Cu1	O2[1]	87.24(10)	C13	C9	C10	116.2(3)
N1[1]	Cu1	O2[1]	92.76(10)	C11	C10	C9	120.1(3)
N1[1]	Cu1	N1	180.0	C10	C11	N2	123.9(3)
N4	Cu1	O2[1]	89.24(9)	C13	C12	N2	123.7(3)
N4	Cu1	O2	90.76(9)	C12	C13	C9	120.3(3)
N4[1]	Cu1	O2[1]	90.76(9)	C15	C14	N3	123.1(3)
N4[1]	Cu1	O2	89.24(9)	C16	C15	C14	120.1(3)
N4[1]	Cu1	N1	90.03(8)	C17	C16	C15	116.7(2)
N4[1]	Cu1	N1[1]	89.97(8)	C19	C16	C15	122.2(3)
N4	Cu1	N1	89.97(8)	C19	C16	C17	121.0(3)
N4	Cu1	N1[1]	90.03(8)	C18	C17	C16	119.7(3)
N4[1]	Cu1	N4	180.0	C17	C18	N3	123.7(3)
O1[2]	Cu2	O1	180.0	C20	C19	C16	111.1(2)
N2	Cu2	O1	89.06(9)	C21	C20	C19	113.2(2)
N2	Cu2	O1[2]	90.94(9)	C22	C21	C20	111.7(2)
N2[2]	Cu2	O1	90.94(9)	C23	C22	C21	121.9(3)
N2[2]	Cu2	O1[2]	89.06(9)	C26	C22	C21	121.9(3)
N2[2]	Cu2	N2	180.0	C26	C22	C23	116.2(2)
N3	Cu2	O1[2]	91.73(10)	C24	C23	C22	119.9(3)
N3[2]	Cu2	O1[2]	88.27(10)	C23	C24	N4	123.7(3)
N3[2]	Cu2	O1	91.73(10)	C26	C25	N4	123.5(3)
N3	Cu2	O1	88.27(10)	C25	C26	C22	120.5(3)
N3[2]	Cu2	N2	93.15(8)	O4	N7	O3	122.6(7)
N3[2]	Cu2	N2[2]	86.85(8)	O5	N7	O3	112.5(5)
N3	Cu2	N2[2]	93.15(8)	O5	N7	O4	124.5(6)
N3	Cu2	N2	86.85(8)	O7	N8	O6	123.9(4)
N3	Cu2	N3[2]	180.0	O8	N8	O6	118.1(4)

C1	N1	Cu1[1]	125.40(19)	O8	N8	O7	117.8(4)
C5	N1	Cu1[1]	118.27(17)	C31	N5	C27	116.7(3)
C5	N1	C1	116.0(2)	C38	N6	C37	115.8(3)
C11	N2	Cu2	125.03(19)	C28	C27	N5	123.0(4)
C12	N2	Cu2	117.96(18)	C29	C28	C27	120.3(3)
C12	N2	C11	115.7(2)	C30	C29	C28	117.4(3)
C14	N3	Cu2[2]	122.17(18)	C32	C29	C28	123.4(3)
C18	N3	Cu2[2]	121.15(18)	C32	C29	C30	119.2(3)
C18	N3	C14	116.7(2)	C31	C30	C29	118.3(3)
C24	N4	Cu1	120.98(18)	C30	C31	N5	124.3(3)
C25	N4	Cu1	121.91(19)	C33	C32	C29	112.1(3)
C25	N4	C24	115.6(2)	C34	C33	C32	112.6(3)
C2	C1	N1	123.6(3)	C35	C34	C33	112.9(3)
C3	C2	C1	119.8(3)	C36	C35	C34	123.4(3)
C4	C3	C2	116.5(3)	C39	C35	C34	120.5(3)
C6	C3	C2	122.0(3)	C39	C35	C36	116.1(3)
C6	C3	C4	121.5(3)	C37	C36	C35	120.1(3)
C5	C4	C3	120.2(3)	C36	C37	N6	123.5(3)
C4	C5	N1	123.7(3)	C39	C38	N6	125.0(3)
C7	C6	C3	113.2(3)	C38	C39	C35	119.4(3)
C8	C7	C6	112.5(3)				

[1]1-X,1-Y,-Z; [2]-X,1-Y,1-Z

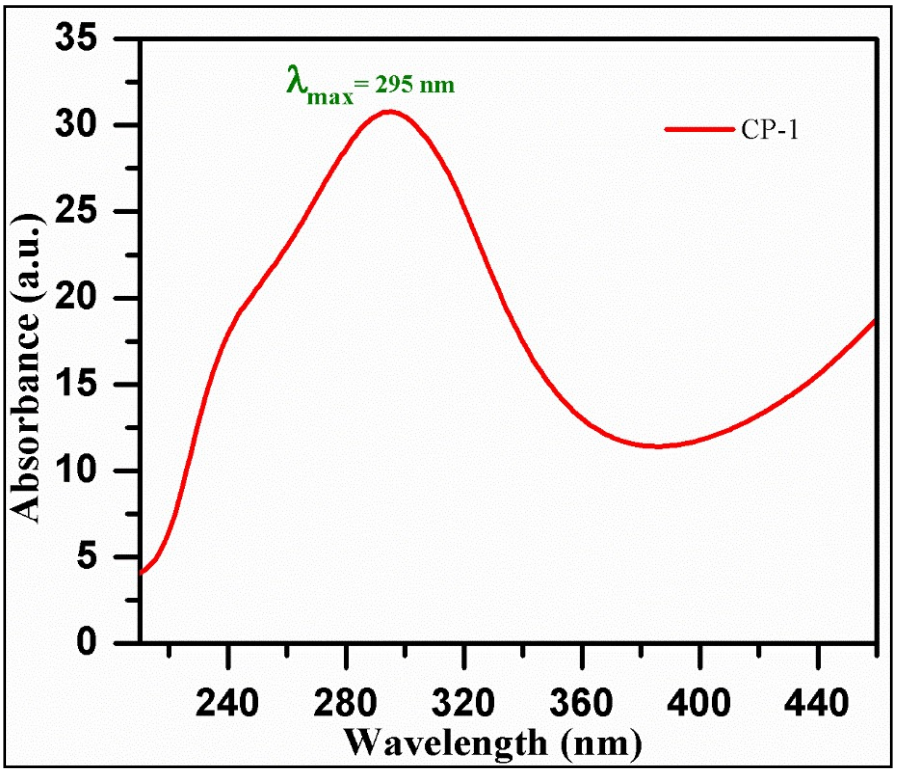

Figure S1. UV-DRS spectrum of CP-1.

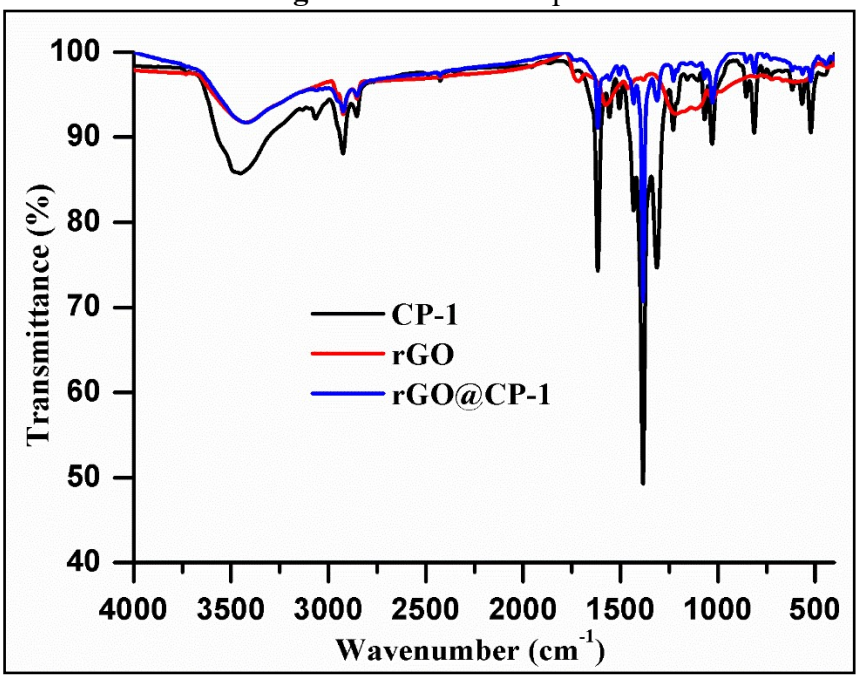

Figure S2. FTIR spectra of CP-1, reduced graphene oxide (rGO), and composite (rGO@CP-1).

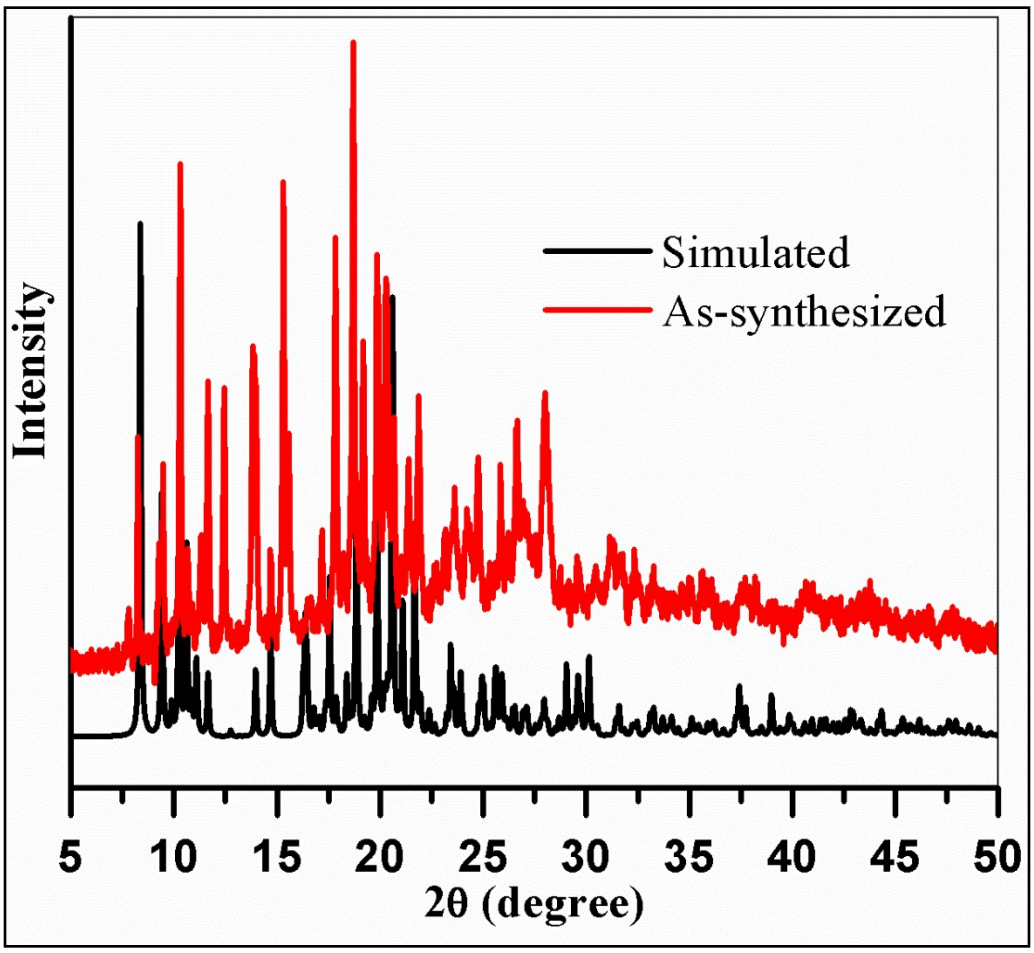

Figure S3(a). PXRD patterns of simulated and as-synthesized of CP-**1.**

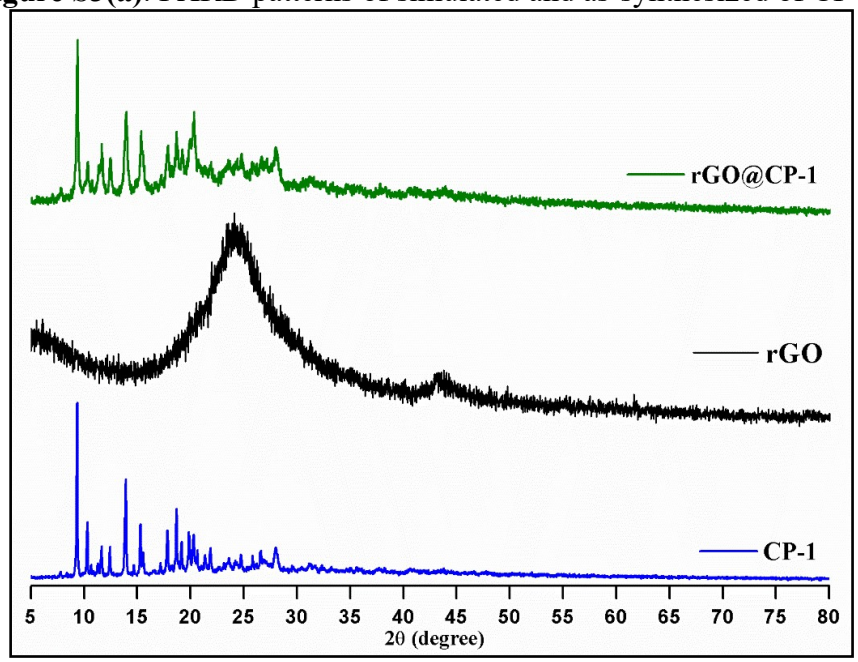

Figure S3b. PXRD patterns of as-synthesized CP-**1**, reduced graphene oxide (rGO), and rGO@CP-**1**.

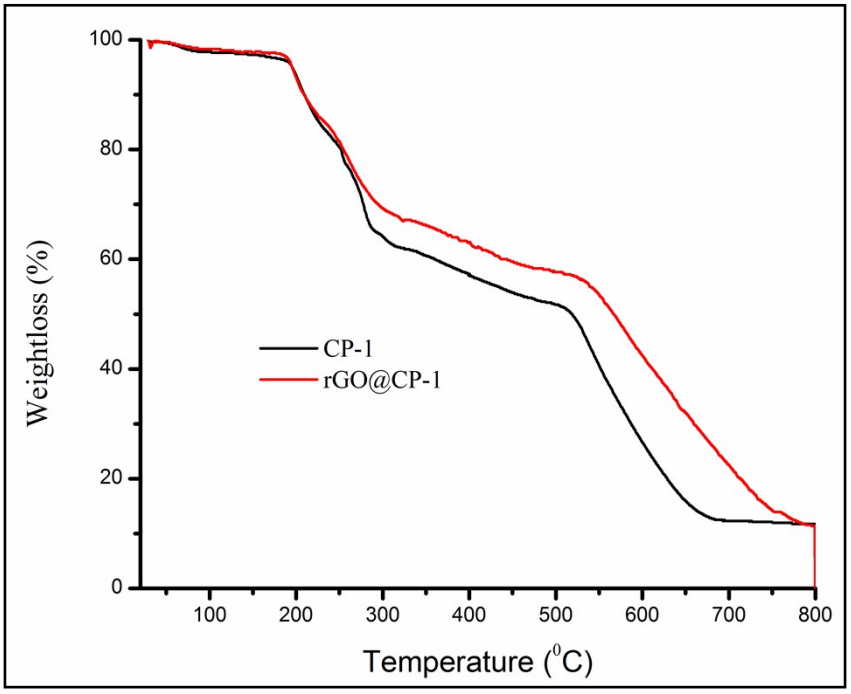

Figure S4. Thermogravimetric curves of as-synthesized coordination polymer (CP-**1**), and composite (rGO@CP-**1**).

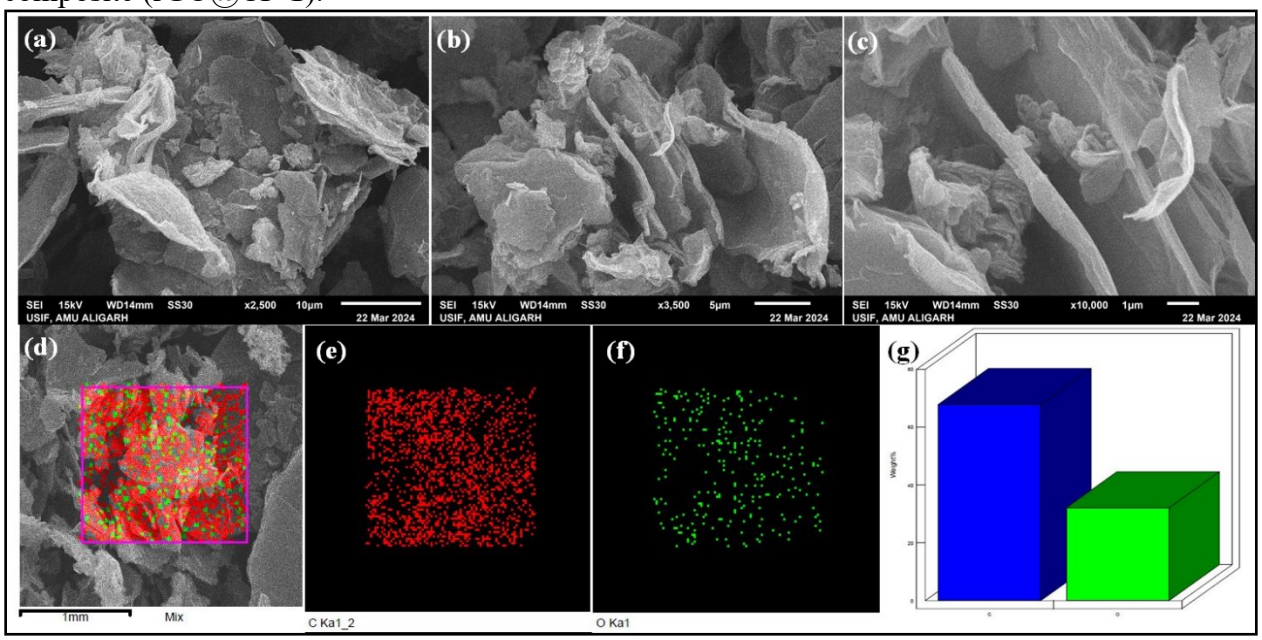

Figure S5a. SEM images of reduced graphene oxide at different magnification range (a-c) with mapping at 1mm selective area (d-f) and EDX (g).

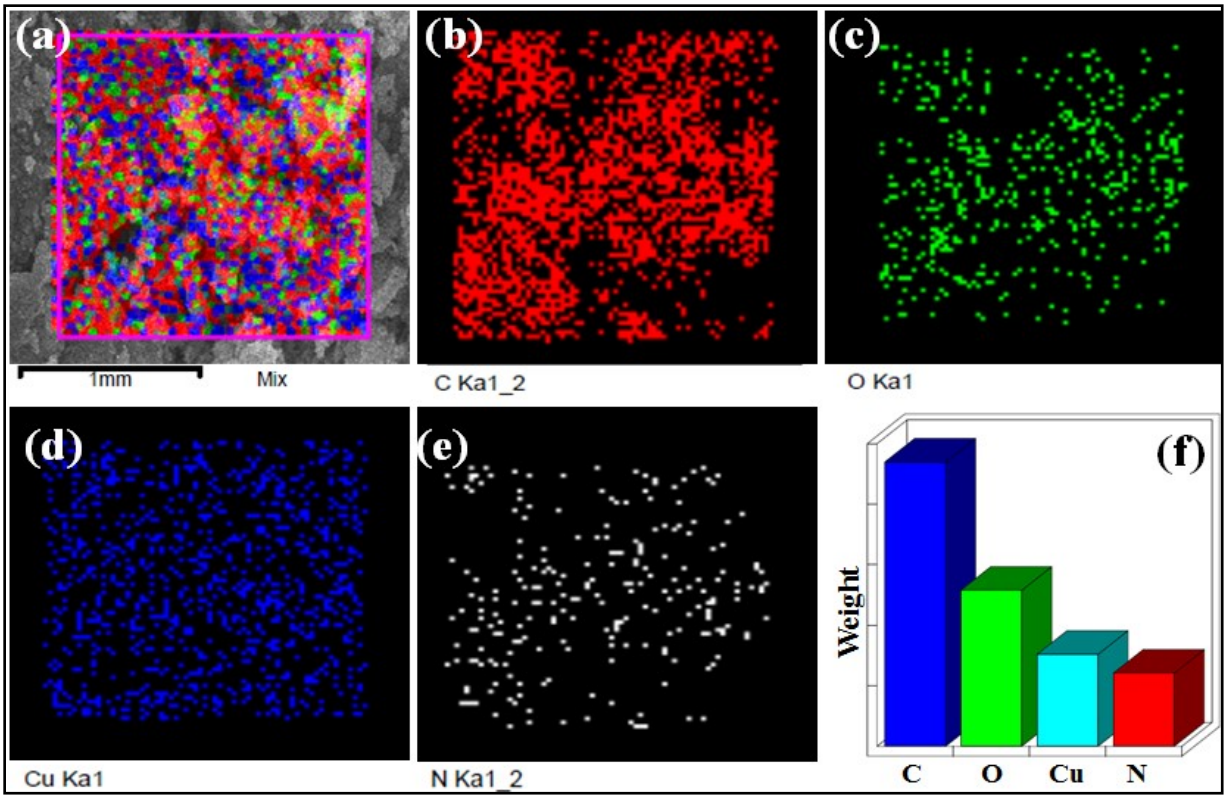

Figure S5b. SEM images of rGO@CP-1 on 1mm mixed selective area for elemental mapping (a-e) and EDX (f).

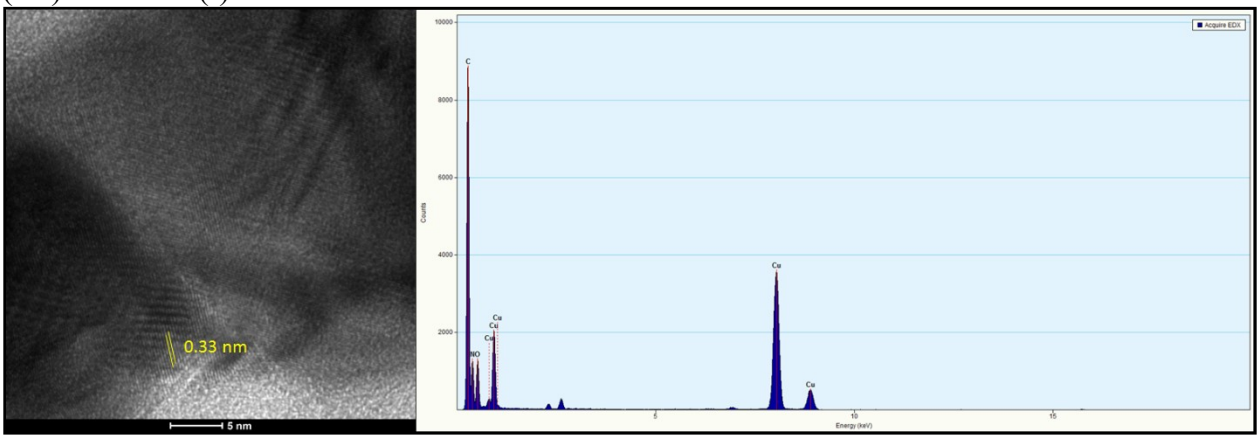

Figure S5c. HR-TEM image of rGO@CP-1 for lattice fringes with EDX spectrum.

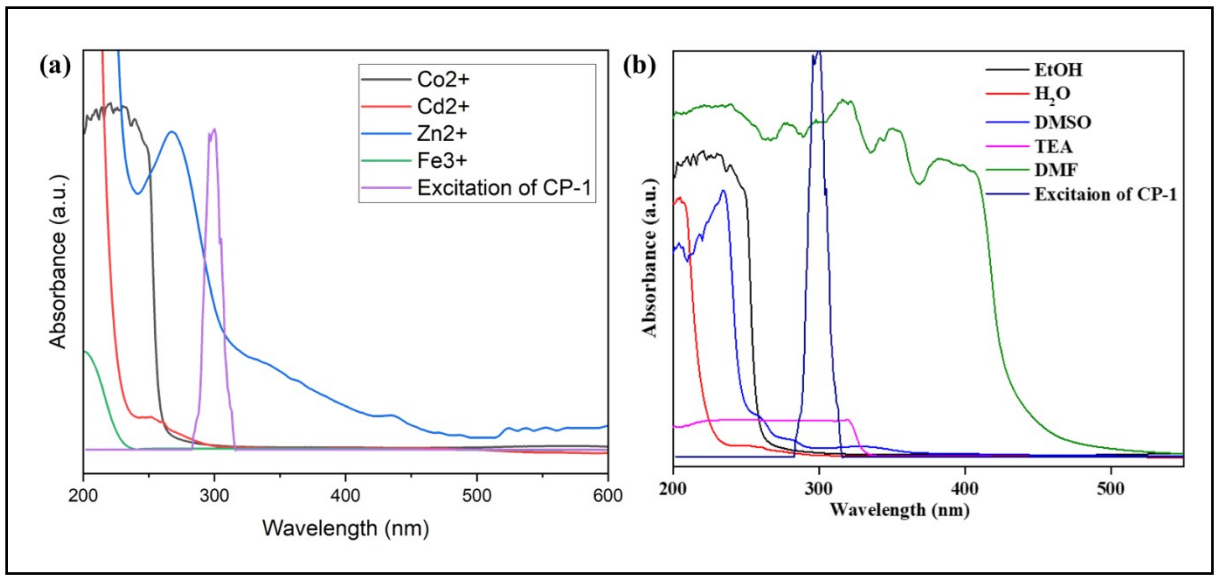

Figure S6. Spectral overlap between the UV-Vis absorption spectra of various analytes and the excitation spectra of **CP-1**.

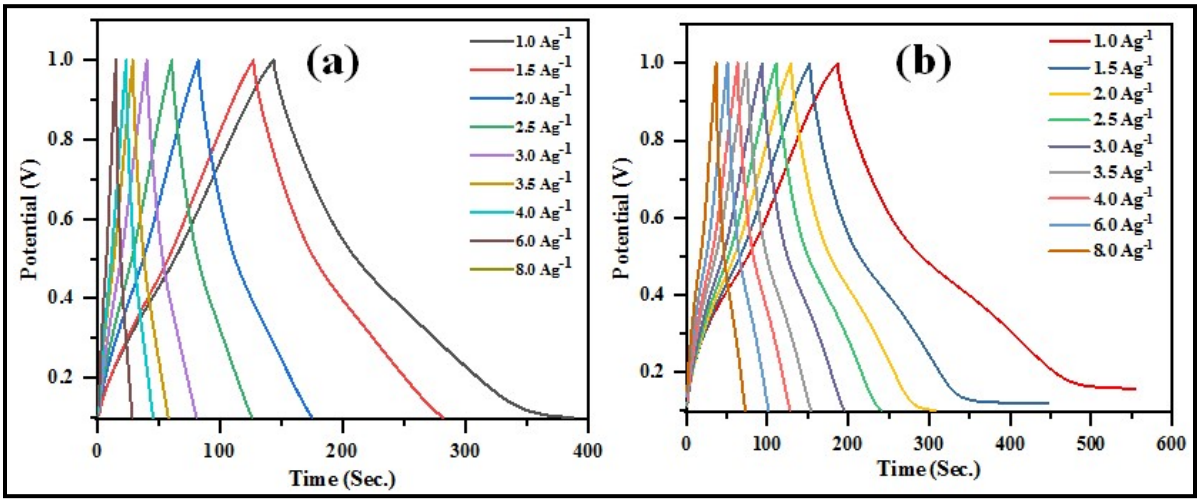

Figure S7. GCD curves of **(a)** CP-1 and **(b)** rGO sheet.