

Tuning the electrochemical performance of copper-based 2D rectangular layered Metal Organic Framework by incorporating reduced-graphene oxide and polyaniline

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Supplementary Information

Table 1: Crystal data and structure refinement parameters for **Cu-PDA MOF**.

Empirical formula	C ₇ H ₇ CuNO ₆
Formula weight	264.68
Crystal system	Monoclinic
Space group	C2/c
<i>a</i> (Å)	10.101(3)
<i>b</i> (Å)	11.843(3)
<i>c</i> (Å)	7.0691(19)
β (°)	105.308(6)
<i>V</i> (Å ³)	815.6(4)
<i>Z</i>	4
<i>D_c</i> (g cm ⁻³)	2.155
μ (mm ⁻¹)	2.69
θ range (°)	3.1-28.2
Measured refls.	9406
Independent refls.	758
<i>R</i> _{int}	0.034
<i>S</i>	1.10
<i>R</i> ₁ / <i>wR</i> ₂	0.041/0.116
$\Delta\rho_{\max}/\Delta\rho_{\min}$ (eÅ ⁻³)	1.95/-0.56
CCDC	2389095

Table 2: Selected bond distances and angles(Å, °)

Cu1-N1	2.102(4)	Cu1-O1 ⁱ	2.188(2)	Cu1-O3	1.932(3)
C3-C2	1.386(4)	C4-O2	1.242(4)	C1-N1	1.345(4)
C1-N1-Cu1	121.21(19)	O3-Cu1-N1	88.64(7)	O3-Cu1-O1 ⁱⁱ	94.49(10)
N1-Cu1-O1 ⁱ	137.67(7)	O1-C4-C2	119.5(3)	O2-C4-O1	122.9(3)

Symmetrycodes: (i) $-x-1/2, y+1/2, -z-1/2$; (ii) $x+1/2, y+1/2, z$.

Table 3: Hydrogen bond parameters (Å, °)

D-H...A	D-H	H...A	D...A	D-H...A
C1—H1...O2 ^{iv}	0.93	2.26	2.981 (5)	134
O3—H3A...O2 ^v	0.80 (2)	1.93 (2)	2.717 (4)	169
O3—H3B...O1 ^{vi}	0.81 (2)	1.95 (2)	2.755 (3)	173

Symmetrycodes: (iv) $-x-1/2, y+1/2, -z-1/2$; (v) $-x, -y-1, -z$; (vi) $x+1/2, -y-1/2, z+1/2$.

Table.4: PXRD information ofPANI

Samples	2θ(deg.)	θ(deg.)	d (nm)	FWHM (β)	D(nm)
Polyaniline	25.89°	12.94°	0.3622	0.269	63

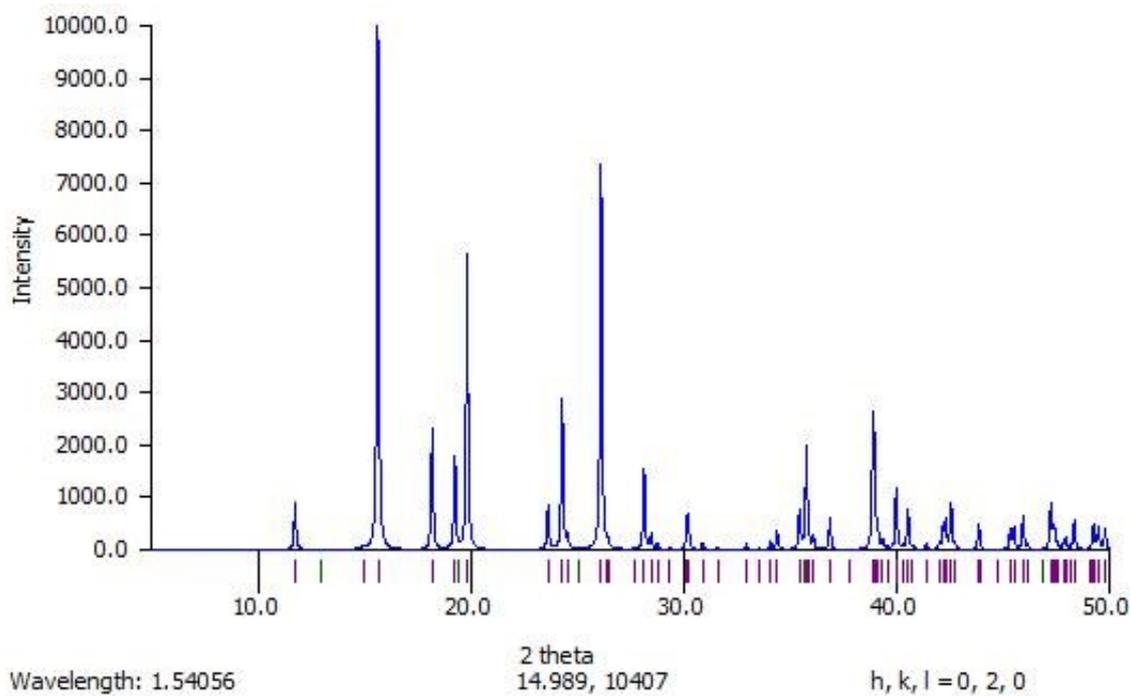


Fig. S1. Simulated XRD diffractogram of Cu-PDA-MOF

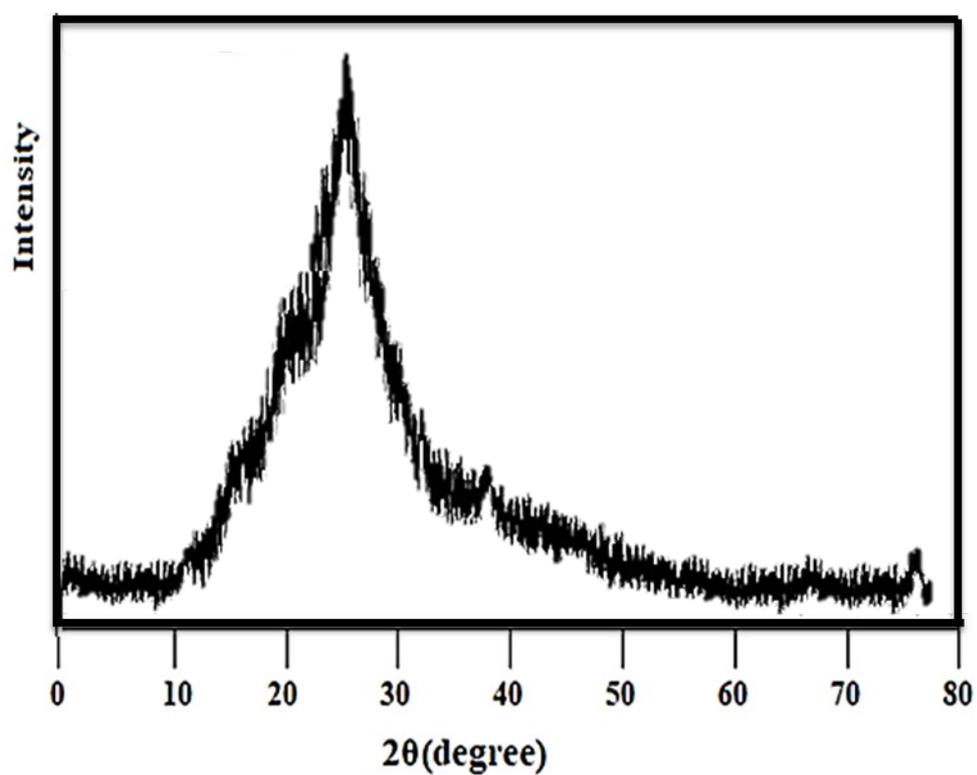


Fig. S2: PXRD spectra of PANI

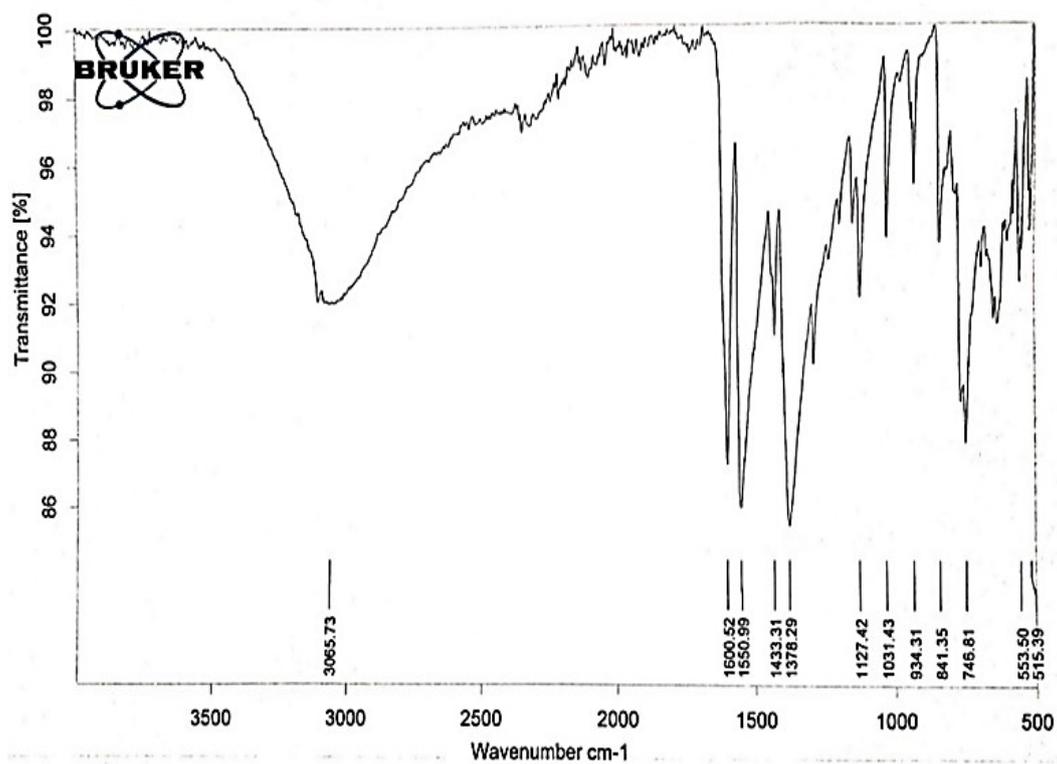


Fig.S3: FTIR spectra of Cu-PDAMOF

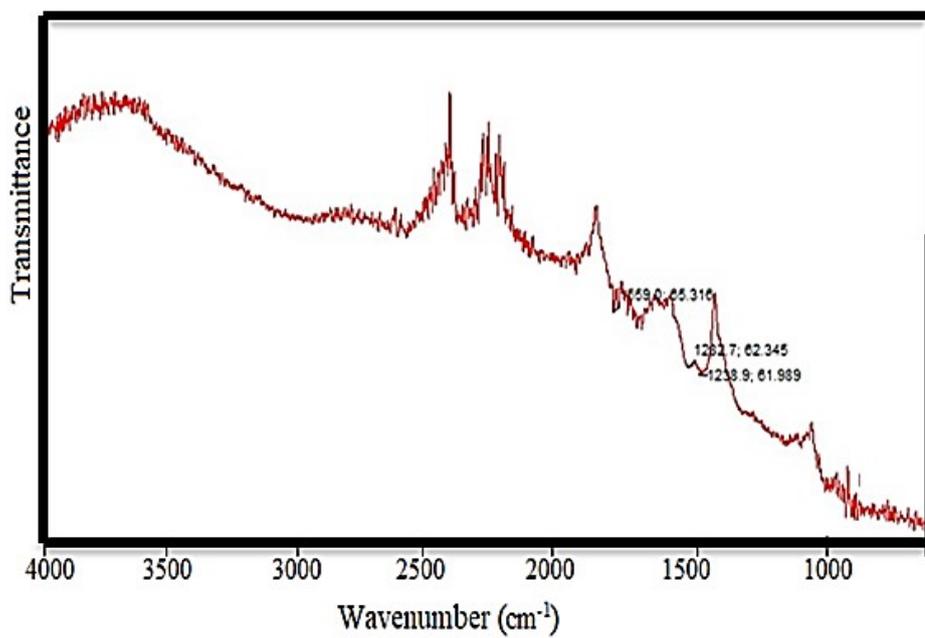


Fig. S4: FTIR spectra of PANI

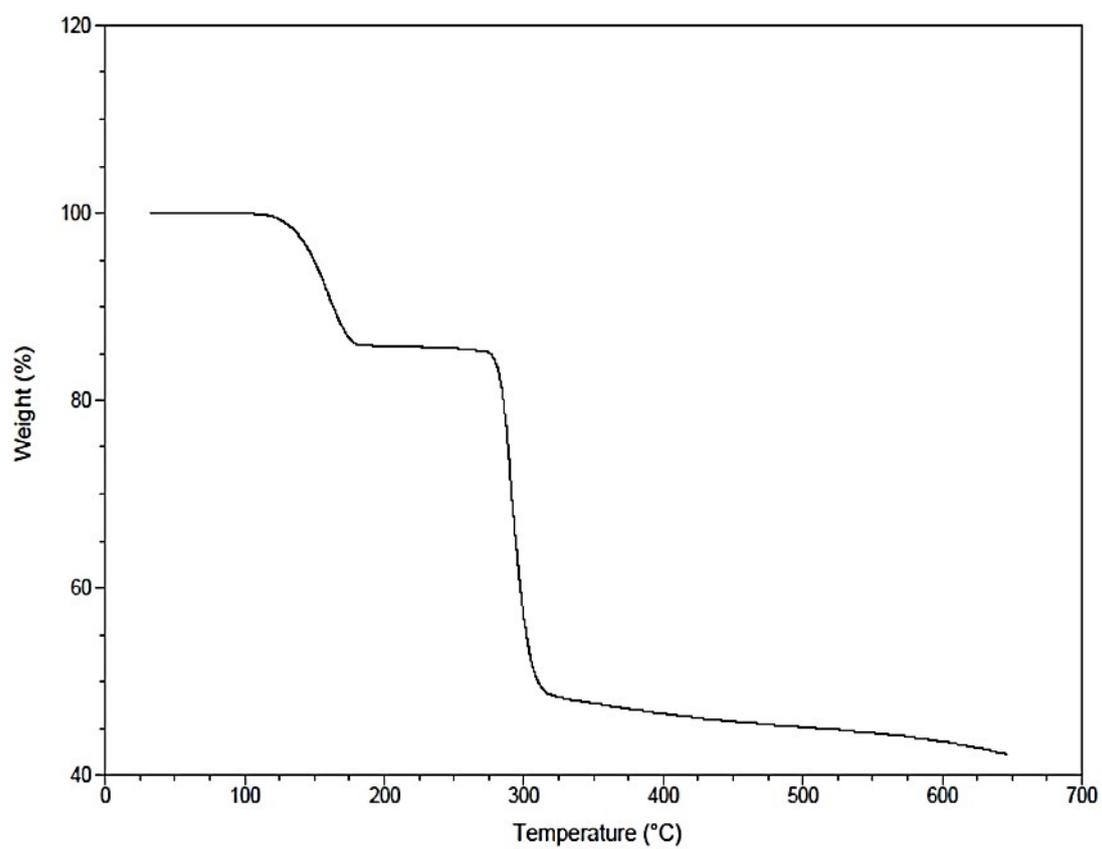


Fig.S5: TGA of Cu-PDAMOF