

Improving electrochemical performance of nitrogen containing copper metal organic framework derived from highly connective 2,4,6-pyridinetricarboxylic acid for hybrid supercapacitor

Supplementary Material

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 2011994 for **Cu-PTA-MOF**. Copy of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or [www: http://www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk)).

Table S1 Crystal data and structure refinement parameters for **Cu-PTA-MOF**.

	Cu-PTA-MOF
Empirical formula	C ₁₆ H ₉ CuKN ₂ O ₁₃
Formula weight	539.89
Crystal system	Monoclinic
Space group	<i>P2/c</i>
<i>a</i> (Å)	11.0915 (3)
<i>b</i> (Å)	19.8193 (3)
<i>c</i> (Å)	11.5477 (2)
β (°)	110.420 (2)
<i>V</i> (Å ³)	2378.96 (9)
<i>Z</i>	4
Diffractionmeter	
λ (Å)	
<i>D_c</i> (g cm ⁻³)	1.507
μ (mm ⁻¹)	3.47
θ range (°)	4.7-71.3
Measured refls.	11490
Independent refls.	4522

R_{int}	0.021
S	1.05
R1/wR2	0.079/0.244
$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}$ ($\text{e}\text{\AA}^{-3}$)	2.06/-0.79

Table S2 Selected bond distances and angles(\AA , $^{\circ}$)

Complex	Cu-				
PTA-MOF					
N1-Cu1	1.921(3)	N2-Cu1	1.968(3)	O6-Cu1	2.060(3)
O7-Cu1	2.298(3)	O1-Cu1	2.093(3)	O12-Cu1	2.316(3)
O2-K1 ⁱ	2.814(4)	O5-K1	2.580(4)	K1-O13	2.854(4)
K1-O7 ⁱⁱ	2.939(4)				
N1-Cu1-O6	80.01(12)	N1-Cu1-O1	78.53(12)	N2-Cu1-O7	76.89(12)
O1-Cu1-O7	86.52(14)	N2-Cu1-O12	75.73(12)	O6-Cu1-O12	85.65(14)

Symmetry codes: (i) $x, y, z-1$; (ii) $-x+1, y, -z+3/2$ for **Cu-PTA-MOF**.

Table S3 Hydrogen bond parameters (\AA , $^{\circ}$)

D-H \cdots A	D-H	H \cdots A	D \cdots A	D-H \cdots A
Cu-PTA-MOF				
C2—H2 \cdots O4 ^{vi}	0.93	2.36	3.199 (5)	150
O4—H4A \cdots O2 ^{vii}	0.82	1.77	2.573 (5)	165
O8—H8 \cdots O13 ⁱⁱ	0.82	1.69	2.497 (5)	166
O9—H9 \cdots O6 ⁱⁱⁱ	0.82	1.80	2.578 (4)	159
O13—H13B \cdots O11 ^{viii}	0.83 (2)	1.85 (2)	2.524 (5)	137
O13—H13A \cdots O1 ^{iv}	0.85 (2)	1.98 (3)	2.665 (5)	136

Symmetry codes: (ii) $-x+1, y, -z+3/2$; (iii) $x, -y+1, z-1/2$; (iv) $x, y, z+1$; (vi) $x, -y+2, z-1/2$; (vii) $x, -y+2, z+1/2$; (viii) $-x, y, -z+3/2$ for **Cu-PTA-MOF**.

Table.S4 XRD information of PPY and PANI

Samples	2θ(deg.)	θ(deg.)	d (nm)	FWHM (β)	D(nm)
Polypyrrole	23.16°	11.58°	0.6941	0.652	56
Polyaniline	25.89°	12.94°	0.3622	0.269	63

FTIR Analysis

Fourier transform infrared spectrum was measured using ATR sample compartment on Bruker Tensor-27 spectrophotometer (Billerica, MA, USA) in the range of 400-4000 cm^{-1} . FTIR spectrum of *Cu-PTA-MOF* is presented in **Fig. S1**. Characteristic band of O-H at 3083 cm^{-1} indicates presence of water molecule. The characteristic bands for the asymmetric and symmetric stretches of carboxylate group were found at 1618, 1597 and 1436 and 1354 cm^{-1} respectively. Shifts of the asymmetric ν_{as} (COO) and symmetric ν_{s} (COO) modes wave numbers upon coordination indicates the binding of PTA ligand to the metal.

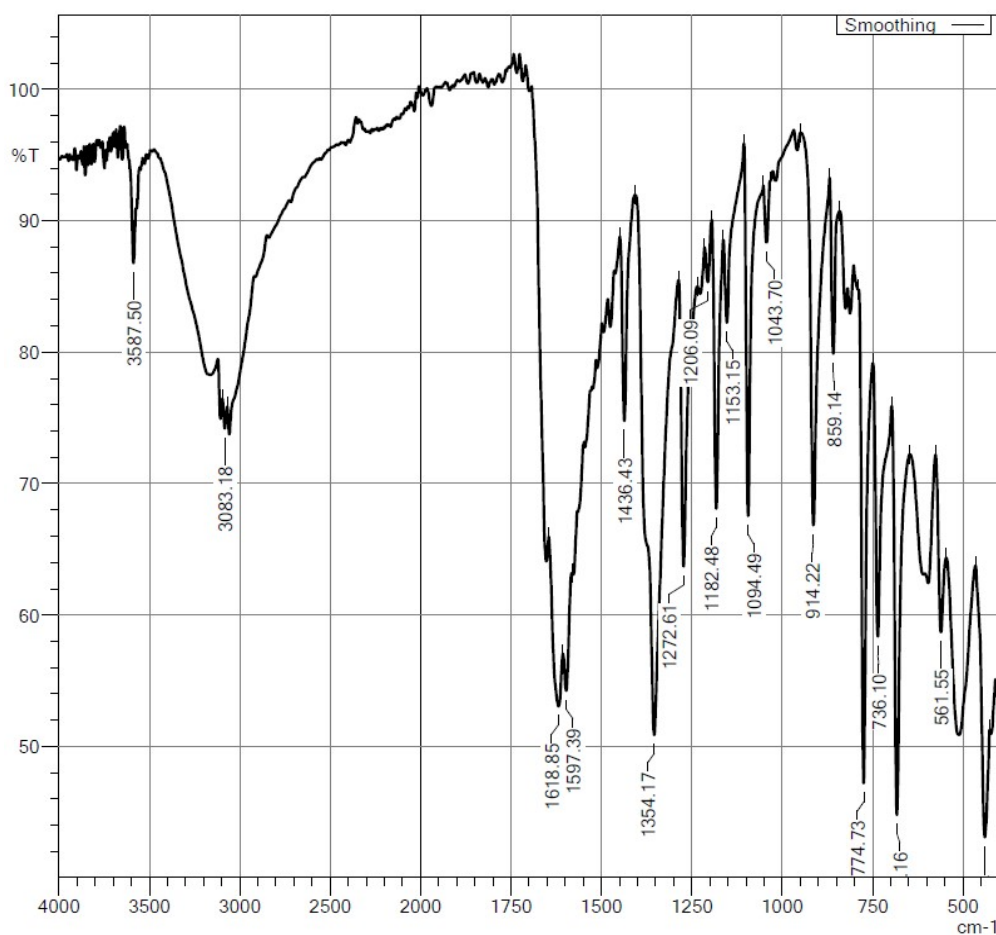


Fig. S1: FTIR spectrum of *Cu-PTA-MOF*

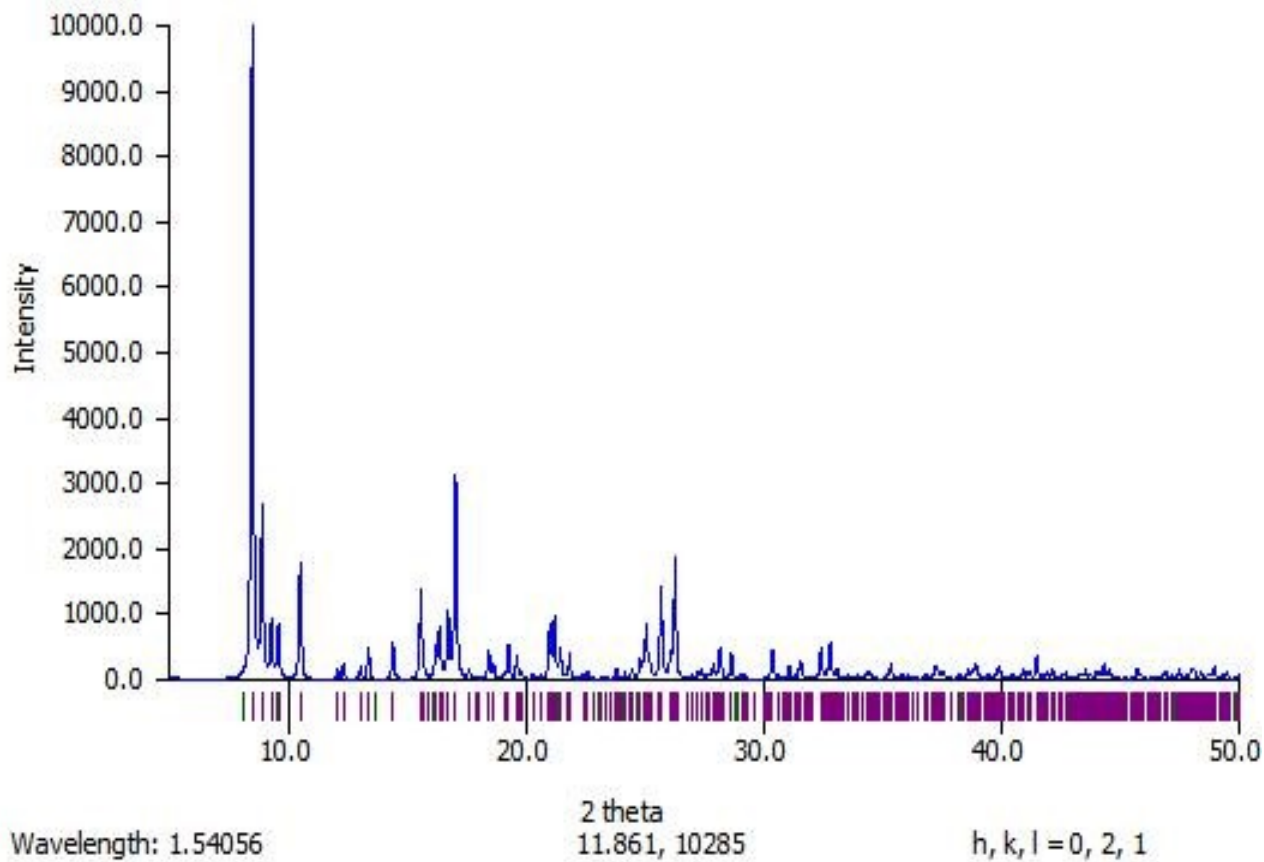


Fig. S2: Simulated powder XRD diffractogram of *Cu-PTA-MOF*

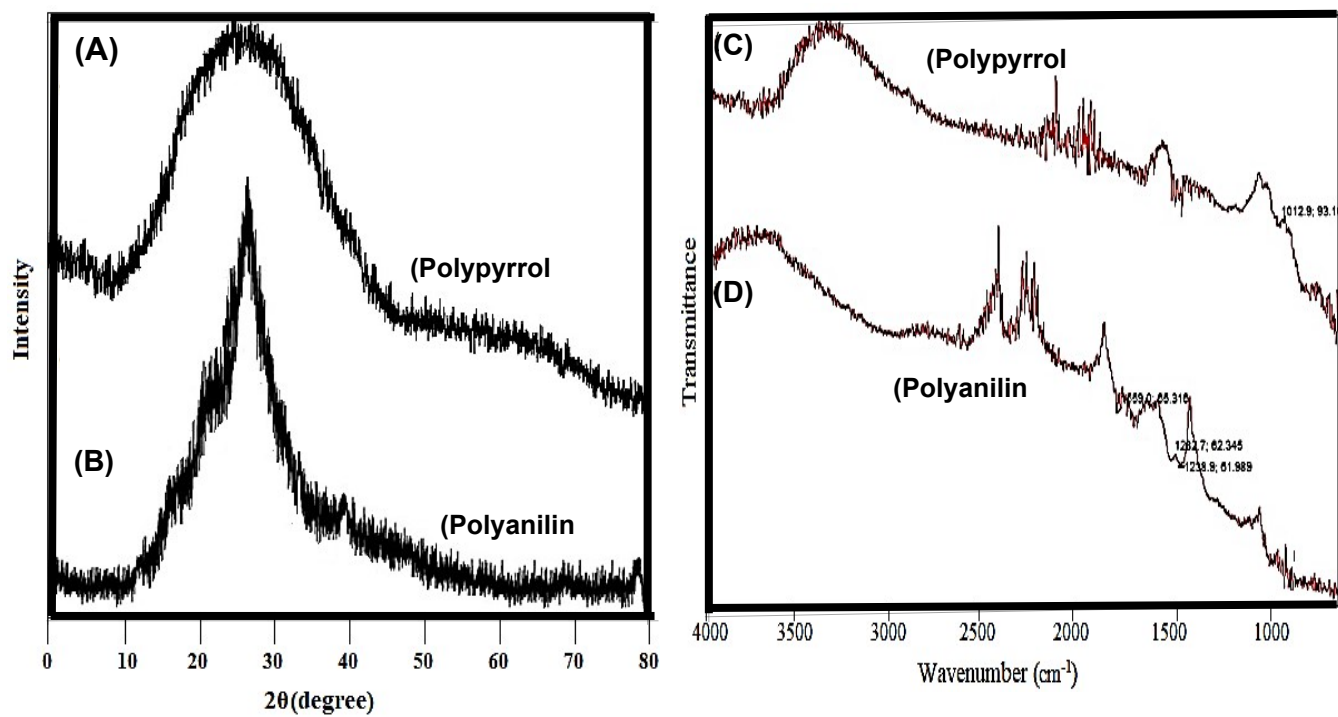


Fig. S3: (A) PXRD spectra of pure PPY and (B) pure PANI. (C) FTIR spectra of pure PPY and (D) pure PANI.

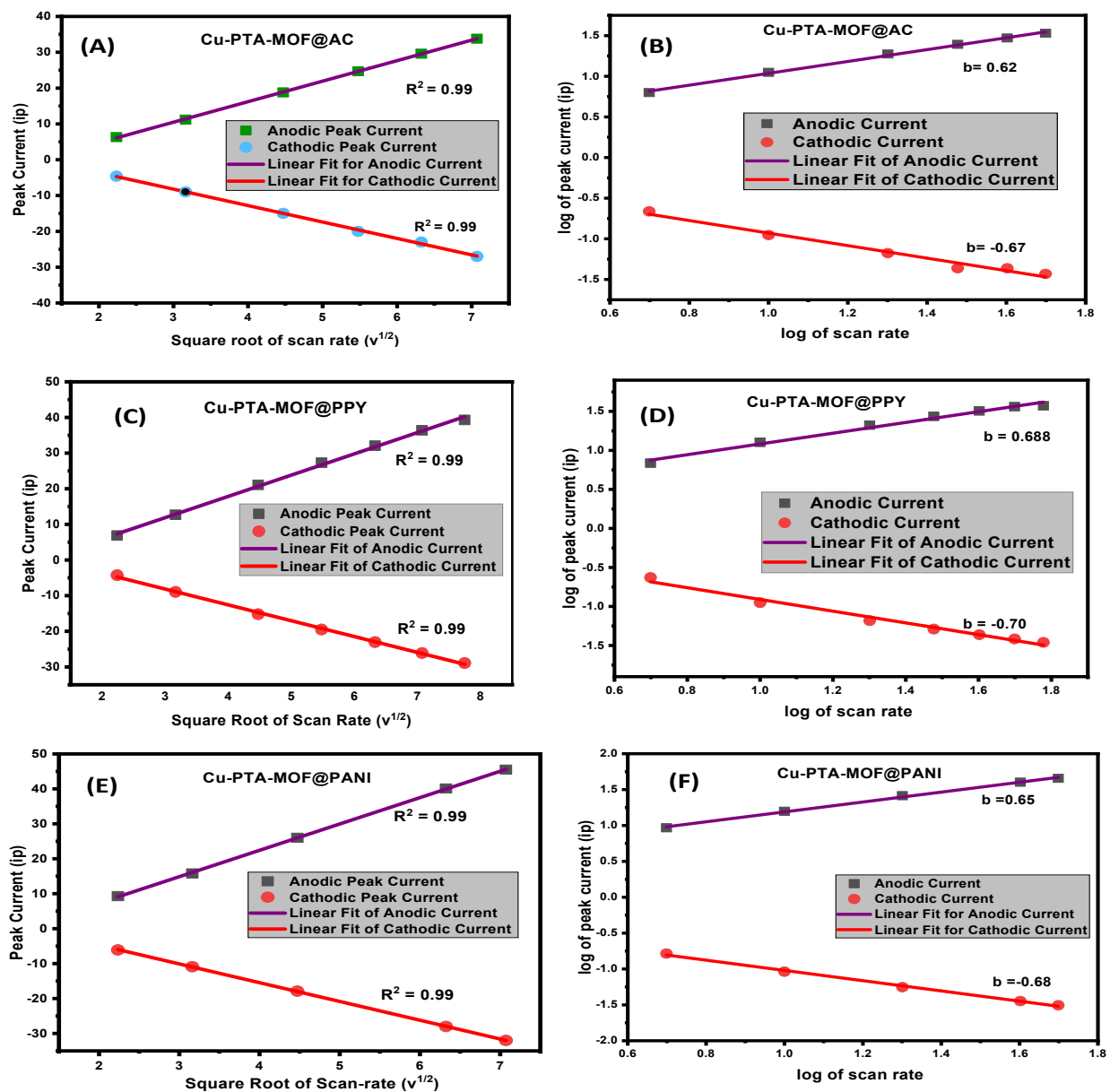


Fig. S4: (A) Cathodic and anodic peaks for Cu-PTA-MOF@AC as a function of scan rate $v^{1/2}$. (B) Slope for peak current log for the Cu-PTA-MOF@AC as a function of scan rates log. (C) As a function of scan rate $v^{1/2}$, Cathodic and anodic peaks for Cu-PTA-MOF@PPY. (D) Slope for peak currents log for the Cu-PTA-MOF@PPY as a function of scan rates log. (E) Cu-PTA-MOF@PANI cathodic and anodic peaks as a function of scan rate $v^{1/2}$. (F) Slope for peak currents log for the Cu-PTA-MOF@PANI as a function of scan rates log.