Electronic Supplementary Material (ESI) for Dalton Transactions

Novel Metal(II) Coordination Polymers Based on N,N'-bis-(4-pyridyl)phthalamide as Supercapacitor Electrode Materials in Aqueous Electrolyte

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Table S1 Selected bond lengths (Å) and angles (º) for complexes **1-2**

Complex 1			
Zn(6)-O(19)	1.913(6)	Zn(5)-O(25)	1.912(7)
Zn(3)-O(17)	1.951(6)	Zn(2)-O(6)	2.036(6)
Zn(4)-O(22)	2.439(7)	Zn(2)-O(5)	2.394(6)
Zn(5)-N(12)#1	1.976(8)	Zn(4)-N(8)#1	2.075(8)
O(6)-Zn(2)-O(5)	58.7(2)	O(9)-Zn(2)-O(5)	162.9(2)
O(10)-Zn(1)-O(3)	106.4(3)	N(4)#2-Zn(2)-O(5)	92.4(3)
O(24)-Zn(5)-N(12)#1	115.1(3)	O(3)-Zn(1)-N(1)	100.4(3)
Complex 2			
Cd(1)-N(4)#3	2.288(4)	Cd(1)-N(1)	2.331(4)
Cd(1)-O(11)#4	2.424(4)	Cd(1)-O(10)	2.327(4)
Cd(2)-N(8)#3	2.303(5)	Cd(2)-N(5)	2.309(4)
Cd(2)-O(7)	2.319(4)	Cd(2)-O(5)#5	2.434(4)
N(5)-Cd(2)-O(10)	83.90(14)	N(4)#3-Cd(1)-O(12)#4	96.47(15)
N(5)-Cd(2)-O(9)	88.85(14)	O(7)-Cd(2)-O(9)	130.75(14)

O(8)-Cd(1)-O(7)	50.68(12)	O(11)#4-Cd(1)-O(7)	166.94(13)
N(4)#3-Cd(1)-N(1)	173.89(16)	N(8)#3-Cd(2)-N(5)	175.40(17)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 x-1,y,z #3 x-1,y,z #4 x,-y+3/2,z-1/2 #5 x,-y+1/2,z+1/2

Table S2 The dihedral angles (°) of the two phenyl rings of **BPC**$^{2-}$ in complex **1**

Plane 1	*Plane 2*	*Dihedral angle*
C20-C25	C20A-C25A	0
C41-C46	C41B-C46B	0
C108-C113	C114-C119	2
C66-C71	C72-C77	25.6
C86-C91	C80-C85	35.7
C100-C105	C94-C99	30.5
C27-C32	C33-C38	9

Symmetry transformations used to generate equivalent atoms:

A -x, -y+2, -z+1; B -x, -y+2, -z

The specific capacitance (SC), specific power density (SP) and specific energy (SE) based on the active materials were estimated from the discharge process using **Equations 1-3** as follows: [1]

$$\mathrm{SC}\ (\mathrm{F{\cdot}g^{-1}}) = \frac{I \times \Delta t}{\Delta E \times m} \qquad \textbf{(1)}$$

$$\mathrm{SP}\ (\mathrm{W{\cdot}kg^{-1}}) = \frac{I \times \Delta E}{m} \qquad \textbf{(2)}$$

$$\mathrm{SE}\ (\mathrm{W{\cdot}h{\cdot}Kg^{-1}}) = \frac{I \times t \times \Delta E}{m} \qquad \textbf{(3)}$$

where I, $\triangle t$, $\triangle E$ and m represent the current density, discharge time, potential range and the active mass of the material, respectively.

The energy deliverable efficiency (η/%) was obtained from **Equation 4.** [2]

$$\eta(\%) = \frac{t_d}{t_c} \times 100 \qquad \textbf{(4)}$$

where t_d and t_c are discharge time and charging time, respectively.

Table S3 Supercapacitive properties of **1-GCE**, **2-GCE** and the bare **GCE** determined using the galvanostatic discharge method at different current densities.

Current Density/ mA·g^{-1}	Potential Range/ V	Electrode	Supercapacitive parameters				
			SC/ F·g^{-1}	SC/ mF· cm^{-2}	SP/ W· kg^{-1}	SE/ W·h ·kg^{-1}	η
2.5	0~1.2	1-GCE	23	93	3	1.9	55%
	0~1.3	2-GCE	22	88	3.3	2.1	91%
	0~0.6	Bare GCE	0.6	2.3	1.5	0.01	16%
6.25	0~2.0	1-GCE	5.2	21	12.5	1.2	40%
	0~1.7	2-GCE	8.6	36	10.6	1.4	95%
	0~1.2	Bare GCE	0.5	2.0	7.5	0.04	23%
18.25	0~2.6	1-GCE	1.4	5.8	48.8	0.5	95%
	0~2.6	2-GCE	1.3	5.0	48.8	0.5	91%
	0~1.2	Bare GCE	0.3	1.3	22.5	0.03	80%

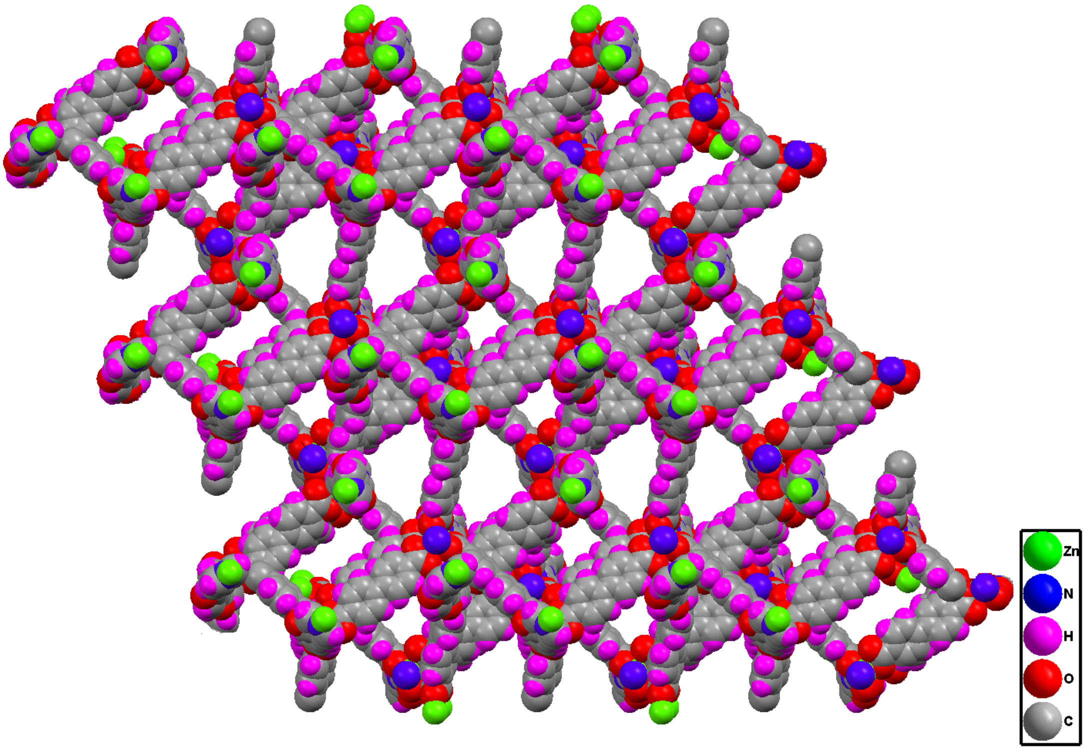

Fig.S1 Space-filling diagram of the 3D host framework in complex **1** (uncoordinated DMF molecules omitted for clarity)

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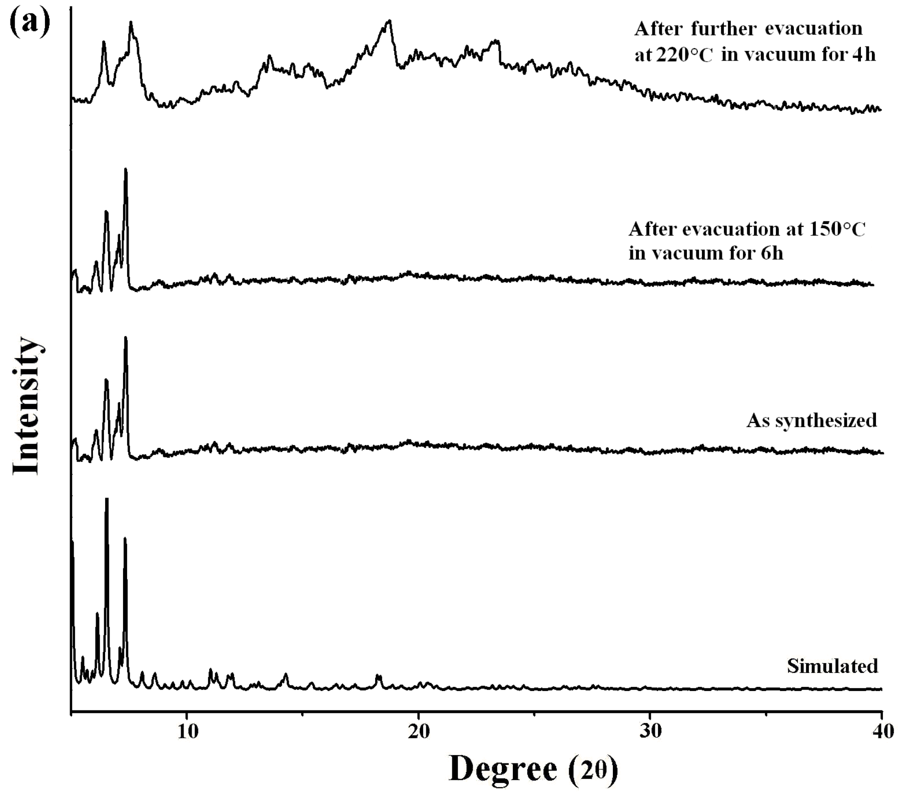

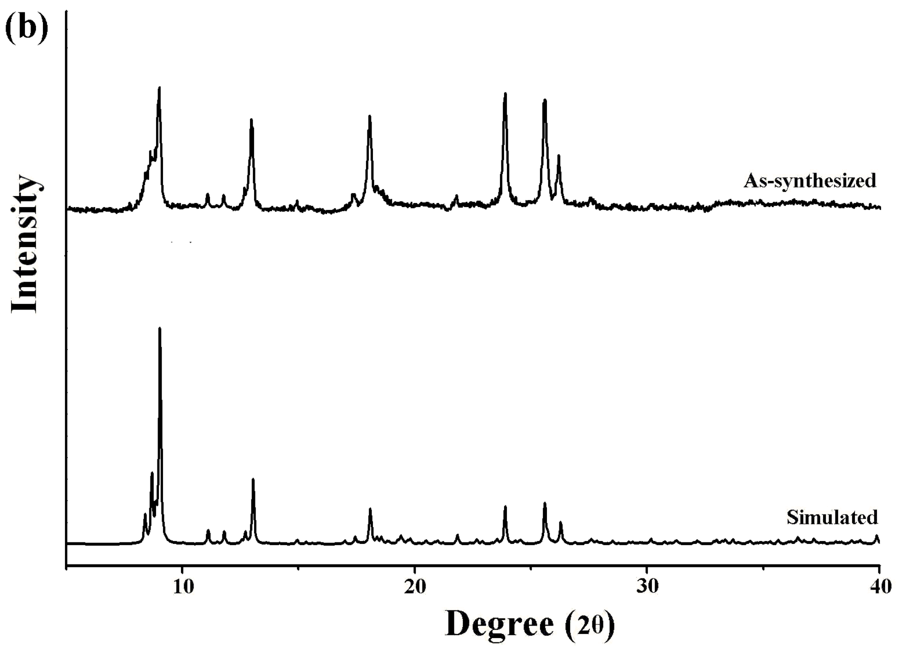

Fig.S2 The PXRD patterns of complexes **1 (a)** and **2 (b).**

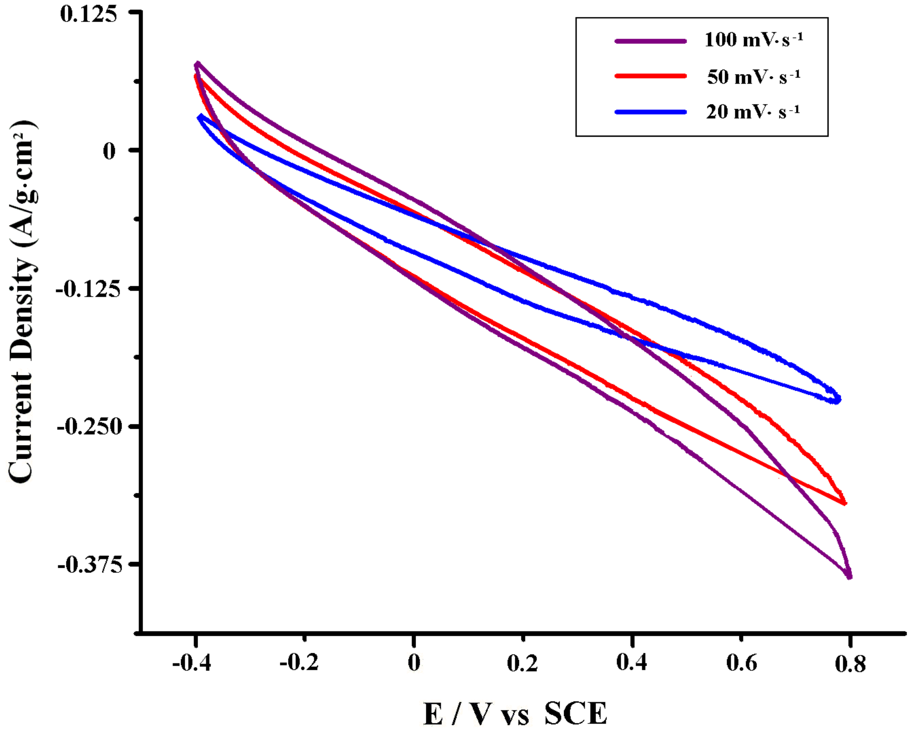

Fig.S3 Cyclic voltammograms (CVs) of the bare **GCE** in 1M Li_2SO_4 aqueous solution at a sweep rate of 100 (purple), 50(red) and 20 $mV{\cdot}s^{-1}$(blue), respectively.

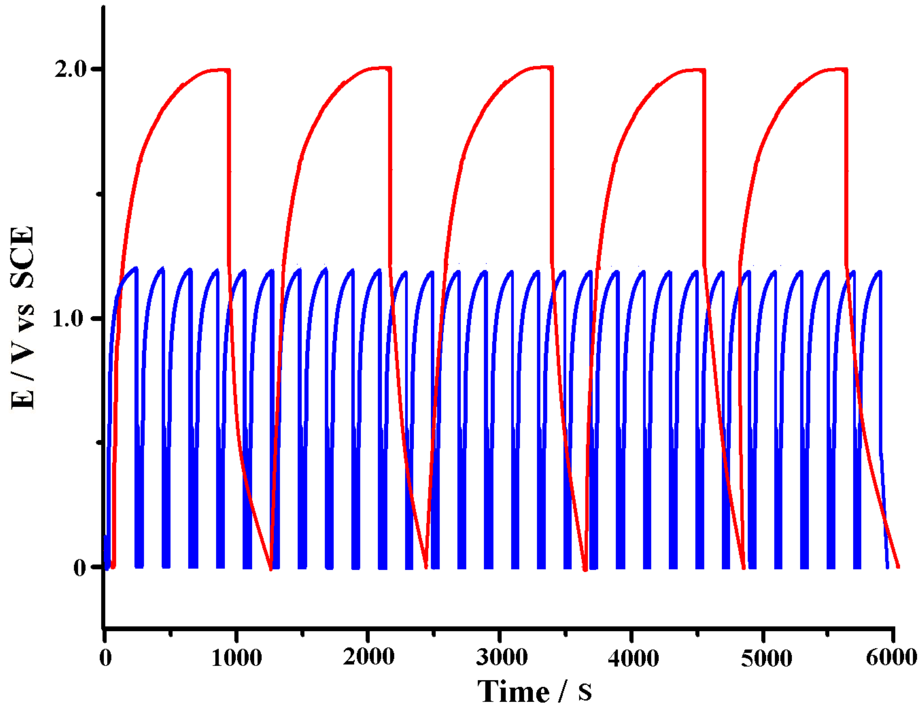

Fig. S4. Typical charge-discharge cycles obtained at **1-GCE** (red) and **bare-GCE** (blue) at 6.25 $mA \cdot g^{-1}$. Supporting electrolyte = 1M Li_2SO_4.

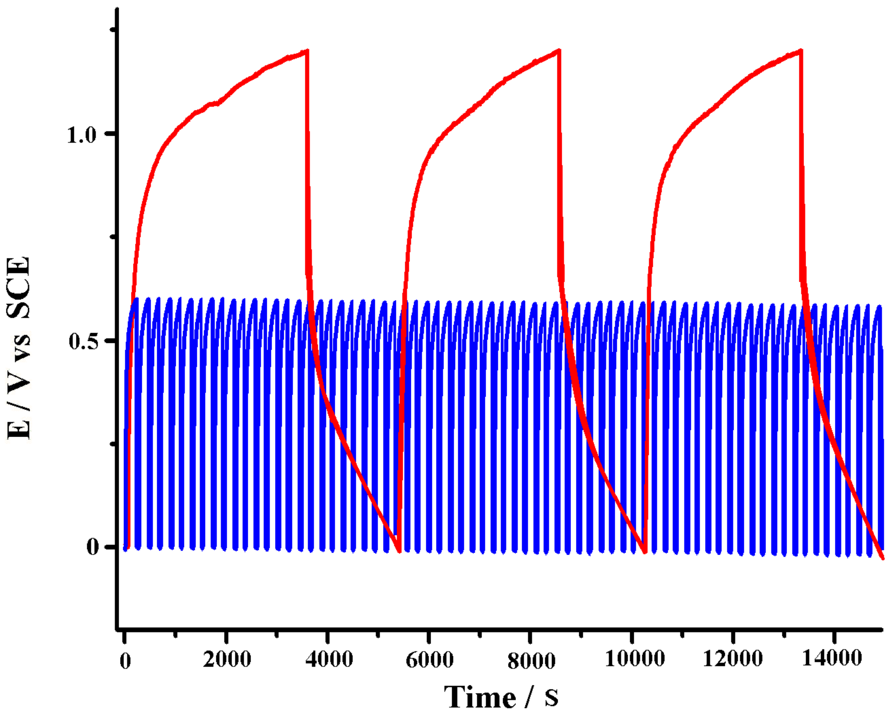

Fig.S5 Typical charge-discharge cycles obtained at **1-GCE** (red) and **bare-GCE** (blue) at 2.5 mA·g^{-1}. Supporting electrolyte = 1M Li_2SO_4.

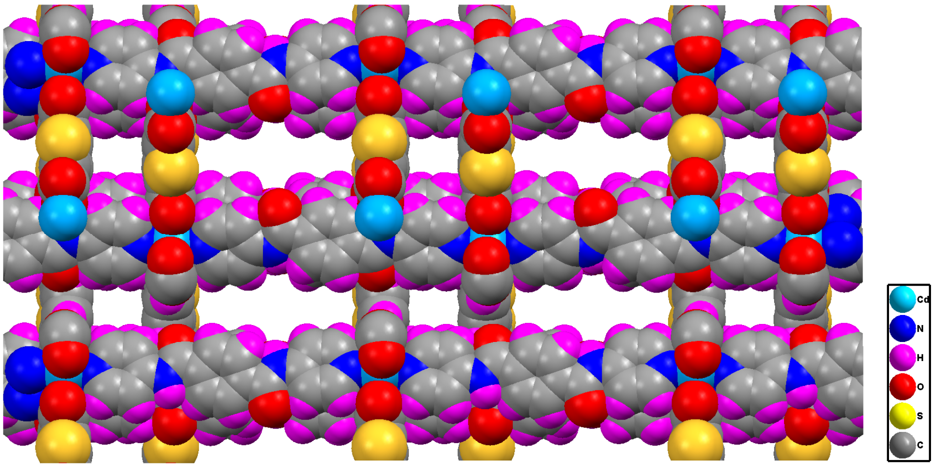

Fig. S6 Space-filling diagram of the 3D host framework in complex **2** (uncoordinated solvent molecules omitted for clarity)

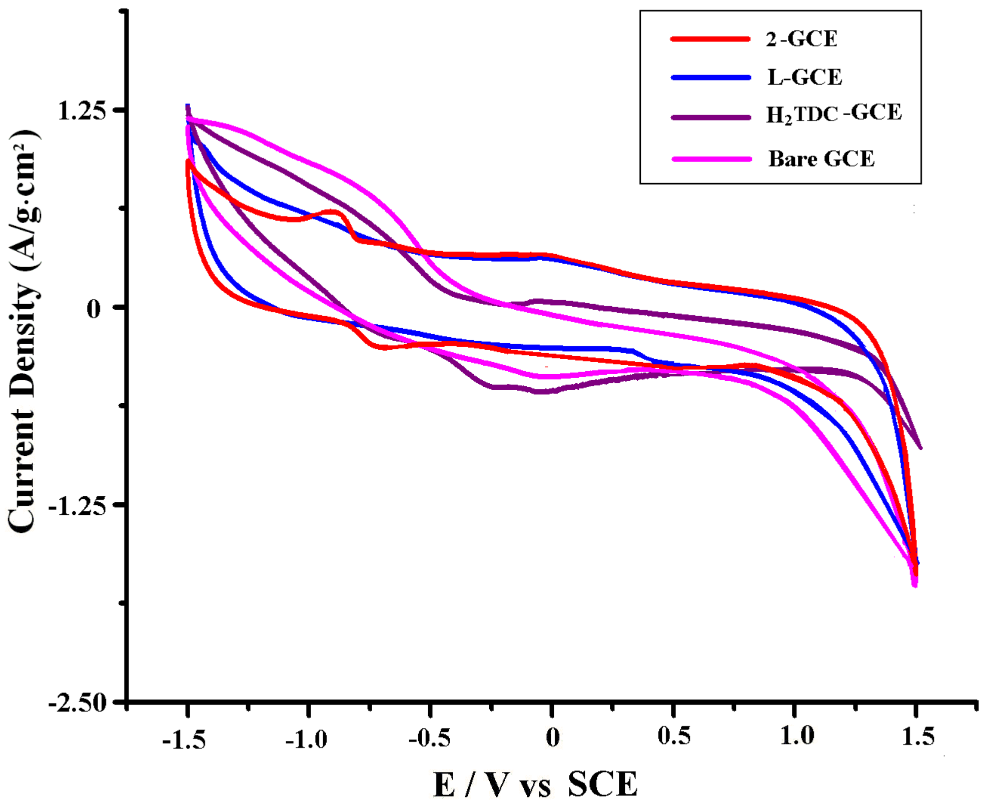

Fig.S7 CVs of the bare **GCE** (pink), **L-GCE** (blue), **H_2TDC-GCE** (purple) and **2-GCE** (red) in 1M Li_2SO_4 aqueous solution at a sweep rate of 50 mV·s^{-1}.

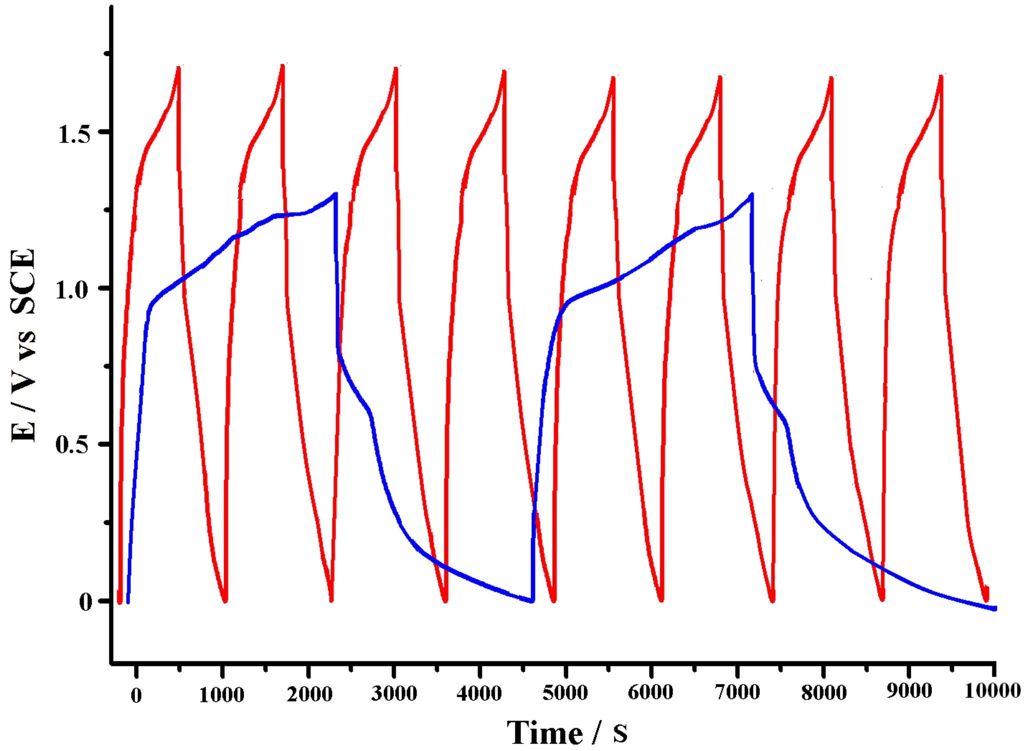

Fig.S8 Typical charge-discharge cycles obtained at **2-GCE** at 6.25 (red) and 2.5 mA·g^{-1}(blue). Supporting electrolyte = 1M Li_2SO_4.

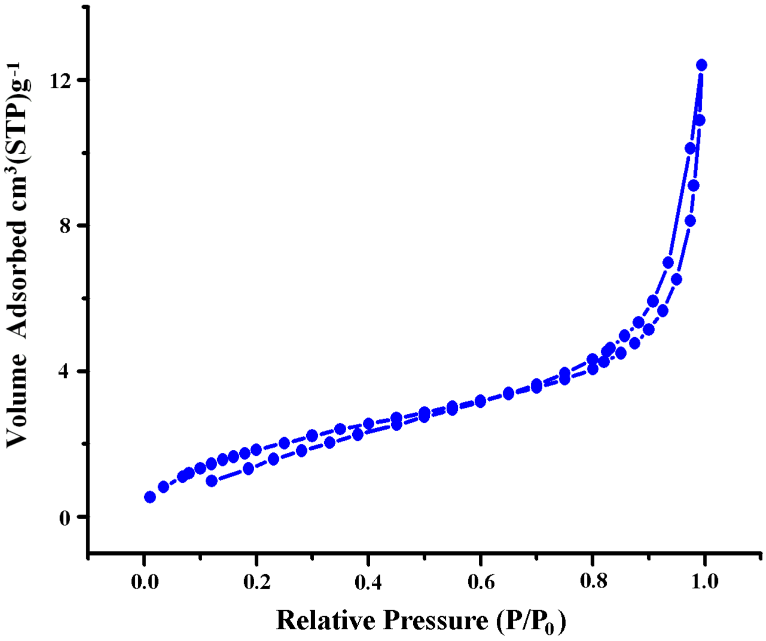

Fig. S9 N_2 adsorption and desorption isotherm at 77 K for evacuated complex **1**.

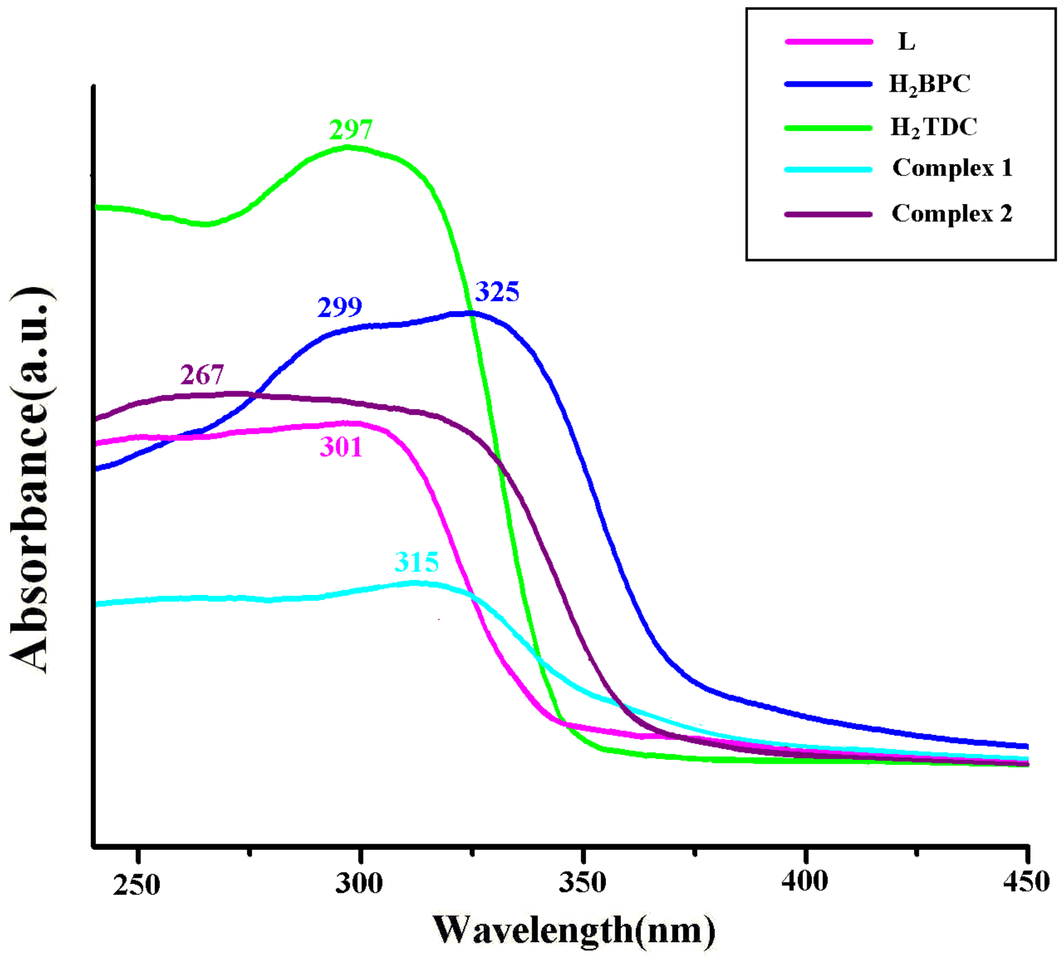

Fig. S10 UV absorption spectra at room temperature for the free ligands and complexes **1-2**.

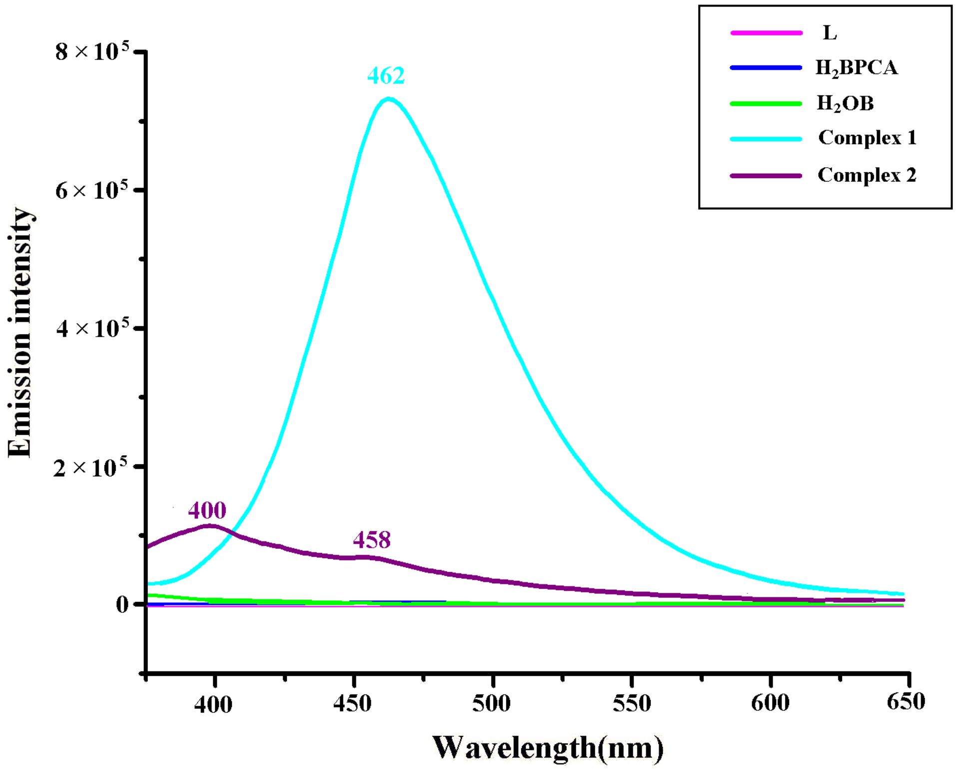

Fig. S11 Solid-state emission spectra at room temperature for the free organic ligands and complexes **1-2**.

References:

1 (a) K. R. Prasad and N. Munichandraiah, *Electrochem. Solid-State Lett.*, **2002**, *5*, A271; (b) V. Gupta, T. Shinomiya, N. Miurain: *Recent Advances in Supercapacitors*, ed. V. Gupta, Transworld Research Network, Kerala, India, **2006**, (ch. 2), 17; (c) V. Ganesh, S. Pitchumani and V. Lakshminarayanan, *J. Power Sources*, **2006**, *158*, 1523; (d) T. Shinomiya, V. Gupta and N. Miura, *Electrochim. Acta*, **2006**, *51*, 4412.

2 S. G. Kandalkar, J. l. Gunjakar and C. D. Lokhande, *Appl. Surf. Sci.*, **2008**, *254*, 5540.