

Electronic Supplementary Information

Development of a promising photosensitive Schottky barrier diode using a novel Cd(II) based coordination polymer

Pravat Ghorai,^a Arka Dey,^b Paula Brandão,^c Joaquín Ortega-Castro,^d Antonio Bauza,^d Antonio Frontera,^{*d} Partha Pratim Ray,^{*b} Amrita Saha^{*a}

^a*Department of Chemistry, Jadavpur University, Kolkata- 700032, India.*

E-mail: amritasahachemju@gmail.com; Tel. +91-33-24572941

^b*Department of Physics, Jadavpur University, Kolkata- 700032, India.*

E-mail: partha@phys.jdvu.ac.in; Tel: +91-9475237259

^c*Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal.*

^d*Departament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca, Balears, Spain. E-mail: toni.frontera@uib.es.*

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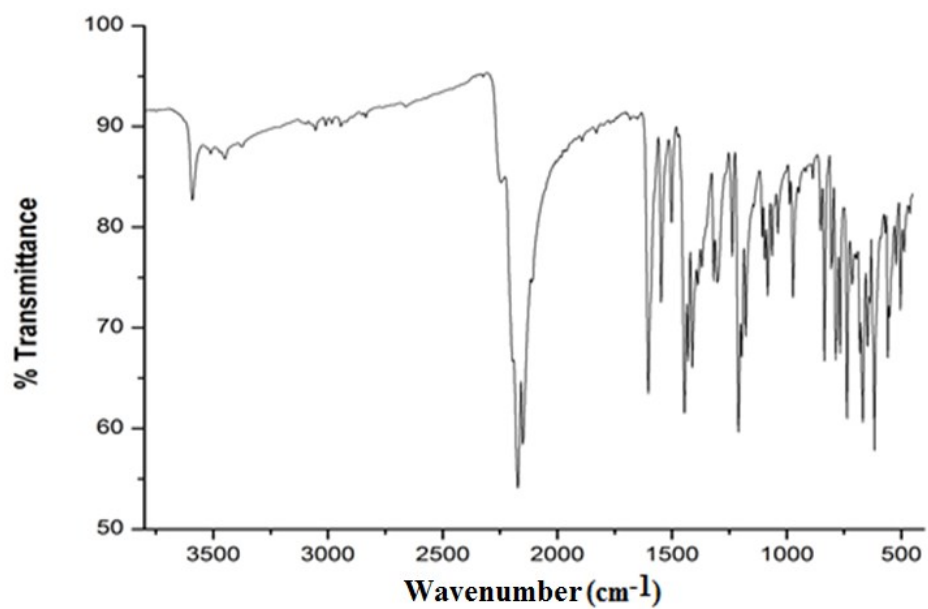


Fig. S1 FTIR spectrum of complex **1**.

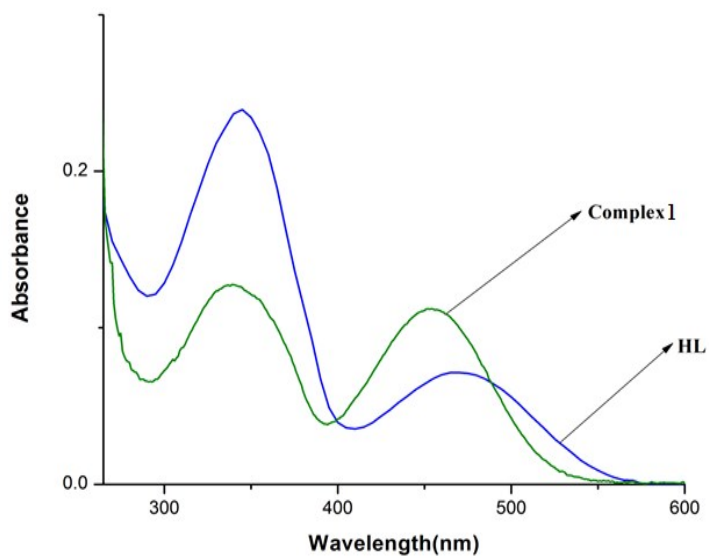


Fig. S2 UV-Vis spectra of **HL** and complex **1** at concentration 10 μ M.

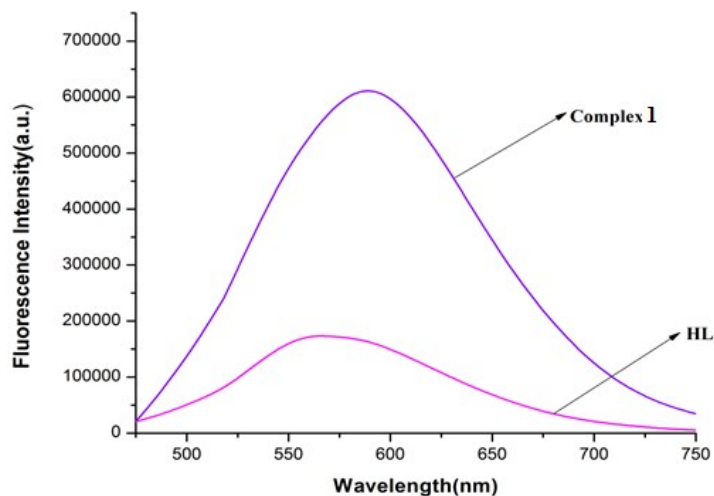


Fig. S3 Fluorescence emission spectra of **HL** and **Complex 1** in DMSO at concentration 10 μ M.

TGA (Thermo Gravimetric Analysis)

TGA of the complex is measured under Nitrogen atmosphere (150ml/min) using Platinum crucible with alpha alumina powder as reference in a PerkinElmer (SINGAPORE) instrument (Model No. - Pyris Diamond TG/DTA). The result showing good stability of the complex up to 350 $^{\circ}$ C.

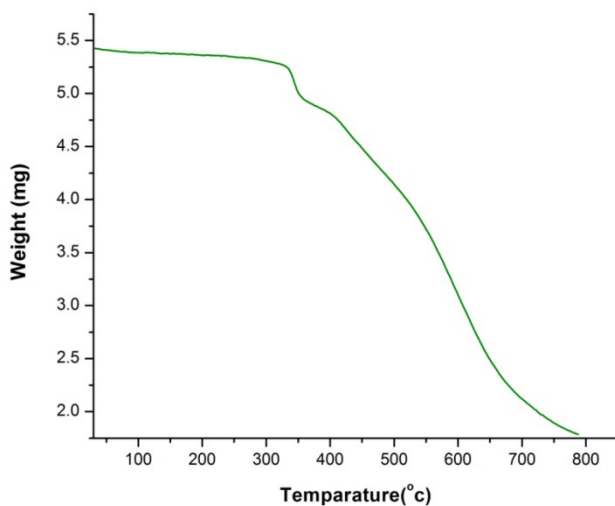


Fig. S4 Thermo Gravimetric Analysis of complex **1** under nitrogen atmosphere showing stability of complex is very appreciable up to 350 $^{\circ}$ C

Powdered X-ray diffraction

The bulk purity of the complex **1** has been confirmed. It is shown in Fig. S5. The simulated pattern is obtained from cif file of the complex and experimental pattern is collected from powdered XRD.

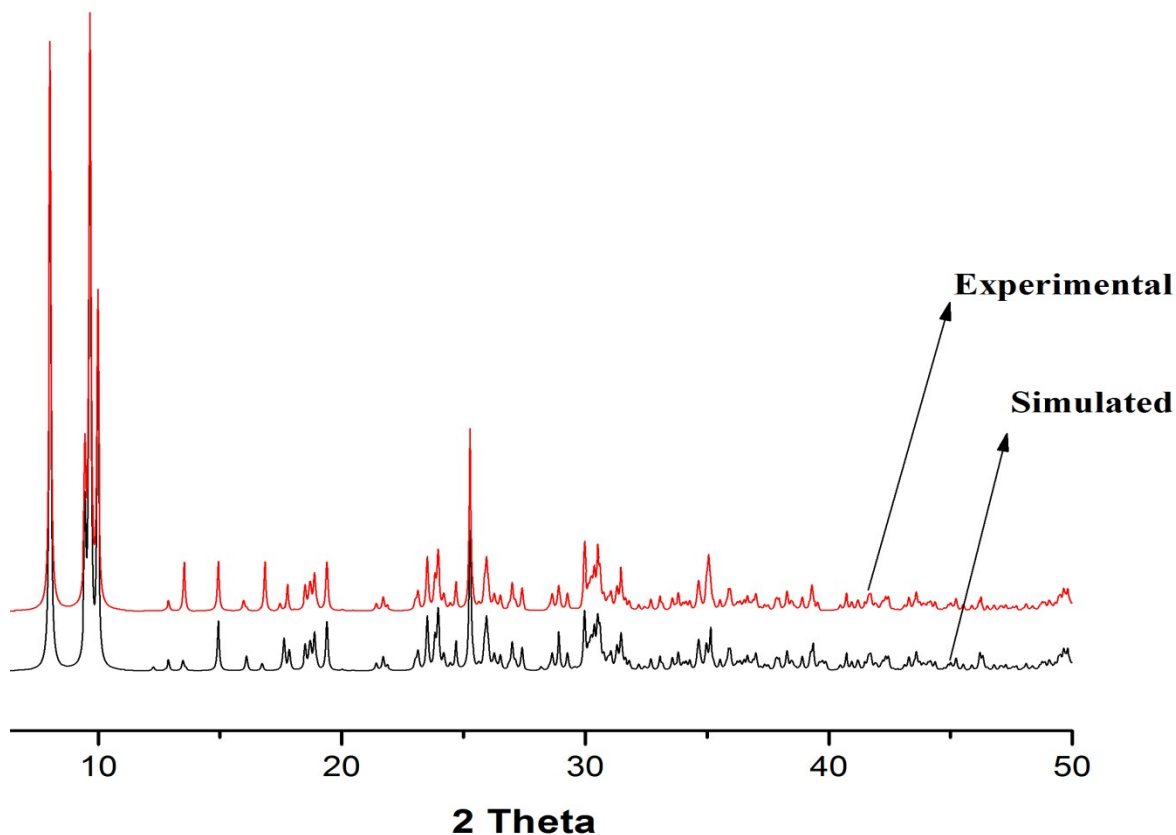


Fig. S5 Simulated and experimental powdered XRD pattern indicating the purity of the bulk materials of complex **1**.

Table S1. Crystal parameters and selected refinement details of the complex **1**.

Complex 1	
Empirical formula	C ₂₀ H ₁₃ Cd ₂ N ₅ O ₅
Formula weight	628.15
Temperature (K)	150(2)
Crystal system	Monoclinic
Space group	<i>C2/c</i>
<i>a</i> (Å)	28.5633(17)
<i>b</i> (Å)	10.0564(6)
<i>c</i> (Å)	18.6924(11)
$\alpha(^{\circ})$	90
$\beta(^{\circ})$	129.554(2)
$\gamma(^{\circ})$	90
Volume (Å ³)	4139.8(4)
<i>Z</i>	8
<i>D</i> _{calc} (g cm ⁻³)	2.016

Absorption coefficient (mm ⁻¹)	2.098
<i>F</i> (000)	2432
θ Range for data collection (°)	2.90-26.15
Reflections collected	19932
Data / restraints / parameters	4581/0/290
Goodness-of-fit on <i>F</i> ²	1.002
Final indices[I>2σ(I)]	R1= 0.0330 wR1= 0.0563
<i>R</i> indices (all data)	R1= 0.0571 wR1= 0.0634

Table S2. Selected bond lengths (Å) and bond angles (°) for complex.

Complex 1			
Cd1-O2	2.231(2)	O1-Cd2- N4	93.10(1)
Cd1-N1	2.266(3)	O2-Cd1-N1	83.54(10)
Cd1-N2	2.331(2)	O2-Cd1-N3	78.39(10)
Cd1-N3	2.336(4)	O2-Cd2-N3	77.68(10)
Cd1-N5	2.254(4)	N1-Cd1-N2	72.84(11)
Cd2-O1	2.581(3)	N2-Cd1-N3	105.00(11)
Cd2-O2	2.300(3)	Cd2-N4	2.293(3)
Cd2-N3	2.303(2)	Cd1-Cd2	3.509
Cd2-Cd2a	3.513		

Table S3. Dielectric parameters of complex **1**.

	Charge Transfer Resistance (K Ω)	D.C. Conductivity (10 ⁻⁶ S m ⁻¹)	Electron Lifetime (10 ⁻⁷ s)	Dielectric Constant (F m ⁻¹)
1	17.25	8.2	1.03	1.93

Table S4. Schottky diode parameters of the device.

	ON/OFF	PHOTOSENSITIVITY	CONDUCTIVITY (S.m ⁻¹)	IDEALITY FACTOR	BARRIER HEIGHT (eV)	R _s FROM dV/dlnI (K Ω)	R _s FROM H (K Ω)
DARK	12.44	2.56	8.26 X10 ⁻²	3.47	0.526	53.06	46.81
LIGHT	27.74		22.07X10 ⁻²	2.11	0.446	16.85	13.61

Table S5. Schottky device parameter of SCLC region.

	μ_{eff} (m ² V ⁻¹ s ⁻¹)	σ (S.m ⁻¹)	N (m ⁻³)	τ (sec)	$\mu_{\text{eff}}\tau$	D	L _D (m)	N' (eVm ⁻³)
DARK	1.619 x 10 ⁻¹²	1.49 X 10 ⁻⁵	5.75 x 10 ²⁵	1.81 x 10 ⁻¹	2.93 x 10 ⁻¹³	4.05 x 10 ⁻¹⁴	1.21 x 10 ⁻⁷	4.71 x 10 ³⁸
LIGHT	3.67 x 10 ⁻¹²	3.62 X 10 ⁻⁵	6.17 x 10 ²⁵	8.25 x 10 ⁻²	3.03 x 10 ⁻¹³	9.17 x 10 ⁻¹⁴	1.23 x 10 ⁻⁷	6.74 x 10 ³⁸