

**Electronic Support Information**

**Cd(II)-based MOF as a photosensitive Schottky diode: experimental and theoretical studies**

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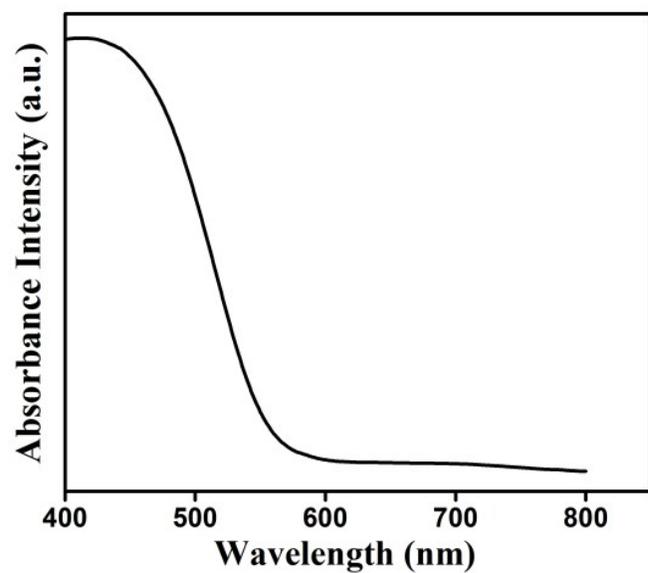
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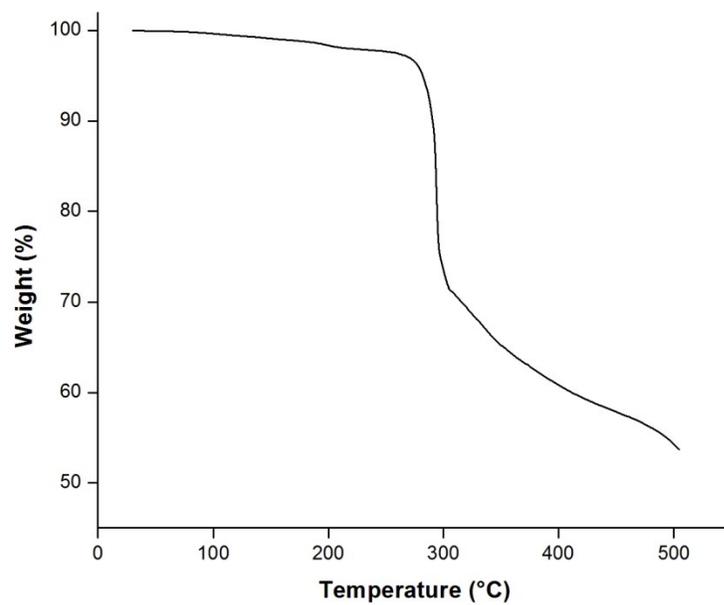
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[partha@physics.jdvu.ac.in](mailto:partha@physics.jdvu.ac.in) (PPR) and

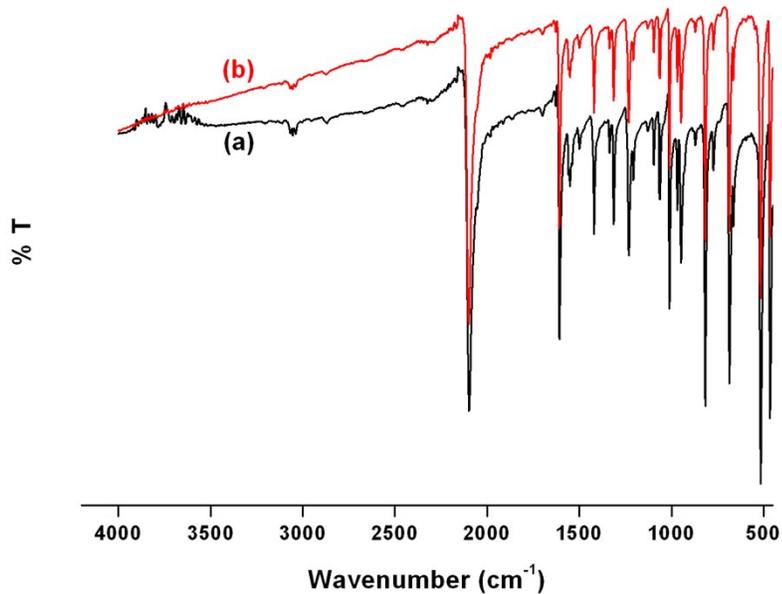
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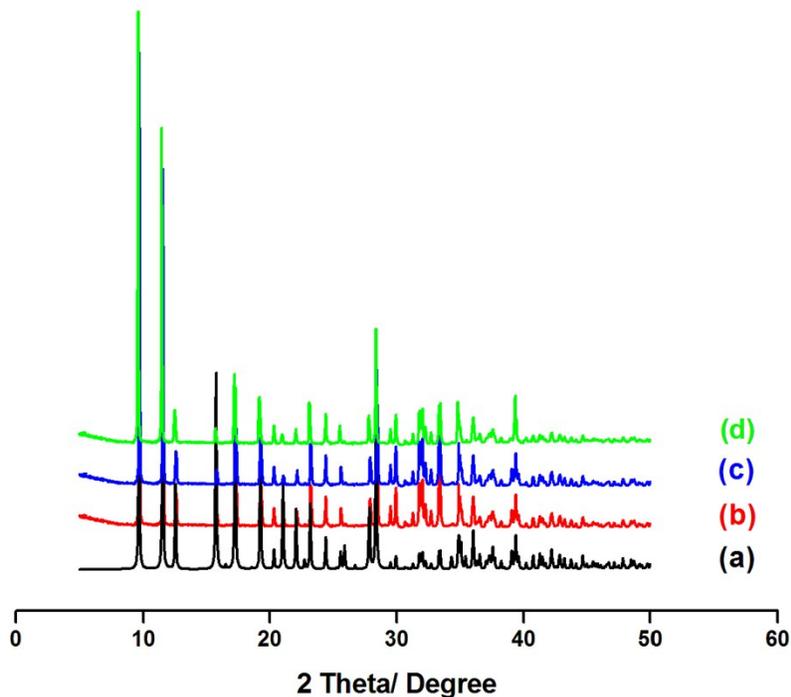
**Fig. S1.** Solid state UV-vis spectrum of **1**.



**Fig. S2.** TGA of **1**.

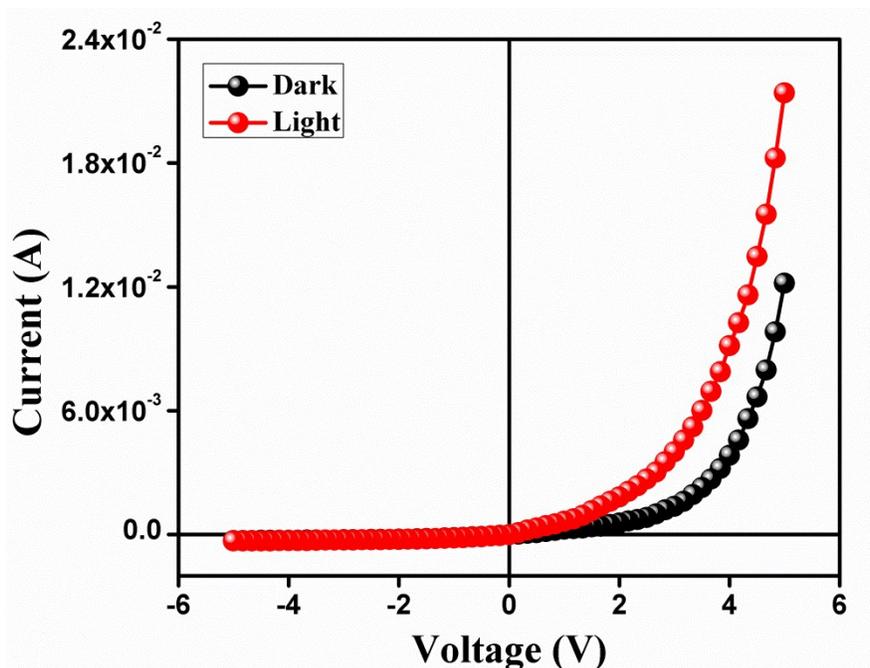


**Fig. S3.** FT-IR spectra of **1** before (a) and after (b) heating the complex at 120 °C indicating the stability of the material.



**Fig. S4.** Powder X-ray diffraction patterns of **1** in different states. (a) Simulated from single crystal X-ray diffraction data, (b) bulk material, (c) bulk material after heating at 120 °C and (d) thin film deposited on glass surface.

To ensure that the Complex 1 type material exhibits better electrical performances after exposed under illumination of incident radiation, we performed another experiment. Here we took another compound containing same 4-bpd ligand,  $\{[\text{Cd}(4\text{-bpd})(\text{N}(\text{CN})_2)_2]\}_n$  (complex 2) and fabricated same type of device with configuration ITO/2/Al. The I-V characteristics of that device were recorded under dark and under illumination of incident light and presented in Fig. S5 with the measured data in Table S1.

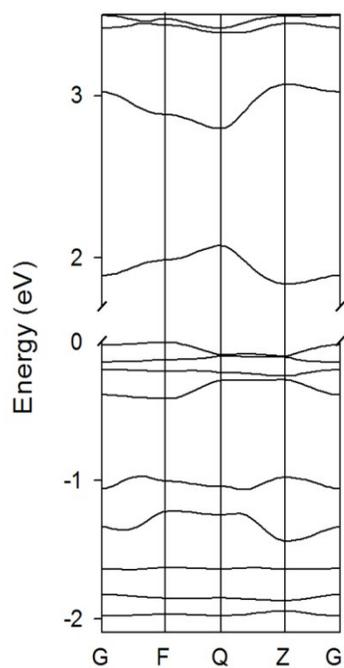


**Fig. S5.** Current–voltage (I–V) measurement of the ITO/Complex 2/Al sandwich structure

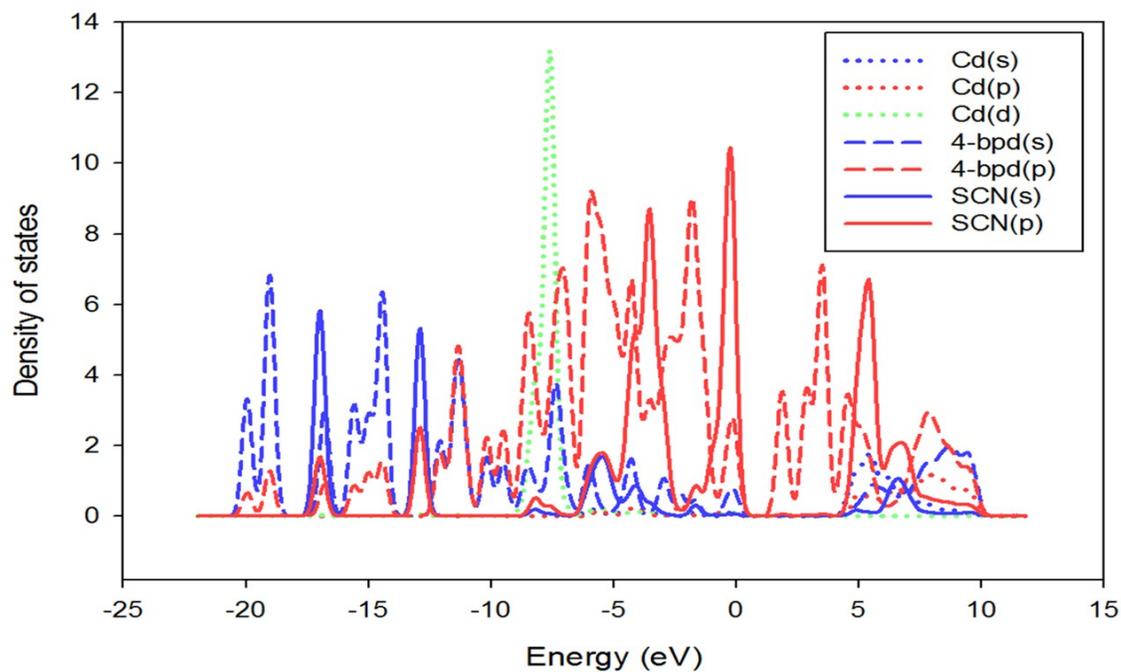
**Table S1:** Electrical parameters of ITO/ Complex 2/Al device

Condition	On/Off Ratio	Photosensitivity	Conductivity
Dark	41.28	1.75	$6.05 \times 10^{-5} \text{ S.m}^{-1}$
Light	69.03		$1.82 \times 10^{-4} \text{ S.m}^{-1}$

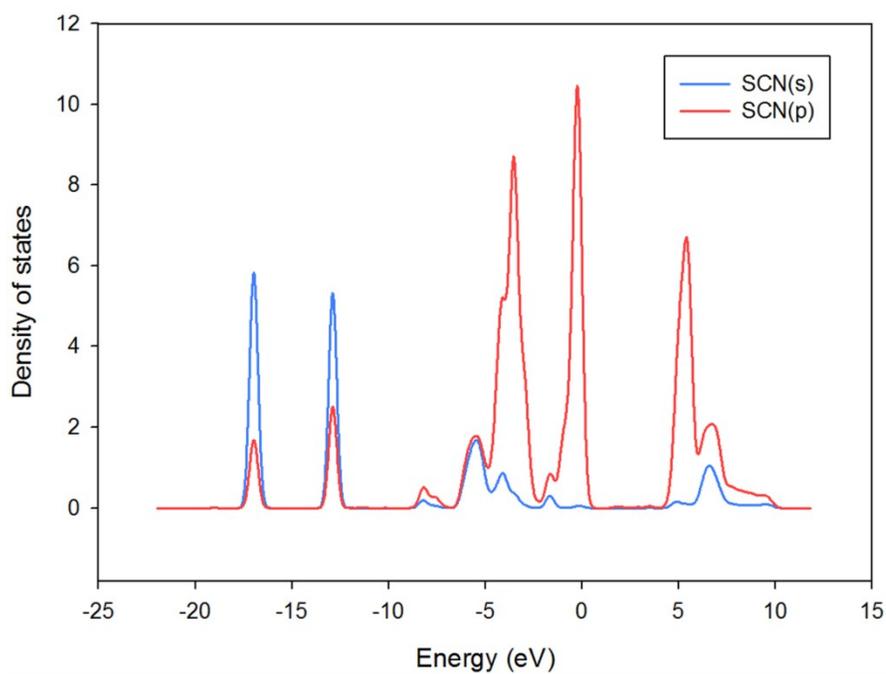
From Fig. S5 it can be seen that complex 2 shows the same kind of non-linear rectifying nature like complex 1. The measured parameters from Table S1 illustrate the enhancement in rectification ratio (on/off ratio) as well as conductivity under illumination of incident light. But comparing this obtained value of complex 2 based devices with complex 1 based device, it can be easily seen that the complex 1 based device shows better performance under same kind of experimental conditions.



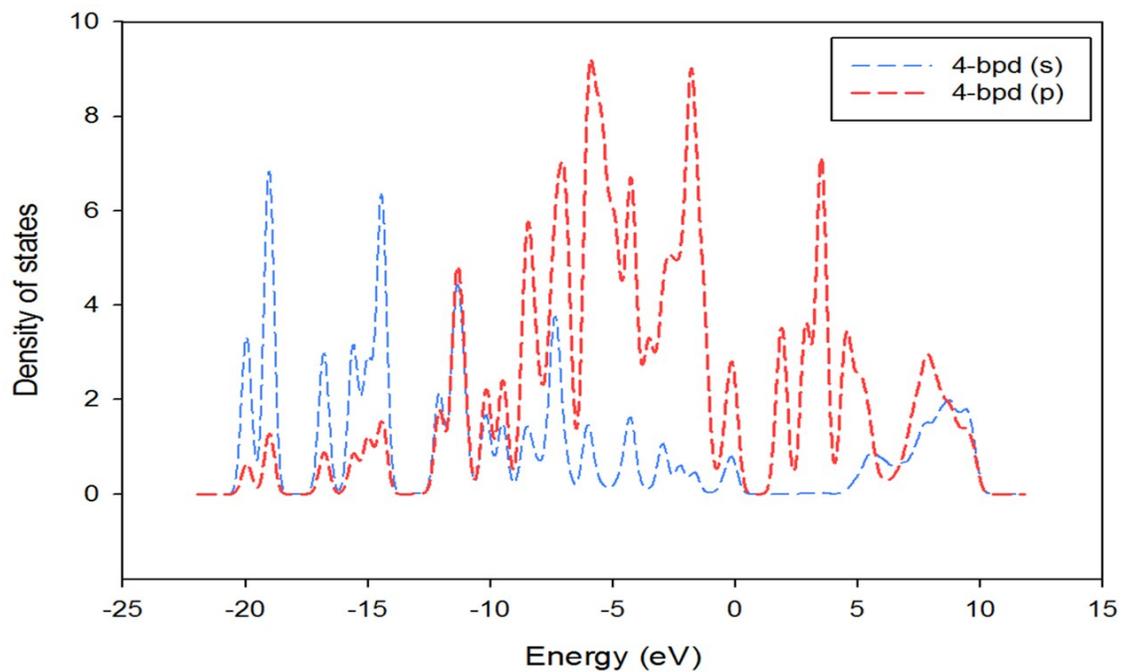
**Fig. S6.** Some electronic bands of ground state of **1**.



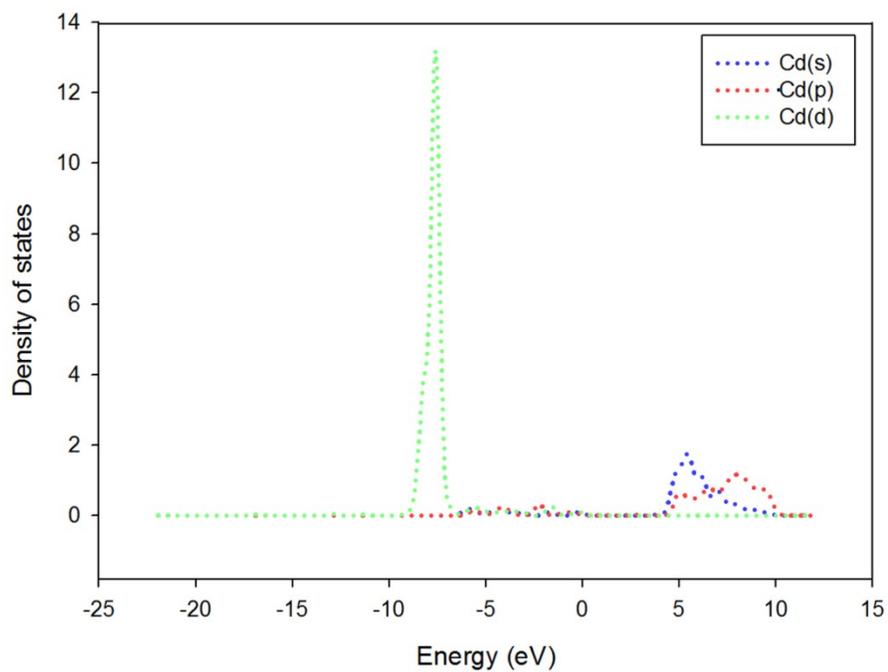
**Fig. S7.** Calculated Full Partial DOS of Cadmium atom (point lines), SCN atoms (solid lines) and 4-bpd molecule (dashed lines) of **1**.



**Fig. S8.** Calculated Full Partial DOS of SCN ‘p’ (red line) and ‘s’ (blue line) of **1**.



**Fig. S9.** Calculated Full Partial DOS of 4-bpd ‘p’ (red line) and ‘s’ (blue line) of **1**.



**Fig. S10.** Calculated Full Partial DOS of Cd ‘d’ (green line), ‘p’ (red line) and ‘s’ (blue line) of **1**.