

## **Facile fabrication of polycaprolactone/h-MoO<sub>3</sub> nanocomposites and their structural, optical and electrical properties**

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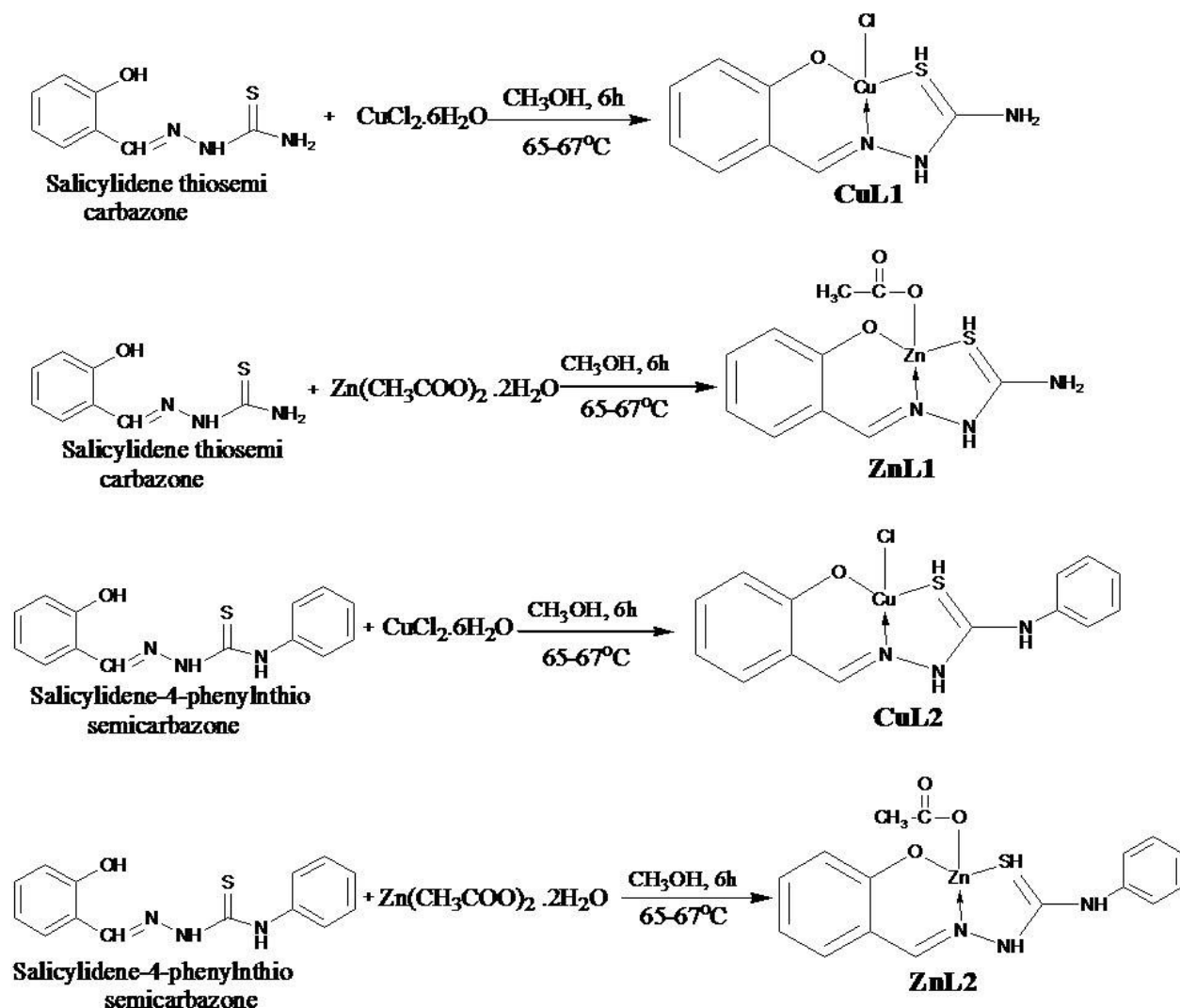
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## Electronic Supplementary Information (ESI)

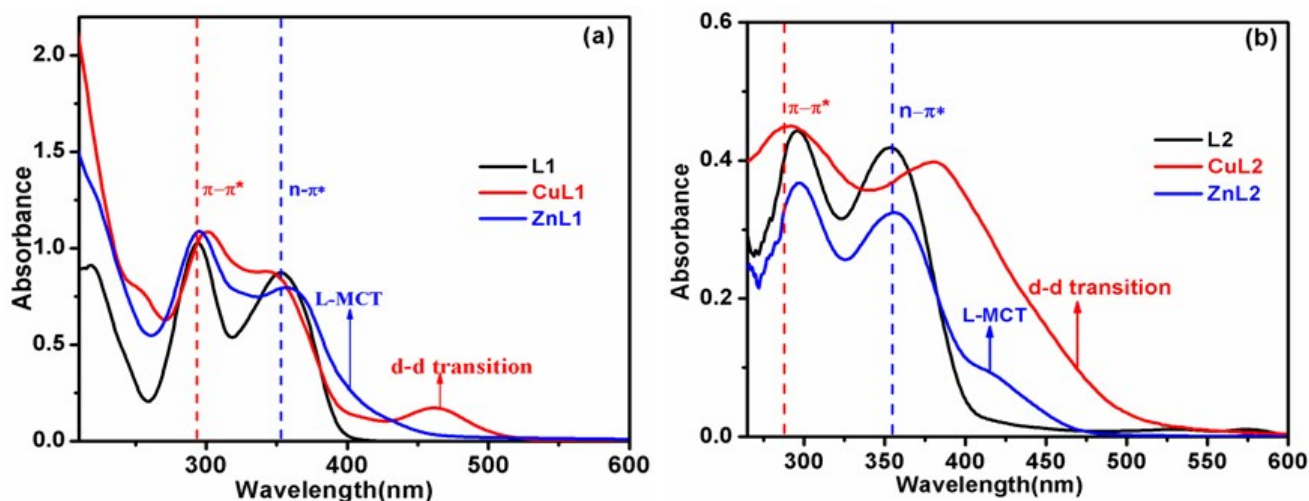


Scheme S1. Preparation of metal complexes **CuL1**, **ZnL1**, **CuL2** and **ZnL2**.

### 3.1 Characterization of catalyst

The UV-Visible spectra were recorded for **L1**, **L2**, **CuL1**, **CuL2**, **ZnL1** and **ZnL2** and the results are shown in Figure S1. The **L1** (Fig. S1 a) shows two absorption bands at 292 nm

( $\pi \rightarrow \pi^*$ ) and 352 nm ( $n \rightarrow \pi^*$ ). The **ZnL1** shows an intense band with an observable red shift at 358 nm. The shift towards longer wavelength is a consequence of coordination of ligand to the metal i.e. due to the formation of  $Zn^{2+}$  complex of **L1**. This result signifies that the  $\pi$ -bonding interactions become stronger in response to Cu(II) and Zn(II) coordination. These findings suggest that the lone pair from the oxygen atom is delocalized throughout the aromatic system, sulfur and  $-C=N$  functionalization of the phenyl ring effectively allows for an extension of  $\pi$ -conjugation. The appearance of a new broad band at 402 nm is attributed to charge transfer from ligand to metal (LMCT) transition.<sup>1</sup> For **CuL1**, an additional weak band appears at 462 nm which ascribed to d-d transition.<sup>2</sup> In Fig. S1.b the pure ligand (**L2**) shows; two different absorption bands at 294 nm ( $\pi \rightarrow \pi^*$ ) and 354 nm ( $n \rightarrow \pi^*$ ). For **ZnL2**, new bands appear at 416 nm, which ascribed to ligand to metal charge transfer spectra (LMCT). In CuL2, a new band is seen 470nm, which indicates d-d transition.



**Fig. S1.** UV-Visible spectra of (a) **L1**, **CuL1** and **ZnL1** (b) **L2**, **CuL2** and **ZnL2**.

**Table S1** Reusability nature of catalyst **ZnL1**

Entry	Cycle	[M]/[C] <sup>a</sup> ratio	Temp (°C)	Time (h)	Mn <sup>b</sup> x10 <sup>3</sup> (g/mol)	Mw <sup>c</sup> x10 <sup>3</sup> (g/mol)	Yield <sup>d</sup> %	PDI <sup>e</sup>
1	1	112:1	125	24	9.79	11.38	91	1.16
2	2	112:1	125	24	6.06	8.03	90	1.32
3	3	112:1	125	24	5.60	7.39	86	1.32
4	4	112:1	125	24	4.89	6.36	81	1.30

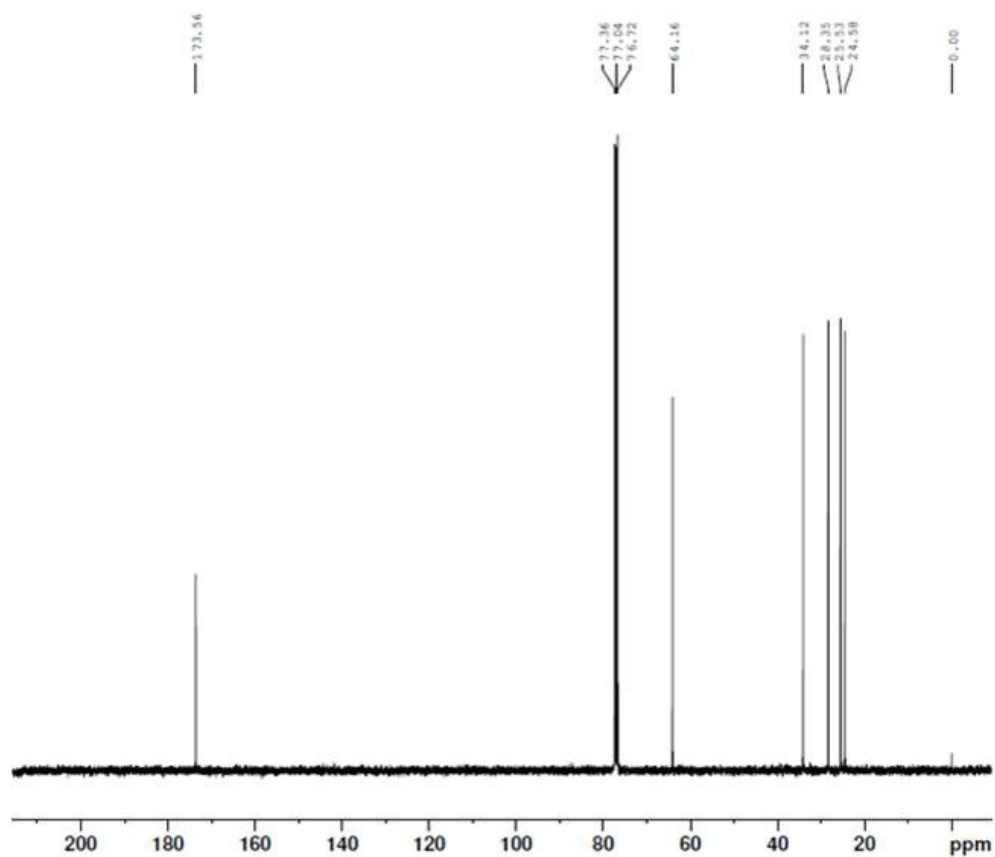
<sup>a</sup> [M]/[C] ratio is the molar ratio of monomer and catalyst.

<sup>b</sup>Mn is the relative number-average molecular weight.

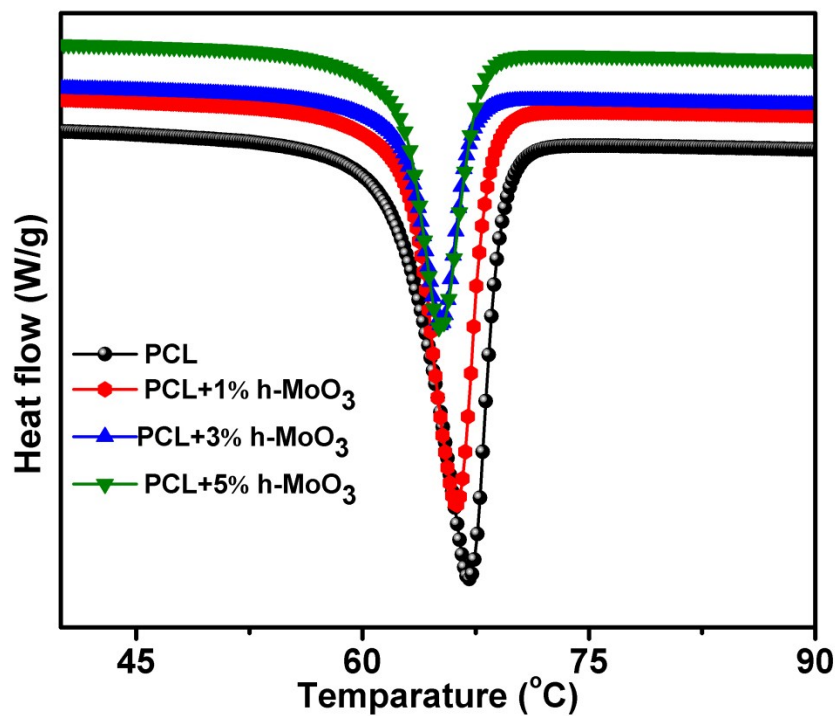
<sup>c</sup>Mw is the relative weight-average molecular weight.

<sup>d</sup> Calculated on the basis of the polymer weight.

<sup>e</sup>PDI = Mw/Mn



**Fig. S2** <sup>13</sup>C NMR spectrum of PCL



**Fig. S3.** Differential scanning calorimetry spectra of pure PCL, PCL+1% h-MoO<sub>3</sub>, PCL+3% h-MoO<sub>3</sub> and PCL+5% h-MoO<sub>3</sub>

## References

1. A. Majumder, V. Gramlich, G. M. Rosair, S. R. Batten, J. D. Masuda, M. S. El Fallah, O. J. Ribas, O. J. P. Sutter, C. Desplanches and S. Mitra; *Crystal Growth & Design*, 2006, **6**, 2355-2368.
2. K. M. Lincoln, M. E. Offutt, T. D. Hayden, R. E. Saunders, and K. N. Green, *Inorg. Chem.* 2014, **53**, 1406–1416