Facile fabrication of polycaprolactone/h-MoO$_3$ nanocomposites and their structural, optical and electrical properties

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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
(π→π*) and 352 nm (n→π*). 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 Zn²⁺ complex of L1. This result signifies that the π-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 π-conjugation. The appearance of a new broad band at 402 nm is attributed to charge transfer from ligand to metal (LMCT) transition.¹ For CuL1, an additional weak band appears at 462 nm which ascribed to d-d transition.² In Fig. S1.b the pure ligand (L2) shows; two different absorption bands at 294 nm (π→π*) and 354 nm (n→π*). 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.](image-url)
Table S1 Reusability nature of catalyst ZnL1

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<th>Entry</th>
<th>Cycle</th>
<th>[M]/[C] (^a) ratio</th>
<th>Temp (°C)</th>
<th>Time (h)</th>
<th>Mn(^b) x10(^3) (g/mol)</th>
<th>Mw(^c) x10(^3) (g/mol)</th>
<th>Yield(^d) %</th>
<th>PDI(^e)</th>
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\(^a\) [M]/[C] ratio is the molar ratio of monomer and catalyst.  
\(^b\)Mn is the relative number-average molecular weight.  
\(^c\)Mw is the relative weight-average molecular weight.  
\(^d\)Calculated on the basis of the polymer weight.  
\(^e\)PDI = Mw/Mn

Fig. S2 \(^{13}\)C NMR spectrum of PCL
Fig. S3. Differential scanning calorimetry spectra of pure PCL, PCL+1% h-MoO₃, PCL+3% h-MoO₃ and PCL+5% h-MoO₃

References
