

Supporting Information

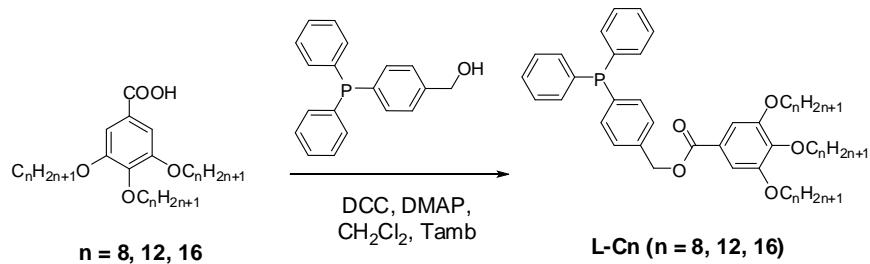
Mechanochromic Luminescence and Liquid Crystallinity of Molecular Copper Clusters

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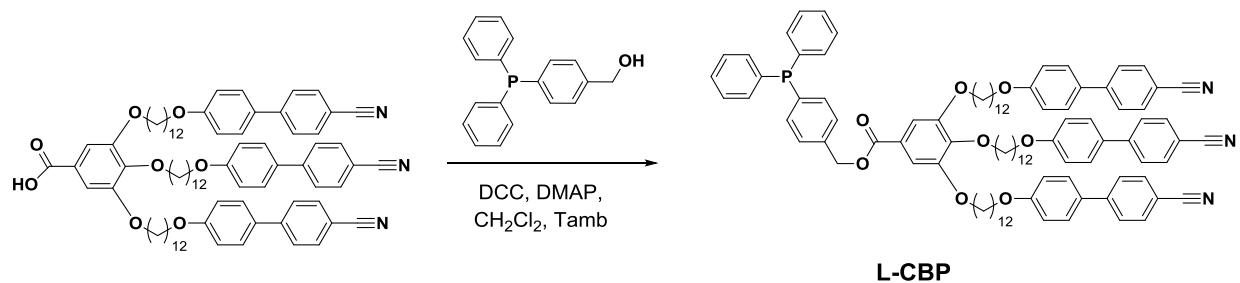
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Scheme S1. Synthesis of **L-Cn** (n = 8, 12 and 16) ligands.



Scheme S2. Synthesis of **L-CBP** ligand.

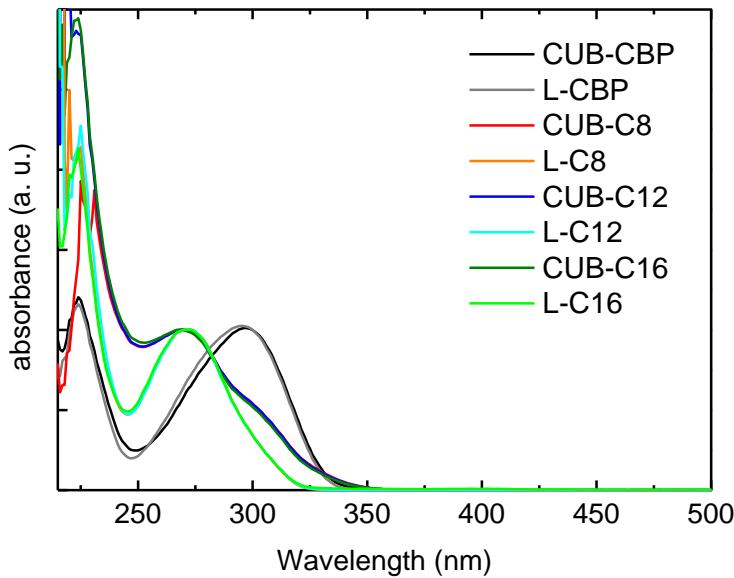


Figure S1. Normalized UV-vis. absorption spectra of clusters and ligands in dichloromethane.

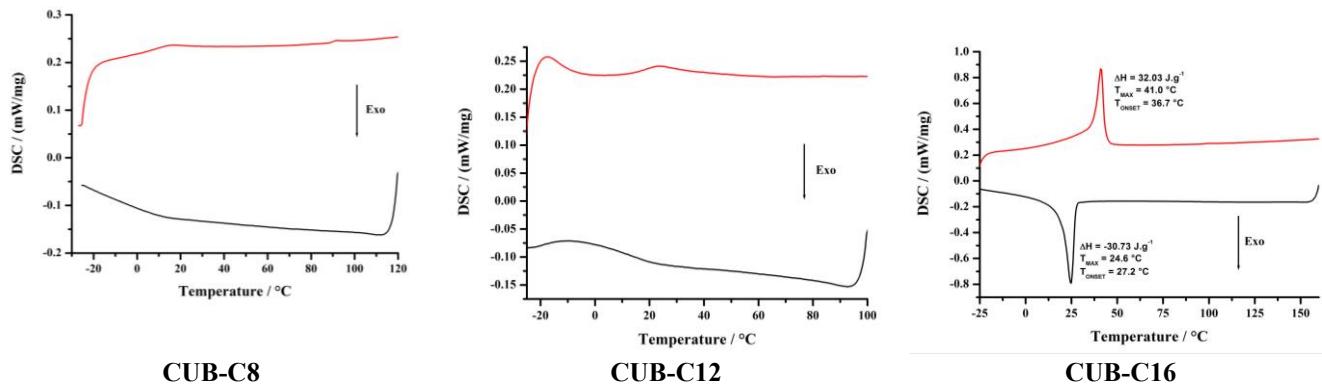


Figure S2. DSC curves of CUB-C_n ($n = 8, 12$ and 16) compounds (red: second heating curve, black: first cooling curves, $10\text{ }^{\circ}\text{C}/\text{min}$).

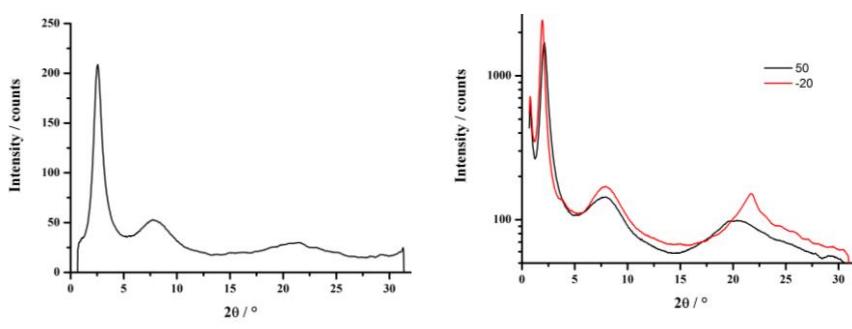


Figure S3. XRD pattern of CUB-C_n ($n = 8$ and 16) compounds.

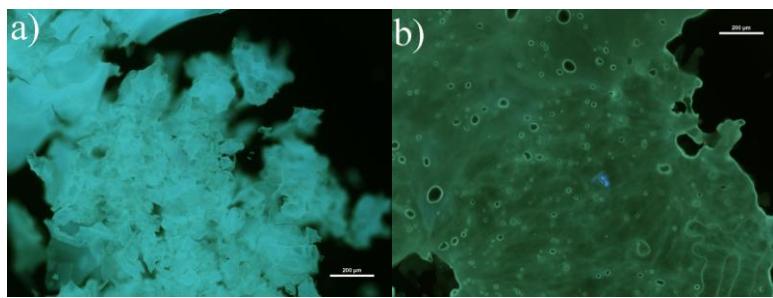


Figure S4. Pristine powder of CUB-CBP observed by optical microscopy under UV irradiation (350–400 nm) (a) at room temperature and (b) after melting at 79 °C (first heating).

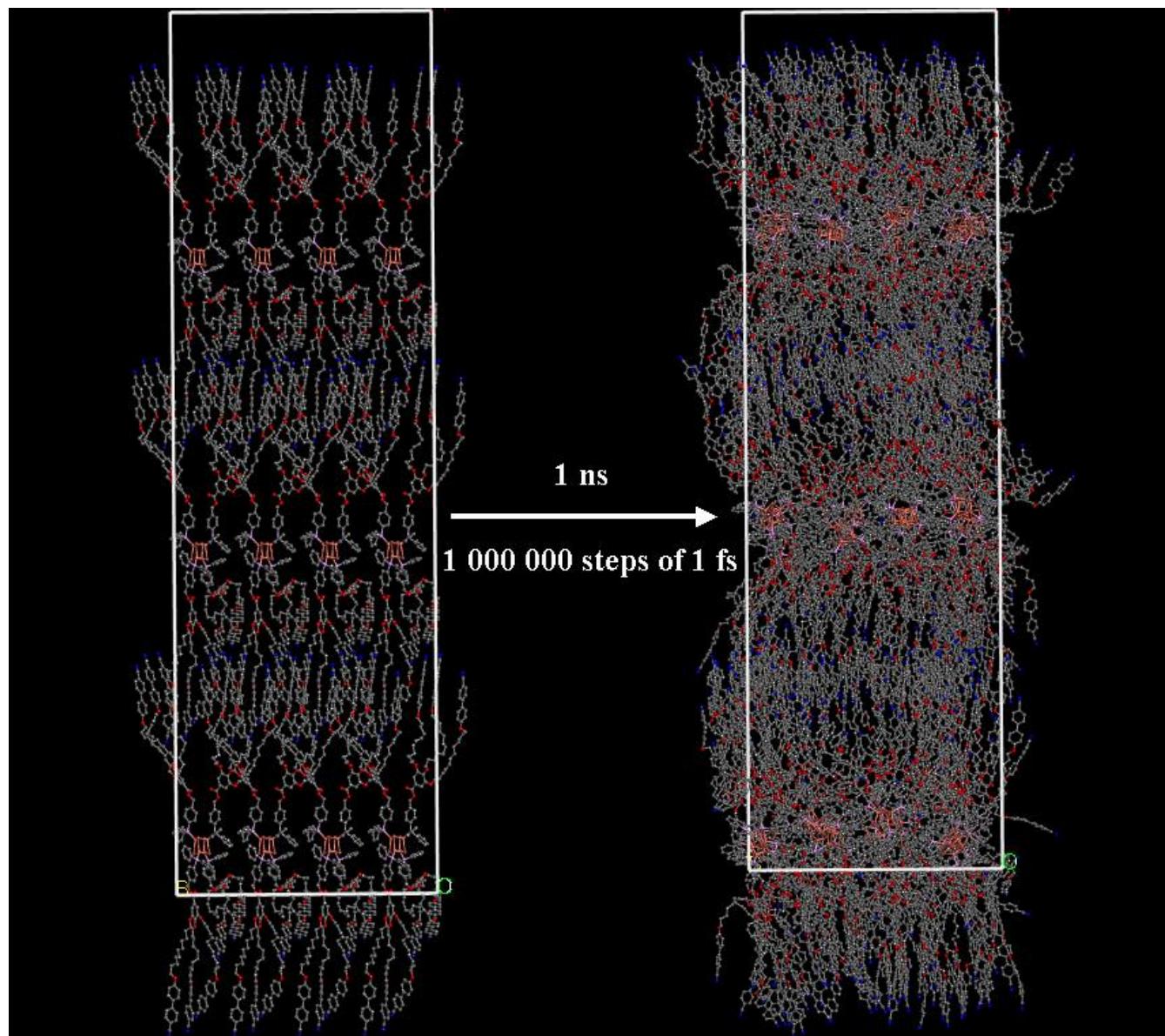


Figure S5. Packing of the CUB-CBP before and after MD in the Smectic A phase (nitrogen in blue, oxygen in red, carbon in grey, phosphorus in purple and copper and iodine in pink).

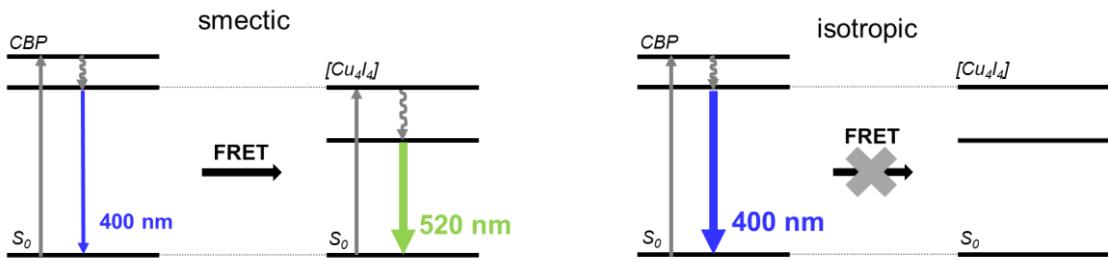


Figure S6. Simplified energetic diagram of CUB-CBP and the possible FRET mechanism with the CBP as the donor and the $[Cu_4I_4]$ cluster core as the acceptor.

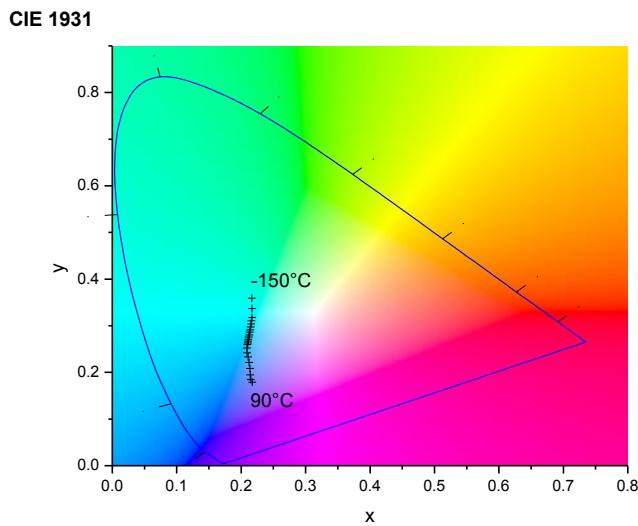


Figure S7. CIE chromaticity diagram (Commission Internationale de L'Eclairage 1931) showing the temperature-dependent emission color of CUB-CBP from 90 down to -150 °C at $\lambda_{ex} = 280$ nm.

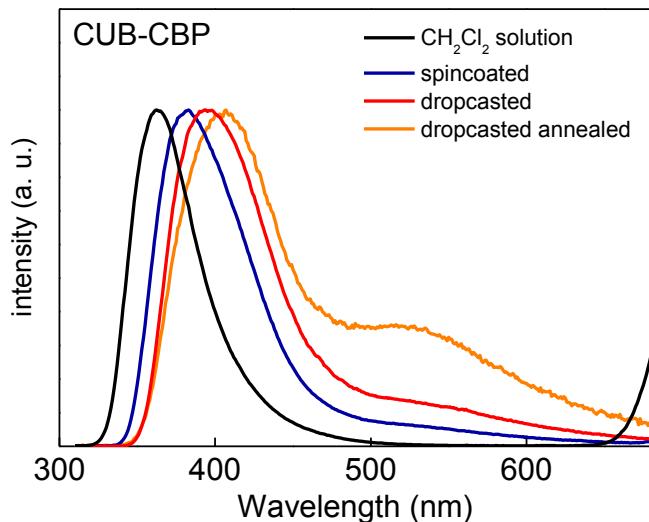


Figure S8. Normalized emission spectra of CUB-CBP in CH_2Cl_2 solution, spincoated and dropcasted on quartz substrate before and after annealing at $\lambda_{ex} = 280$ nm.