

*Dependence of optoelectronic & mesophasic properties on crystal-packing in OPEs*Sohini Bhattacharyya<sup>1</sup>, Tapas Kumar Maji<sup>1</sup><sup>1</sup>Chemistry And Physics Of Materials Unit, JNCASR, Bangalore, India

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Oligo-(p-phenylene) ethynelenes (OPE) are an intriguing class of organic molecules with rigid, highly conjugated backbone, ideal for charge/ electron transfer and brilliant luminescence. Herein we report the synthesis of a series of OPE based novel organic molecules with dialkoxypentyl side-chains and different end groups (pyridinic for 1, acetate for 2 and carboxylic acid for 3).

1 yields highly emissive light green needle shaped crystals when crystallized by a vapour diffusion method where the molecules pack in a unique staggered morphology. The interactions involved are parallelly displaced  $\pi$ - $\pi$  stacking in the longitudinal direction and weak CH...N bonding in the lateral direction. Corresponding to the crystal packing, we observed a conductivity of  $1.75 \times 10^{-7}$  S.cm<sup>-1</sup> in the longitudinal direction and  $3.31 \times 10^{-9}$  S.cm<sup>-1</sup> in the lateral direction obtained from the single crystal. Also, the compound shows mechanochromic and solvatochromic properties, along with liquid crystalline behaviour with a columnar phase.

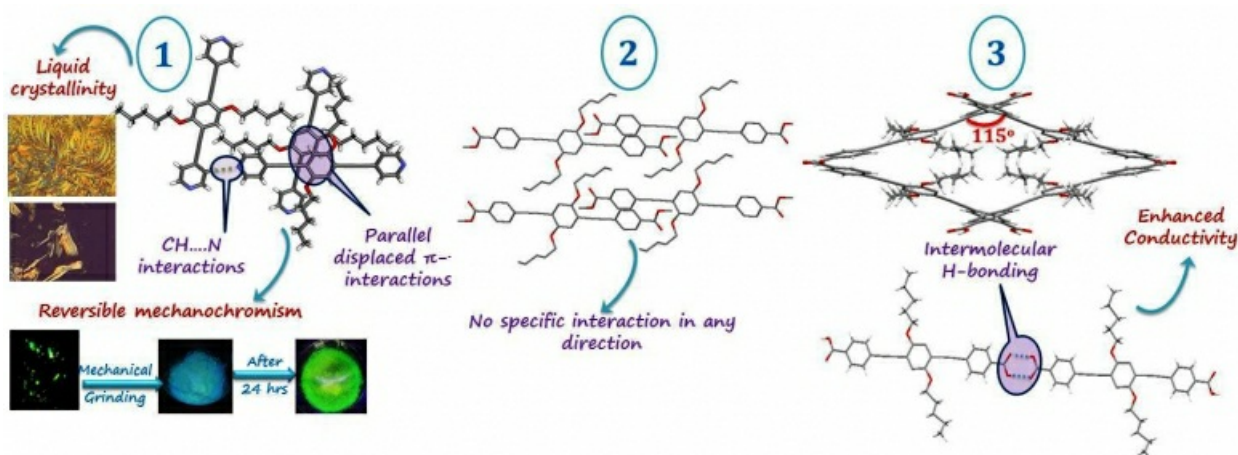
However, once the end group is changed to acetate, the crystal packing and the interactions change significantly. In the absence of any significant interaction in the crystal packing, the conductivity in both longitudinal lateral directions is rather less in 2. 2 exhibits a polymorph at 383 K, but does not have any liquid crystalline property.

Next, 2 was hydrolysed to form 3, an OPE dicarboxylic acid with dialkoxypentyl side chains. 3 has a very rigid network, where two infinite chains of hydrogen bonded molecules are aligned at 115° to one another. Owing to the inflexible structure, liquid crystalline phase is not observed in this case. But the strong interaction accentuates and enhances the longitudinal conductivity. The mechanochromic and solvatochromic properties present in 1 are absent in both 2 and 3. 1 and 3 both have metal coordination sites in the form of pyridinic nitrogens, and can be assembled to Metal-organic frameworks (MOFs) with enhanced conductivity.

1. Collis, G.E., et al. (2015). Chem. Mater., 27, 112-118.

2. Bunz, U. H. F. (2000). Chem. Rev., 100, 1605-1644

3. Dinca, M., et al. (2016). Angew. Chem. Int. Ed. 55, 3566-3579.



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