Multiscale molecular modelling of structural-electronic relationship in discotic liquid crystals

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Discotic Liquid Crystals (DLCs) have been of research interest, due to their potential applications in electronics, such as organic field effect transistors (OFETs), organic photovoltaics (OPVs) and organic light emitting diodes (OLEDs). Structurally, DLCs comprise of a rigid planar core surrounded by several aliphatic chains, which are able to self organise into columnar stacks in the liquid crystalline phase. These columnar stacks are analogous to one dimensional molecular wires, as charge transfer is enabled along the columnar axis, due to delocalisation of the pi-orbitals within the cores. In this paper, we introduce a multiscale modelling approach which integrates molecular mechanics and quantum mechanics in order to correlate the structural parameters in a DLC column, with its bandgap, density of states (DOS) and electron population characteristics. An all-atom model of two stacked HAT6 (2,3,6,7,10,11-hexahexyloxytriphenylene) molecules within a periodic cell unit was simulated using the Materials Studio simulation package. The structural parameters investigated were core-core spacing (D), lateral twist (θ) and lateral slide (L). The investigation of geometrical and energetic stabilities of HAT6 were investigated using the density functional spin polarized calculations and Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional. The DOS calculations was carried out using the Kohn–Sham equation expanded in a double numeric quality basis set (DNP ver. 4.4) with polarization functions. The DFT semi-core pseudo-potentials were used for the treatment of the electron population. In particular, electron population analysis provided vital information on the structural conditions which provide optimal intracolumnar charge transfer in DLCs. This knowledge will be useful for future use in rational design of DLCs.

Speaker Biography

Suhana Mohd Said is currently an Associate professor in the Department of Electrical Engineering, Faculty of Engineering, University of Malaya. She obtained her M.Eng. in Engineering Science from the University of Durham, United Kingdom, in 1997. She then gained her D.Phil. from the University of Oxford, United Kingdom, in Liquid Crystal Technology in 2003. Her research interests in the field of liquid crystals include ferroelectric liquid crystals, blue phase liquid crystals and discotic liquid crystals for electronics applications. She is also actively conducting research in the field of lead free solders, and thermoelectric materials and devices. She has published over 70 scientific papers, filed 5 patents, and has been invited speaker in several international conferences in the field of liquid crystals and thermoelectrics.