Density Functional Theory Study of Solid-Sate Structure and Optoelectronic Properties of Fluorene-Based Conjugated Polymers

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ABSTRACT: Using the dispersion corrected density functional theory (DFT-D/B97D) approach, we have performed molecular and solid-state calculations to study the influence of intra- and inter-molecular interactions on the bulk structure and the electronic and optical properties of fluorene based conjugated polymers. In particular, we investigate the role of side-chain length on the molecular packing and optical properties of poly (9, 9-di-n-alkylfluorene-alt-benzothiadiazole) or FnBT's where n is the number of CH$_2$ units in the alkyl side-chains. The results indicate that for the FnBT with longer side-chains, due to the significant inter-molecular interactions between the side-chains the packing of these polymers forms a lamellar structure. On the other hand, for the FnBT with shorter side-chains, the cylindrical phase is more favorable and the corresponding crystals are almost hexagonal. These different packing structures can be attributed to the microphase separations between the flexible side-chains and the rigid backbones and are in agreement with previuos investigations for other hairy-rod polymers. In addition, as a result of the efficient inter-chain interactions for the lamellar structures, the dihedral angle between the F and BT units is reduced by about 30° providing a more planar backbone which in turn leads to a decrease, of about 0.2 eV and 0.3 eV, in the band gap of the lamellar structure relative to its value for the gas and cylindrical phases respectively. Time-dependent DFT is also used to study the excited states of the monomer of FnBT with various lengths of side chains.

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