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The Effect of Side-Chain Length on the Solid-State Structure and Optical Properties of F8BT: A DFT Study<sup>1</sup> MOHAMMAD JAVAD ES-LAMIBIDGOLI, JOLANTA B. LAGOWSKI, Memorial University of Newfoundland — Using the long-range corrected hybrid density functional theory (DFT/B97D) approach, we have performed bulk solid state calculations to investigate the influence of side-chain length on the molecular packing and optical properties of poly (9,9-din-octylfluorene-alt-benzothiadiazole) or F8BT. Two different packing structures, the lamellar and nearly hexagonal, were obtained corresponding to longer and shorter side-chains respectively. This behavior can be attributed to the micro-phase separations between the flexible side-chains and the rigid backbones and is in agreement with previous investigations for other hairy-rod polymers. In addition, as a result of the efficient inter-chain interactions for the lamellar structure, the dihedral angle between the F8 and BT units is reduced providing a more planar configuration for the backbone which leads to the decreased band gap (by 0.2-0.3 eV) in comparison to the hexagonal phase and the gas phase with no side-chain. Time-dependent DFT (TDDFT/B3LYP) was also used to study the excited states of the monomer of F8BT optimized in solid-state structures with different side-chain lengths. It is found that the absorption spectrum is red shifted for the polymers with lamellar structure relative to the polymers in hexagonal and gas phases.

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