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Conformational Dependence of Charge Transport and Band Gap in Poly (3-Hexyl Thiophene) Oligomers RAM BHATTA, Department of Chemistry, The University of Akron, OH 44325-3601, YENENEH YIMER, MESFIN TSIGE, Department of Polymer Science, The University of Akron, OH 44325-3909, DAVID PERRY, Department of Chemistry, The University of Akron, OH 44325-3601 — Structural defects will affect the charge transport properties and the band gap in the Poly (3-Hexylthiophene) (P3HT) polymer, a promising electron donor for organic solar cells. In the present work, such effects are modeled by density functional theory (DFT) calculations on P3HT oligomers up to 12 monomer units in planar and non-planar conformations. DFT calculations were performed at B3LYP/6-31++G(d,p) treating both backbone and hexyl chains explicitly. The structural properties of the oligomers change significantly for 2 to 8 unit isolated oligomers but reach asymptotic values by a 10 unit P3HT chain. The dependence of charge transfer integral on chain length and on the backbone torsional angle is reported. The band gap approaches ∼2.0 eV asymptotically as the chain length is increased, which is close to the experimental value. Comparison of the charge transport integral for P3HT with polythiophene (PT) shows that the hexyl chains enhance electronic coupling across the P3HT chain. The charge transport integral declines exponentially as the oligomers are lengthened with a half-length of 4.4 units.

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