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Frontier Orbital Energy Change of Poly(3-Hexylthiophene) Oligomers: Effect of Large Amplitude Torsional Motion[1] RAM BHATTA, Department of Chemistry, The University of Akron, MESFIN TSIGE, Department of Polymer Science, The University of Akron, DAVID PERRY, Department of Chemistry, The University of Akron — Poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61-butyric acid methylester (PCBM) based solar cells remain the most promising organic photovoltaics so far. Despite their promise for organic solar cells, practical application is hindered by low efficiency, associated with poor electron transport from P3HT to PCBM. For isolated P3HT oligomers, we investigate the torsional dependence of electronic properties by performing DFT calculations and extrapolate to the long chain limit. The fully relaxed isolated P3HT oligomers are non-planar with a 47 degree twist angle between each pair of rings and are lower in energy by 0.03 eV per monomer unit than the fully planar oligomers. The non-planarity lowers highest occupied molecular orbital (HOMO) energy by 1 eV and rises lowest unoccupied molecular orbital (LUMO) energy by 0.6 eV compared to the respective orbital energies in a planar P3HT. The shifts in HOMO and LUMO energies increase the band gap from 1.9 eV in planar P3HT up to 3.3 eV when all backbone angles are non-planar and point to a reduced electrical conductivity. The larger band gap in non-planar P3HT accounts for the observed blue shift in the visible P3HT absorption band in P3HT/PCBM mixtures.

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