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First Principles Calculations of Conformational and Electronic Properties of PTB7[1] RAM BHATTA, DAVID PERRY, MESFIN TSIGE, The University of Akron — The thieno[3,4-b]thiophene-altbenzodithiophene copolymer (PTB7) is a promising electron donor in organic photovoltaic (OPV) devices with a power conversion efficiency (PCE) of about 9 percent. Further enhancement of the PCE is required for the practical realization and successful commercialization, which, in turn relies on the core understanding of structure-property relationships in OPV materials. Here, we present large-scale density functional calculations of the torsional and electronic properties of PTB7 oligomers. These first principles results include the chain length dependence of the torsional potential, the nearest neighbor torsional coupling, the band gap and the electronic conjugation length. PTB7 was found to have weaker nearest-neighbor torsional coupling, a lower band gap and a longer conjugation length compared to the other conjugated polymers like polythiophene and poly(3-alkylthiophene). These results help to explain the relative efficiency of OPV devices in which PTB7 is the electron donor.

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Ram Bhatta
The University of Akron

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