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Chain Shapes and Ordering of Conjugated Polymers from Atomstic Simulations WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Pennsylvania State Univ — Conjugated block copolymers, such as P3HT-b-PFTBT, are candidates for optimizing the efficiency of OPVs due to their self-assembly on different length scales. With microphase separated domains, and sharp interfaces between donor and acceptor blocks, transfer of excitons and free charge carriers is enhanced and charge recombination is reduced. To better understand mesocopic and interfacial packing and ordering of these materials, homopolymers are first investigated via atomistic simulations. We proposed a numerical averaging method and an analytical approach to estimate single chain dimensions of semiflexible polymers based on DFT computed dihedral potentials. Estimations are compared to our MD simulation results of polymer melts. Shorter persistence lengths from MD simulations indicate side groups and inter-chain interactions bring flexibility to polymer backbones. By assuming molten polymers as persistent chains of rods, nematic phase transitions and orderings of these materials are also discussed.

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