

Atomistic Simulations to Predict Semiconducting Polymer Blend Morphology Effect on Charge Transport

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Blends are crucial for many organic electronic devices, including electrochemical transistors, light-emitting diodes, and solar cells. For example, the performance of organic photovoltaics (OPVs) depends on the electronically active layer blend morphology, which influences the charge transfer rate and exciton dissociation. Yet a faithful representation of the interface and the local structure of polymers is lacking. In principle, molecular dynamics simulation can represent these blend morphologies. However, semiconducting polymers with aromatic rings are large, stiff, and slowly relaxing, which makes equilibration challenging. We develop a new coarse-graining (CG) method, which improves simulation efficiency ten-fold by representing aromatic rings as rigidly bonded moieties, in which we represent several atoms as virtual sites. We use this method to characterize the morphology of a typical OPV blend: P3HT (donor) and O-IDTBR (acceptor). We find that moieties with solubilizing side-groups have fewer electronic contacts because of steric hindrance. On slow cooling, the fast simulation method allows us to observe crystallization, which occurs more readily in pure P3HT than in the blend. Our simulations represent the local structures of small mixed regions; on larger scales, P3HT and O-IDTBR demix. To describe the resulting interface, we need the Flory-Huggins χ parameter. We measure χ using a new “push-pull” technique, which applies robustly to polymer blends of any architecture. The method applies equal and opposite potentials to polymers in a blend to induce a concentration variation, which is more pronounced for polymers with repulsive interactions ($\chi > 0$). We test the method by blends of bead-spring chains, then apply it to estimate χ for a blend of P3HT and O-IDTBR. Combining local structures from our CG representation and the χ parameter using the “push-pull” technique, we obtain a comprehensive view of the OPV blend morphology.