High-throughput molecular simulations into the morphology of P3HT:PCBM blends

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Introduction

Organic solar cells are advantageous because they can be processed cost and energy efficiently out of abundant materials and roll-to-roll printed onto flexible substrates. However, they currently suffer from low efficiency.

The goal of this research is to understand the effect of temperature, solvent quality, solvent amount, and concentrations of organic/porous donor molecules on active layer morphology. This morphological control is critical to device efficiency because it impacts the mobility of charge carriers through the active layer to the electrodes (see Figure 1).

We use HOOMD-blue, a particle simulation Python package including molecular dynamics, to simulate P3HT:PCBM blends (PC61BM and PC71BM) on a supercomputing cluster. We run simulations of several hundred molecules for up to 48 hours at a time.

Molecular Model

We use a united atom model and rigid bodies to simulate the molecules in our systems. The P3HT model is a 15-mer with the thiophene rings (rings of blue and orange atoms in Figure 2) treated as rigid bodies. The PC61BM molecule is approximated by two rigid bodies, one for the endocycle and one for the benzenoid ring, while the PC71BM is made up of one rigid body containing the bucylic unit and benzenes ring.

We use the Optimized Potential for Liquid Simulation for United Atoms (OPLS-UA) force field to approximate the bonded, non-bonded, angle, and dihedral interactions within and between molecules. Our O is 3.90 Å as prescribed by OPLS-UA.

Morphology Characterization

In order to characterize the morphology of our systems, we use the following tools:
- Visual Molecular Dynamics (VMD): molecular visualization program useful for 3D-rendered eye observations and rough measurements of structure
- Clustering algorithm: calculates and shows visualization of molecular aggregation
- Radial distribution function (RDF): calculates the occurrence of inter-structure distances, peaks in the graph correspond to distances with high probability.
- Simulated grazing incidence X-ray scattering (GIXS) patterns: help reveal the characteristic length scales and directionality of periodic features in a morphology.
- Structure factor: radial average of a GIXS pattern that, like the RDF, yields characteristic length scales of a morphology, but in frequency space rather than coordinate space.
- Potential energy: a flat potential energy over time can indicate system equilibration, a downward trend indicates movement toward more energy minimizing configurations.
- P3HT end-to-end distance: provides information about the shape of the oligomers which can affect their ability to stack.

Results - P3HT:PCBM Blend

In Figure 6, we compare the results of nominallyidentical PC61BM and PC71BM blends. The phase transition is evident above the appearance of the (001) peak representing the distance between neighboring P3HT oligomers within a stack. A second nearest neighbor peak is also visible in Figure 4.

The potential energy in the disordered system decreases by only 0.2% compared to 1.2% in the semi-ordered system since the system that self-assembles is progressing into a lower energy nanodomall morphology whereas the disordered system has an implicit solvent strong enough to dissolve the P3HT and prevent self-assembly.

Future Work

- Sampling parameter space at finer intervals
- Running higher throughput simulations
- Morphology Characterization
- Potential energy vs. time: the melt temperature vs. time curve used to calibrate the simulation temperature to the experimental temperature.
- Charge transport calculations
- The project of this purpose is to connect device morphology to device efficiency. The next step involves simulating devices and testing the simulations' morphology and eventually simulating entire devices using these morphologies.
- Quantitative characterization of difference in two PCBS systems
- The two systems look qualitatively similar but will likely differ in electronic properties (e.g. charge transport) due to minor differences in ordered morphologies.

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References:


