Multiscale Modeling of Organic Solar Cells

Chun-Wei Pao
Academia Sinica

Organic solar cells (OSCs) are promising sources for solar energy harvesting because of their low production costs, mechanical flexibilities, and light weight comparing with their pure inorganic counterparts. The key toward OSC device performance is the nanomorphology of the bulk hererojunction (BHJ) layer - the photoactive layer comprising an interpenetrating, bicontinuous network of electron donor/acceptor materials. In OSCs, the electron donor materials are usually semiconducting organic polymers/small molecules, whereas electron acceptor materials are usually fullerenes or their derivatives such as PCBM, or semiconductor nanocrystals such as TiO2. The formation of BHJ layer relies on phase separation between electron donor and acceptor phases, which critically depends on the device fabrication conditions. Hence, comprehensive insights into the correlations between device fabrication conditions and resultant BHJ nanomorphologies are important for optimizing device performances. Nevertheless, experimental characterization of the nanomorphologies of the BHJ layer is never trivial. In this work, we will present our works in developing multiscale coarse-grained model to simulate the morphology evolution of the BHJ layer during thermal annealing, solution processing, and vacuum co-deposition processes, with system size compatible with those in experiments. Our simulation results can provide multi-resolution morphological details - ranging from mesoscale morphological properties to molecular scale packings, which are not yet available from experiments. Hence, the multiscale molecular simulation platform we constructed can potentially be helpful to reveal the correlations between device fabrication protocols and resultant device performance, thereby helping experimental teams optimize OSC fabrication protocols to further promote device performance of next-generation OSC devices.