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NANOMORPHOLOGY OF ORGANIC SOLAR CELLS FROM MULTISCALE MOLECULAR SIMULATIONS

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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. Electron donor materials are usually semiconducting polymers/small molecules, whereas electron acceptor materials are usually fullerenes or semiconducting nanocrystals (e.g. TiO_2 nano rods). 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 talk, we will present our works in developing a multiscale molecular simulation platform to simulate the morphology evolution of the BHJ layer under various electron donor/acceptor blends (polymer/fullerene, and polymer/inorganic nano crystals) and device fabrication processes (thermal annealing and solvent evaporation), with system size compatible with those in experiments [1, 2]. Our simulation results were in excellent agreements with available experimental data, and we 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 carry out *in silico* OSC device fabrication experiments to help experimental teams optimize OSC fabrication protocols to further promote device performance of next-generation OSC devices.

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