CENTER FOR EXCITONICS SEMINAR SERIES

Polymer-Acceptor Bulk Heterojunction Solar Cells: from Chemical Structure to Packing and Efficiency

Jean-Luc Bredas

Georgia Institute of Technology

Department of Chemistry

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The morphology of the active layer of a bulk heterojunction (BHJ) solar cell, made of a blend of an electron-donating polymer and an electron-accepting fullerene or nonfullerene derivative, is known to play a determining role in device performance. Here, based on the results of molecular dynamics simulations and long-range corrected density functional theory calculations, we first describe the nature of the binding interactions at the donor–acceptor interfaces, the molecular-level packing in the pure phases as well as at these interfaces, and the impact of the system dynamics on the interfacial electronic structure.

We then discuss how even minor changes in the chemical structure of the polymer backbone have been shown experimentally to change substantially the blend morphology and the resulting solar-cell efficiency. Taking a series of representative systems based on benzothiadiazole-quaterthiophene polymers and $PC_{71}BM$, we elucidate the impact of the chemical changes on the "local" morphology. We focus on the extent of polymer-fullerene mixing, on their packing, and on the characteristics of the fullerene-fullerene connecting network in the mixed regions, which are all aspects that are difficult to access experimentally. We are able to rationalize the evolutions in power conversion efficiencies within the polymer series. Finally, we address the peculiarities observed in the PIPCP-fullerene blends.RC - Starting Investigator Award (2009) and the ERC - Consolidator Grant (2013).

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