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Impact of polymer/fullerene intermolecular interactions on the performance of organic solar cells

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In this presentation, we seek to provide a rationalization of the impact that intermolecular arrangements and interactions at the polymer/fullerene interfaces have on the performance of bulk-heterojunction solar cells. We discuss the results of combined electronic-structure calculations and molecular-dynamics simulations both for representative systems reported in the literature and new systems synthesized in our Center. In particular, we examine:

(i) the propensity of the fullerene molecules to dock preferentially on top of the electron-poor moiety or electron-rich moiety of the polymer, as a function of the nature and location of the polymer side chains; and

(ii) the impact that the packing arrangements have on the energetic distribution of the charge-transfer interfacial electronic states and their localization/delocalization characteristics.

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