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Microscopic simulations of electronic excitations in donor-acceptor heterojunctions of small-molecule based solar cells BJOERN BAUMEIER, Max Planck Institute for Polymer Research — Fundamental processes involving electronic excitations govern the functionality of molecular materials in which the dynamics of excitons and charges is determined by an interplay of molecular electronic structure and morphological order. To understand, e.g., charge separation and recombination at donor-acceptor heterojunctions in organic solar cells, knowledge about the microscopic details influencing these dynamics in the bulk and across the interface is required. For a set of prototypical heterojunctions of small-molecule donor materials with C_{60}, we employ a hybrid QM/MM approach[1] linking density-functional and many-body Green's functions theory[2] (DFT/GW-BSE) to polarizable force-fields[3] and analyze the charged and neutral electronic excitations therein. We pay special attention the spatially-resolved electron/hole transport levels, as well as the relative energies of Frenkel and charge-transfer excitations at the interface. Finally, we link the molecular architecture of the donor material, its orientation on the fullerene substrate as well as mesoscale order[4] to the solar cell performance.

[1]JCTC **7**, 3335 (2011)
[2]JCTC **8**, 2790 (2012)
[3]JCTC **10**, 3140 (2014)
[4]Nat. Mater., **in print** (2014)

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