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Multiscale modeling of excitation dynamics in molecular materials with GW-BSE/MM BJOERN BAUMEIER, Department of Mathematics and Computer Science Institute for Complex Molecular Systems, Eindhoven University of Technology — 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 heterojunctions of small-molecule donor materials with C60, we employ a hybrid QM/MM approach [JCTC 7, 3335 (2011)] linking density-functional and many-body Green's functions theory [JCTC 8, 2790 (2012)] (DFT/GW-BSE) to polarizable force-fields [JCTC 10, 3140 (2014)] and analyze the charged and neutral electronic excitations therein. We develop models for both static and dynamic properties of the excitations, including (a) the diffusion of Frenkel excitons and (b) the relative energies of Frenkel and charge-transfer excitations at the donor-acceptor interface and the resulting charge separation dynamics. Our simulations allow linking the molecular architecture of the donor material, its orientation on the fullerene substrate as well as mesoscale order [Nat. Mater. 14, 434 (2015)] to the solar cell performance.

Bjoern Baumeier
Department of Mathematics and Computer Science
Institute for Complex Molecular Systems, Eindhoven University of Technology

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