

# In silico characterization of polymer-fullerene organic photovoltaic bulk heterojunctions

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In organic photovoltaic materials an ultrafast electron transfer starts the (eventual) charge separation process. The morphology of the active layer impacts the different pathways which this first step can lead to. This is investigated via a range of computational techniques, which allows to consider the relevant length and time scales.

Organic solar cells (OSCs) are among the new generation photovoltaic technologies which could be employed to convert solar energy. The most efficient OSCs fabricated to date require a bulk heterojunction, an active layer composed of intimately intermixed electron acceptors – molecules with a high electron affinity such as fullerene derivatives – and electron donors – such as semiconducting polymers. The morphology of this layer has been shown to be crucial for the efficiency of the device because of its decisive impact on the charge separation process. However, a fundamental understanding of the relationship between morphology, electronic properties and efficiency is still sought after.

Coarse-grain (CG) models compatible with the Martini CG force field [1] are used to generate morphologies via large-scale solvent evaporation simulations [2], allowing the study of the morphology as a function of the structure of the molecules. These CG morphologies are then back-mapped to atomistic resolution. The electronic structure of molecules at the interfaces and in the bulk is determined with quantum chemical (QC) calculations. Particular attention is given to the distribution of microscopic properties (excited state energies, local dielectric response, Fig. 1) and how these impact macroscopic properties (exciton binding energy, dielectric constant) and the charge separation process.

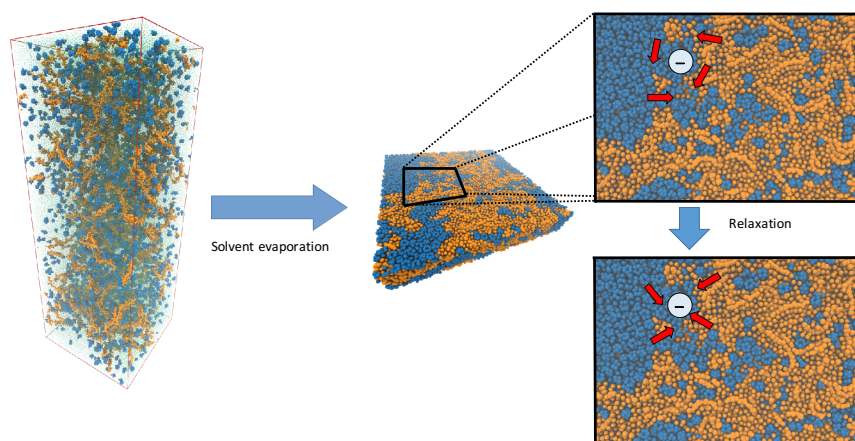


Fig 1. A coarse-grain morphology is obtained by solvent evaporation simulations (left-hand side; the polymer is depicted in orange, while the fullerene in blue). The local dielectric response of the blend around a charge can then be investigated (a schematic of an electron is depicted as a light blue particle, in the right-hand side of the picture, while relevant dipoles on the donor and acceptor molecules are shown as red arrows).

- [1] S. J. Marrink, H. J. Risselada, S. Yefimov, D. P. Tieleman, A. H. de Vries, *JPCB*, **111**, 7812 (2007).  
[2] R. Alessandri, A. H. de Vries, R. W. A. Havenith, S. J. Marrink, *in preparation*.