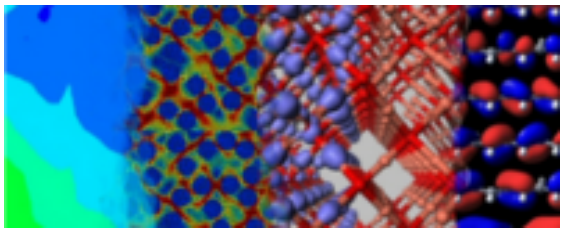

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Three-dimensional modelling of transport, injection and recombination in organic light-emitting diodes

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Charge transport in organic semiconductors can be described by hopping of charge carriers between localized states. The energetic disorder present in those organic semiconductors leads to the percolation of charge carriers, resulting in an inhomogeneous filamentary three-dimensional current density. We present a complete Monte Carlo modelling study of charge transport, injection and recombination in organic light-emitting diodes. The effects of space charge, image-charge potentials close to the electrodes, finite injection barriers, and the complete dependence of the mobility on the temperature, the carrier density and the electric field are taken into account. While the obtained 3D current density is very inhomogeneous, the total current through the devices agrees quite well with existing analytical models. The inclusion of short-range Coulomb interactions leads to a slight change of the total current due to two effects: blocking of filaments and declotting of charge carriers. The recombination rate in a bulk organic semiconductor can be well described by the Langevin recombination formula when the correct mobility, correcting for the presence of both electrons and holes, is used. All these results were obtained while assuming a cubic lattice of sites, a Miller-Abrahams hopping formalism and a Gaussian site energy distribution. Recently, we started with a multi-scale computational scheme in which we integrate several different simulation methods covering one or more length- and/or time-scales. By means of a coarse-grained Monte Carlo method and well established force field parameterizations, the morphology of the organic semiconductor can be simulated. These morphologies are then used in DFT simulations to calculate the site energies of the hopping sites and the transfer integrals between those sites. The corresponding site energies and transfer integrals are then used in a kinetic Monte Carlo program to simulate the three-dimensional charge carrier current density and recombination profiles.

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