Modeling and simulation of organic semiconductor devices: A drift diffusion perspective

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In this contribution we demonstrate how macroscopic models can be used to gain in-depth insight into essential mechanisms governing the performance of organic electronic devices.

As a major working horse, we rely on two-dimensional drift-diffusion based simulations that, in essence, self-consistently solve the current density and continuity equations for electrons and holes and the Poisson equation. Moreover, we self-consistently consider thermionic and tunneling injection currents, as well as interface recombination and back drift currents at the interfaces between metal contacts and the organic semiconductor.

Prototypical challenges in dealing with organic electronic devices are: (i) Organic semiconductors possess only a negligible amount of mobile carriers even at room temperature due to their large energy gap. To establish any current, carriers need to be provided either by injection at contacts or by (photo-) generation. (ii) Transport occurs through a semiconducting layer that often possesses a marked degree of disorder. (iii) In many applications, devices possess a huge aspect ratio; currents may need to be established across several micrometers while the active layer is just a few tens of nanometers thick.

Two illustrative examples from our previous research will be shown in which these specific challenges were tackled successfully with drift-diffusion models: One deals with the role of the polymer:nanoparticle blend ratio on the efficiency organic-inorganic nanocomposite solar cells and a second example with understanding the impact injection on the performance organic thin-film transistors. Beyond discussing the results of the simulations, these examples allow us to comment on the limitations of this macroscopic approach and on the possibilities to incorporate information from models acting on lower length scales.