ORAL presentation

Scale-Bridging Models for Organic Semiconductors

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Small-molecule organic semiconductors are used in a wide spectrum of applications, ranging from organic light emitting diodes to organic photovoltaics. Presently, quantitative ab-initio models to assess the influence of these molecule-dependent properties, including the influence of dopants, are lacking. Here, we present a scale-bridging model, which can quantitatively describe an increasing number of experimentally relevant properties of these materials[1,2]. The model consists of a multi-step procedure, incorporating single molecule parameterization by ab-initio method, generation of atomistic morphologies, DFT based electronic structure calculations yielding site energies, energy disorder, electronic couplings and reorganization energies. These parameters are used in KMC simulations or analytic models to address key properties of the materials. In this talk, I will focus on disorder-compensation effects that provide a quantitative understanding of doping in these materials. While well understood for inorganic materials, the mechanism of doping-induced conductivity and Fermi level shift in organic semiconductors remains elusive despite recent research efforts. In microscopic simulations with full treatment of many-body Coulomb effects, we reproduce the Fermi level shift in agreement with experimental observations. We find that the additional disorder introduced by doping can actually compensate the intrinsic disorder of the material, such that the total disorder remains constant or is even reduced at doping molar ratios relevant to experiment. In addition to the established dependence of the doping-induced states on the Coulomb interaction in the ionized host-dopant pair, we find that the position of the Fermi level is controlled by disorder compensation. Secondly, I will address bimolecular exciton quenching processes such as triplet-triplet annihilation (TTA) and triplet-polaron quenching, which play a central role in phosphorescent organic light-emitting diode (PhOLED) device performance and are therefore an essential component in computational models. We performed virtual photoluminescence experiments on a prototypical PhOLED emission materials and arrive at a phenomenological TTA quenching rate comparable to experimental results experiments in the low-intensity limit. Finally, I will discuss efforts to computionally predict novel pure ETL materials with three orders of magnitude higher mobility than their precursors [6] and elucidate the molecular mechanism of doping these materials with kinetic Monte-Carlo simulations. The availability of first-principles based models to compute key performance characteristics of organic semiconductors may enable in-silico screening of numerous chemical compounds for the development of highly efficient opto-electronic devices.

References:

1. Friederich, P. *et al.* Rational In Silico Design of an Organic Semiconductor with Improved Electron Mobility. *Advanced Materials* **29**, 1703505 (2017).
2. Friederich, P. *et al.* Toward Design of Novel Materials for Organic Electronics. *Advanced Materials* 1808256 (2019). doi:10.1002/adma.201808256