

Molecular Insights on Charge Transport in Conjugated Materials for Applications in Organic Electronics

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Charge transport plays a key role in defining the performance of organic-based devices such as light-emitting diodes, solar cells, or field-effect transistors (FETs). Transport is typically described in two extreme cases, namely the band regime versus the hopping regime. Many electronic effects in organic semiconductors tend to favor a hopping picture in devices at room temperature. In this regime, macroscopic models have been developed over the years to characterize the influence of several parameters (such as temperature, electric field amplitude, disorder, charge carrier density) on the mobility values. Most of them have in common to involve effective parameters that do not take fully into account the nature and relative position of the interacting molecules. On the other hand, quantum-chemical calculations have been extensively used recently to calculate all parameters governing the rate of charge transfer between two interacting molecules in the hopping regime, thus with an explicit account of the chemical structure and actual packing of the molecules [1,2]. We will first survey some of our recent studies aiming at the description of the various transport parameters in a large variety of systems, going from model systems to experimental systems [2,3]. The bridge between the molecular and the supramolecular assemblies is established by calculating the charge carrier mobility via Monte-Carlo (MC) simulations based on the Marcus hopping transfer rates [4]. The influence of energetic and positional disorder on the hole mobility is investigated in model and more realistic systems such as single crystal of pentacene in contact with a polymeric layer encountered in FETs [5].

However, such simulations are often performed on frozen structures, thus neglecting the impact of lattice dynamics. In the last part of the talk, we will examine the way intermolecular vibrations modulate the key transport parameters and the implications for charge transport properties in crystalline as well as liquid-crystalline systems [6,7].

References

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