Computational modeling of organic photovoltaic materials and devices

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Organic semiconductor materials, based on pi-conjugated molecules and polymers, are of intense interest for applications including photovoltaic solar energy conversion. These materials are attractive because of the possibility to control optoelectronic properties through chemical design as well as the potential for low cost device manufacture using high volume processing. Recent developments have led to solar-to-electric power conversion efficiencies of around 10%, but higher performance is believed possible with improved materials and device designs. In order to select and design materials with potential for higher performance, design tools to relate device function to the chemical and physical structure of the materials are needed.

The simulation of organic photovoltaic materials and devices is complicated by the molecular nature of the materials, which leads to slow charge transport, the need for a heterojunction to separate photogenerated charge pairs, and disorder in the density of states for electrons and holes. Consequently, the electrical response of organic donor-acceptor heterojunction solar cells is not readily described by conventional semiconductor device models. Modelling tools are needed that can accommodate disorder in the energies and dynamics of charges and can incorporate two different organic semiconductor materials.

To develop such modelling tools, methods are needed to help understand first, how charge dynamics are related to the chemical and physical structure of the component materials and second, how the dispersive nature of the charge dynamics influences the current-voltage response of a photovoltaic device. We use a multi-scale modelling approach to simulate charge dynamics in organic electronic materials, incorporating molecular modelling of the microstructure of organic films, quantum chemical calculation of intermolecular charge transfer rates and kinetic Monte Carlo simulation of current transport and recombination [1, 2]. The methods are validated by a range of experimental measurements. Moreover, we have adapted continuum models of device behaviour to incorporate disorder in the electronic structure via a density-of-states function that can be related to the microscopic studies [3,4]. We will show how such an approach can be used to help explain the opto-electrical behaviour of organic photovoltaic materials and devices.

ACKNOWLEDGEMENT

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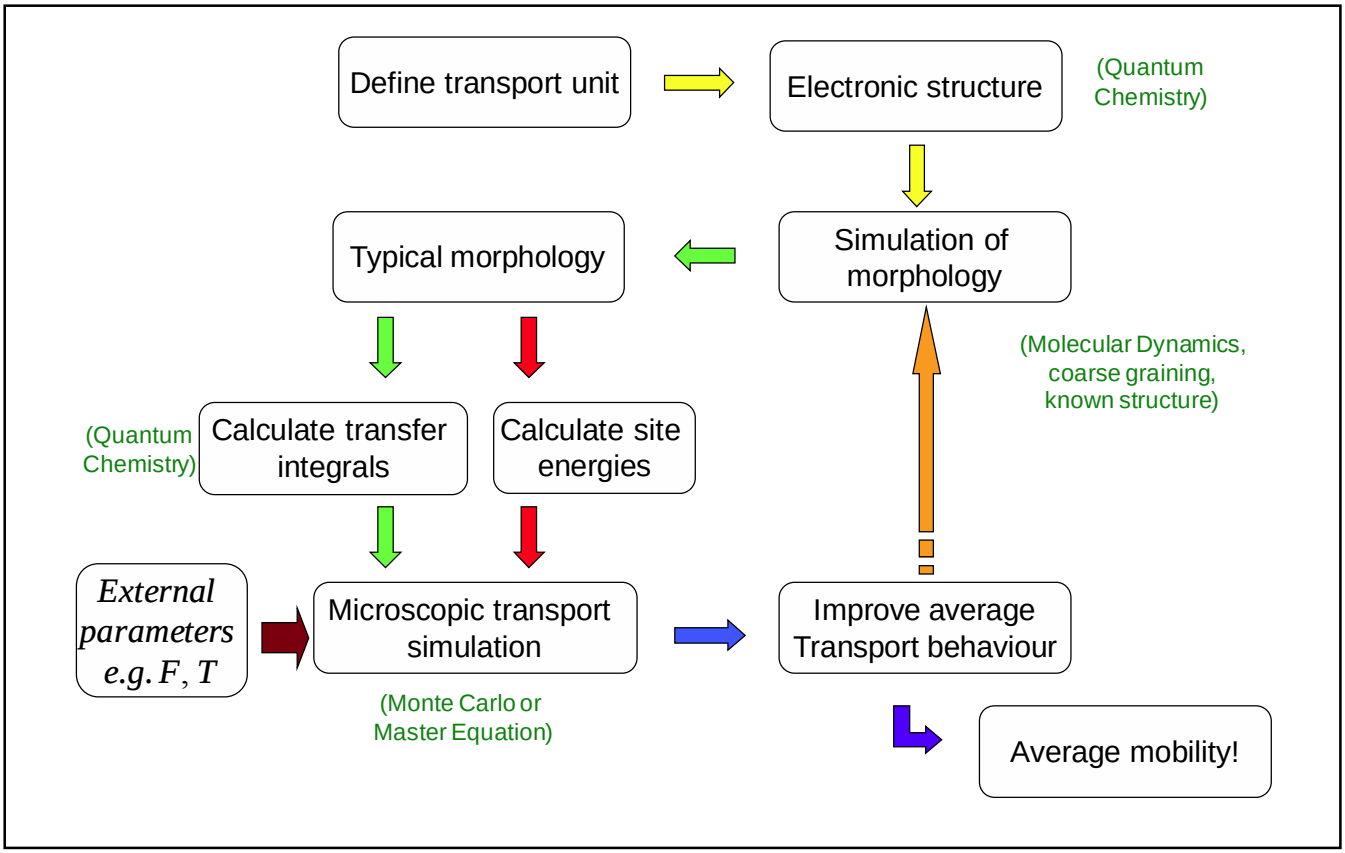

Fig. 1. Schematic of the multi-scale model used to simulate transport properties of organic semiconductors.

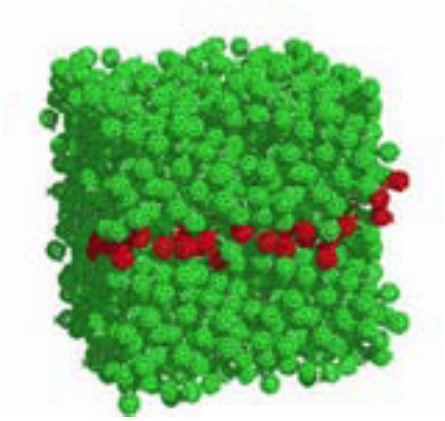

Fig. 2. Visualisation of a time-of-flight mobility simulation in a disordered film of fullerenes.

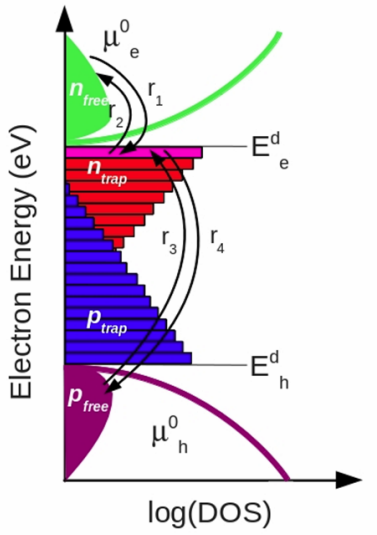

Fig. 3. A distribution of electron and hole trap states is included in device models to explain experimental behavior.