Generation and Transport of Charge Carriers in Organic Solar Cells

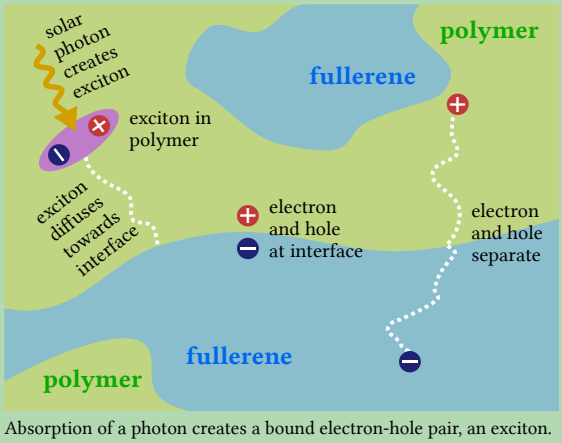
Philipps Universität Marburg

J. O. Oelerich, S. D. Baranovskii, M. Wiemer, D. Hümmer, F. Jansson, F. Gebhard

Many Particle Theory Group, Faculty of Physics, Philipps-Universität Marburg

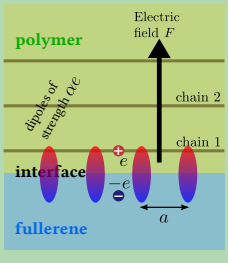
Generation

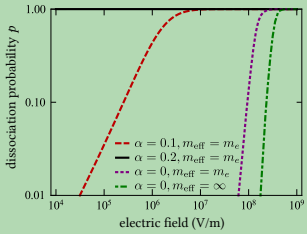
Why is exciton-dissociation so efficient in organic solar cells?



Absorption of a photon creates a bound electron-hole pair, an exciton. These excitons diffuse towards the interface between the two phases of the solar cell and experiments show that they are then separated with about 80% efficiency.

The solution for this is the formation of a chain of permanent dipoles at the interface. This periodic potential results in a repulsive force pushing the hole away from the electron. With rising distance from the interface, the potential also becomes narrower, resulting in a higher kinetic energy. The dissociation efficiency depends both on the dipole strength and the hole's effective mass.





The dissociation probability can be calculated with the formula below. It is plotted for several values of the dipole strength α and the hole's effective mass m_{eff} vs. the size of the electric field. It can be seen that the experimentally observed, high dissociation efficiency can easily be reproduced with this model.

$$p = \frac{\tau_0}{\tau_0 + \sum_{n=1}^{N-1} a_{n\to n+1}^{-1} \exp\left(\frac{E_n - E_1}{kT}\right)}$$

References

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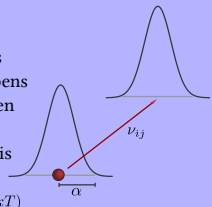
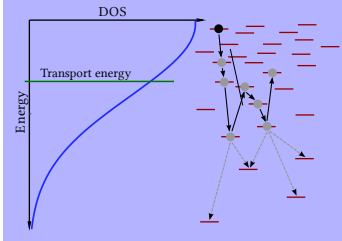
Transport

How do charge carriers move in organic materials?

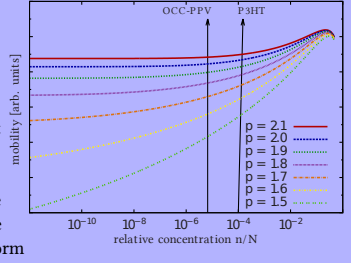
Electronic states in organic semiconductors are highly localized. Charge transport happens via incoherent tunneling transitions between these states, which is called *hopping*. The hopping rate between two sites i and j is usually described by the Miller-Abrahams Expression: $\nu_{ij} = \nu_0 \exp(-2r_{ij}/\alpha) \exp(-\Delta\varepsilon_{ij}/kT)$

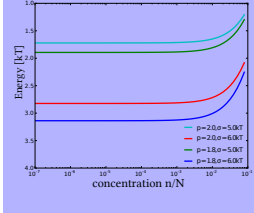




The interplay between the spatial and energetic part of these rates and a DOS that decays energetically lead to an activated behaviour during hopping transport at finite temperatures. The optimal activation energy is called *transport energy*.

The shape of the DOS is a very important property for transport. Experiments show that the charge carrier mobility becomes concentration dependent at a critical concentration n_c. We have shown that by measuring this number one can extract the shape of the DOS, assuming a general form $g(\varepsilon) = g_0 \exp\left[-\left(\frac{\varepsilon}{\sigma}\right)^p\right]$.





The transport energy also becomes n-dependent at a certain concentration. We studied this dependence taking into account the percolative nature of long-range hopping transport. The results are plotted in the figure on the left for different DOS widths σ and DOS exponents p.

Comparison with experimental data shows that the density of states in disordered organic materials is close to a gaussian. This is an important result for further calculations within this field. There are still open questions regarding charge transport mechanisms, e.g. whether or not transport is activated and how decisive the transport energy is for properties like conductivity or charge carrier mobility.

References

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