Séminaire de Chimie Théorique

Salle de Conférence, 3eme Est, bat. A12

Lundi 9 Octobre à 15:00

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Theoretical Insight to Structure and Transport in Organic Materials

Organic semiconductors play an increasing role as materials in electronic devices such as organic-light-emitting diodes (OLEDs), -solar cells and -field-effect transistors. We present computational chemistry protocols which (i) provide realistic estimates of key parameters of such materials (ii) give atomistic insight into transport limitations and (iii) indicate optimization potentials for this type of devices.

Transport of charge and energy is a key property for organic electronics applications. We present protocols for the determination of realistic intermolecular potentials for these systems which are most frequently extended π-systems. Subsequently we present an approach to transport properties based on hopping theory and an efficient solution of the resulting Pauli master equation. Rates for the transfer of electrons, holes or excited states (excitons) between neighbored molecules are evaluated with Marcus theory or with Fermi's golden rule. Quite good performance for exciton and charge transport is demonstrated.

It is well established that inefficient exciton transport is severely limiting the performance of organic solar cells. A comparison of calculated and measured exciton mobilities points to important quenching effects of exciton diffusion. An atomistic picture for exciton trapping was developed on the basis of quantum chemical results. This shows that small motions of neighbored molecules lead to deexcitation processes which are supposed to stop further exciton transport. As this quenching mechanism is a strong function of the flexibility and the mutual orientation of the organic molecules within their crystalline or semi-crystalline environment there is a good chance to find materials with better exciton transport properties.

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