Einladung zum Vortrag von

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Polaron Transport in Organic Crystals: Theory and Modelling

An important class of organic semiconductors are molecular crystals of high purity. Due to their high degree of structural order, such crystals are ideal candidates for the investigation of the intrinsic excitations and charge-carrier transport phenomena in organic solids. A particularly important and challenging topic is the understanding and ab initio description of the charge-carrier mobilities in these crystals, as the mobility is a fundamental material property and a central quantity for the optimization of device performance.

The description of charge transport in organic crystals is a nontrivial task due to the strong coupling of electronic and vibronic degrees of freedom. Very often, one describes the resulting carrier mobility within either the limit of localized small polarons or the limit of delocalized Bloch waves. Both approaches, however, are not satisfying and also appear to be somewhat incompatible. While elaborations of Holstein's small-polaron model are usually restricted to high temperatures and strong electron-phonon coupling, the wide-band theory based upon the Boltzmann equation can neither describe polaronic effects nor hopping motion and is restricted to low temperatures.

This situation is particularly unsatisfying since many interesting organic systems have strong electron-phonon coupling and, simultaneously, also large bandwidths, i.e., strong electronic coupling. Hence, a perturbative treatment of either interaction is not justified. Furthermore, the lack of knowledge concerning the necessary material parameters for simulations has to be overcome by means of first-principles calculations of electrons, phonons, and their mutual interaction.

In my talk, I will present a combined theoretical and numerical ab initio description of charge transport in organic crystals which overcomes the

above-mentioned limitations. It generalizes Holstein's small polaron model to polarons of arbitrary size and allows to calculate the carrier mobility from density-functional theory.

The generalized mobility expression treats coherent band transport and thermally induced hopping on equal footing and reproduces the results of previous theories in the respective limits. As a prototypical example, the theory is applied to herringbone-stacked crystals where the temperature dependence of the mobilities is simulated from first principles and compared to experimental data. Finally, the mobility anisotropy is analyzed by a novel 3D visualization technique for the relevant transport channels.

Der Vortrag wird vom Lehrstuhl für Atomistic Modelling and Design of Materials im Rahmen der *SimNet Multiscale Lectures* und vom Institut für Physik im Rahmen des *Seminars aus Halbleiterphysik und Nanotechnologie* veranstaltet.