HL 40: Invited Talk Hannewald

Time: Thursday 14:00–14:45 Location: ER 270

Invited Talk HL 40.1 Thu 14:00 ER 270

Charge transport in organic molecular crystals — •Karsten Hannewald — European Theoretical Spectroscopy Facility and Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany

An important class of organic semiconductors are molecular crystals of high purity. Besides the overall technological potential (OFETs, OLEDs), these crystals are interesting model systems for fundamental studies of the intrinsic excitations and charge-carrier transport mechanisms. We present a theoretical and numerical description of charge transport in such organic crystals. Our approach is based upon the Kubo formula for electrical conductivity within the framework of a mixed Holstein-Peierls model. Special attention is paid to polaronic effects that arise due to the strong electron-phonon interaction in organic materials. Explicit formulas for the polaron bandwidths and mobilities as a function of temperature are derived. The theory is supplemented by *ab initio* calculations of the relevant material parameters (transfer integrals, electron-phonon coupling, phonons) for various materials (oligo acenes, durene, guanine). Our predictions for the temperature dependence and anisotropy of the electron and hole mobilities agree well with experimental data and provide new insight into several hitherto poorly understood transport phenomena.