NECEM SEMINAR: Explaining Charge Mobility Regimes in Amorphous Materials

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15:00pm-16:00pm, Monday 8th April 2019
Newcastle University, Bedson Building, Lecture Theatre 2.76

Refreshments available after the seminar

Explaining Charge Mobility Regimes in Amorphous Materials

The charge-carrier mobility is presumably the most prominently used parameter to quantify the ability of materials to conduct electric current and whether a material is suited for envisaged electronic device applications. In amorphous materials, such as disordered organic semiconductors, the charge-carrier mobility is commonly evaluated assuming hopping transport, where charge carriers are viewed to migrate via hopping between localised states through the material. Such a hopping motion is governed by a complex interplay of multiple factors, most notably the energetic disorder, the electric field, interactions amongst charge carriers, and temperature. State-of-the-art simulation techniques like kinetic Monte Carlo or the Master equation (ME) account well for this complex interplay and allow us to predict the charge-carrier mobility and related properties such as electric currents. A particular appealing aspect of such simulations is the prospect to determine, how the charge-carrier mobility depends on conditions that can be externally controlled within a device, such as imposed electric fields or the density of available mobile charge carriers. However, the aforementioned contemporary simulation techniques can establish these relations only for each system individually.
Hence, it is desirable to provide a more fundamental point of view, with the help of which we can identify mobility regimes triggered by the electric field and/or by the charge-carrier density in a universal and illustrative manner. Such a distinction would also reveal how transitions from one transport regime to another take place and which conditions would need to apply to realise a transition.
We developed a new simulation technique providing this fundamental view. The technique is reminiscent of ME with the additional benefit that it can directly incorporate correlations and interactions. The separation of field- and charge-density-related effects included in our new technique allows to interpret the corresponding evolution of the mobility. We will explore the mobility regimes from the perspective of steady-state charge-carrier densities

and occupation statistics; i.e., the prevalent perspective in microelectronics dealing with conventional crystalline semiconductors. In this talk, we first will illustrate the main ideas behind our technique and the reasons for the field dependence of the mobility with the help of transport simulations considering a single charge carrier. Second, we will elucidate how the mobility depends on the charge-carrier density by successively increasing the number of considered charge carriers.

Dr. Karin Zojer The group of Karin Zojer, centered at the Institute of Solid State Physics, aims at establishing structure to transport-property relationships in disordered solids. The group engages in modeling and simulation of charge transport in organic electronic devices and, recently, mass transport through paper sheets. Starting out from “numerical experiments”, relying on our own, home-made, method implementations (Drift diffusion solver, KMC simulations), we analyze and extract structure-to-property relationships to identify limitations or realistic tuning handles.

Location
Bedson Building, Lecture Theatre 2.76

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