physikalisches Kolloquium

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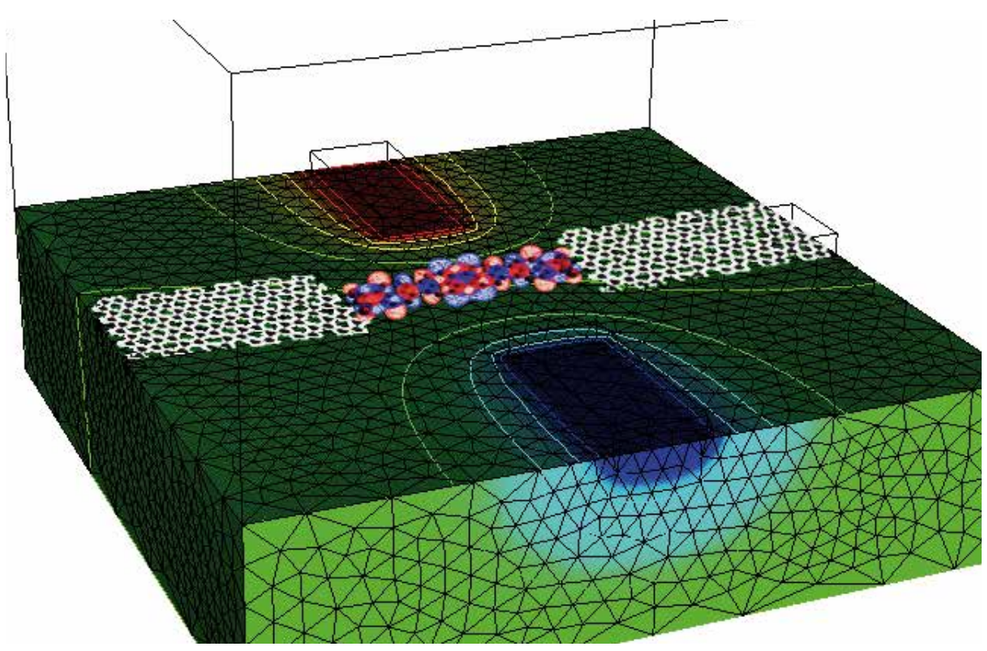
Complex nanoscale modeling: quantum transport in molecular electronics

Mo. 13.04.15
16:00 Uhr
Ort: H34

Nanoscale modeling of realistic systems requires multiscale and multiphysics approach linking atomistic ab initio description, quantum transport methods and 3D electrical fields (in some cases also magnetic fields, stress, thermal flow and other). Quantum electron and phonon (vibron) transport play central roles in molecular electronics. Although the theoretical foundations are in most cases well established, a quantitative and predictive theory is still a challenge. In this talk I want to give the overview of simple models and more realistic approaches. First of all, we discuss carbon nanostructures as an example of relatively simple, noninteracting, but large-scale and disordered quantum conductors. We consider semi-empirical and ab initio based atomistic tight-binding models for electron and phonon transport. Thermoelectric properties and CNT-FET will be considered as applications. The other important problem, if one speaks about a real device geometry, is the influence of the external fields, created by external systems: electrodes, gates, STM tip, etc. In many cases there is no need to consider the external system quantum-mechanically and it is possible to use classical Finite Element Method (FEM) to model the external potentials and currents, as well as thermal flow, mechanical stresses, and many other material dependent physical parameters in the continuum limit. Finally, we consider different levels of theoretical treatment of many-body effects (Coulomb blockade, memory, switching, Kondo effect), starting from a few-level model approach, namely a single-level electron-vibron (polaron) model and Hubbard-Anderson model for Coulomb interaction. I will present a new ab initio approach based on localized molecular orbitals. The aim is to use atomistic DFT calculations, capable for providing the electronic structure, but include only relevant electronic states. This approach helps to describe transport in large-scale systems, get effective-orbital tight-binding model for biological molecules like DNA, formulate a few-level model for many-body effects. In conclusion, I will present some details of the computational approach developed within the open source project for nanoscale modeling.



Above: A model of a planar molecular electronics system combining ab initio and FEM methods.