Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Tuesday, November 8th 2016 - 14:00
CFEL Seminar room I (Bldg. 99)

Stefan Kurth

University of the Basque Country UPV/EHU, San Sebastian
IKERBASQUE, Basque Foundation for Science, Bilbao

Transport through strongly correlated systems described by density functional theory

In this talk I will describe the evolution of our understanding on how to describe transport through strongly correlated systems in the framework of density functional theory (DFT).A first indication that DFT might be useful to tackle this situation came with the realization that the Kondo plateau in the zero-bias conductance may already be captured at the level of standard Landauer theory combined with DFT. Later it has been shown how the description of Coulomb blockade in the zero-bias limit can be achieved within DFT. In a more recent development we have proposed a DFT formalism to describe electronic transport in the steady state which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds.

Finally, I will present a recent parametrization of the xc potentials for the single-impurity Anderson model which correctly incorporates both the Kondo and Coulomb blockade regimes, i.e., both zero and finite temperature. This parametrization allows for calculation of currents and differential conductances at arbitrary bias and temperature at negligible numerical cost but with the accuracy of sophisticated renormalization group methods.

Host: Angel Rubio

MAX-PLANCK-GESELLSCHAFT