Electron transport through molecular junctions and FHI-aims

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In this talk, we will overview an efficient implementation of the non-equilibrium Green's functions formalism merged with non-interacting Kohn-Sham particles to evaluate electron transport characteristics of the nanoscale systems, like organic molecules establishing a contact to metallic electrodes. An efficient approximation for the self-energy will be discussed where metallic reservoirs are modeled by absorbing, energy independent, spacial boundary conditions that the Kohn-Sham wave functions are subject to [1]. A power of the approximate scheme will be demonstrated on the methodological example of the one-dimensional tight-binding wire, as well as on the example of the realistic systems like benzene-dithiol or alkane-dithiol molecular junctions with gold electrodes [2]. A comparison between computational schemes relying on the Gaussian basis functions (TURBOMOLE) and on the numerically tabulated atomic sets (FHI-aims) will be given.

Furthermore, we will discuss more elaborated schemes to constract the self-energies which allow to account for the spin-polarized electronic structure of the transition metal electrodes. We will demonstrate an ability to treat a variety of different magnetic configurations (e.g. nano-scale domain walls) which could appear when a metal-organic molecule with few spins, localized on the open shell *d*-ions, is brought in contact with a ferromagnetic surface and a tip of the spin-polarized-STM. Recent experiments [3,4] on the spin-polarized transport and magnetoresistance effect observed in the hydrogen-phtalocyanine STM molecular junctions will be discussed in detail.

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[4] A. Bagrets, S. Schmaus, A. Jaafar, T. K. Yamada, M. Alouani, W. Wulfhekel, and F. Evers, preprint (2012), under review in Nano Lett.