MAR09-2008-004572

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

**Theoretical aspects of modeling the conductance of molecular junctions**

KURT STOKBRO, QuantumWise A/S

In this talk I will discuss different semi-empirical and ab initio approaches for modeling the coherent electron transport of molecular junctions using the non-equilibrium Greens function formalism [1]. The most important effects for determining the conductance are the energies and coupling of the frontier molecular orbitals to the electrodes. I will discuss the accuracy of different levels of theory for calculating the HOMO-LUMO gap of various molecules, and present a simple correction that improves the accuracy of Density Functional based mean field theories [2]. The physical origin of the correction is illustrated using the Moshinsky atom as test system, and the accuracy is illustrated for a number of small molecules [3]. The coupling of the molecule to the electrodes is controlled by the terminal group on the molecule. We illustrate how a molecule with C60 terminal groups can have a very strong coupling with the electrodes [4].

[1] Mads Brandbyge, Jose-Luis Mozos, Pablo Ordejon, Jeremy Taylor, and Kurt Stokbro, *Density functional method for nonequilibrium electron transport*, Phys. Rev. B. 65, 165401 (2002).
[2] A. Cehovin, H. Mera, J. H. Jensen, K. Stokbro, and T. B. Pedersen, *Role of the virtual orbitals and HOMO-LUMO gap in mean-field approximations to the conductance of molecular junctions*, Phys. Rev. B 77, 195432 (2008)
[3] H. Mera and K. Stokbro, *Using Kohn-Sham-DFT to describe charged excitations in finite systems,* submitted
[4] C. A. Martin et. Al., Fullerene-*Based Anchoring Groups for Molecular Electronics*, J. Am. Chem. Soc. 130, 13198 (2008)