ELECTRON TRANSPORT IN MOLECULAR WIRES

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Molecular electronics represents a large step in device miniaturization and due to advancements in techniques, useful devices have been built on the basis of individual molecules. The aim of this work is to theoretically model the transport properties of newly synthesized, candidate molecular switches that are contacted between gold electrodes. The molecular wires [1] that are studied here have been designed and synthesised based on flourinone structures with added benzene rings. The conductances of molecules with lengths varying from 4 to 10nm are calculated. It is necessary to study these longer molecules, as they will impose a less stringent requirement on the contact lithography in a scalable device.

The computational approach that is used is a combination of the first principles DFT code SIESTA and previously developed transport codes, which uses a Greens function scattering approach to calculate the conductance. The molecule and contact regions are included in the quantum mechanical calculation and the size of the contact region is increased until a convergence in the conduction of the single molecule is found. The results are then compared to recent STM measurements of these molecules.

References:

[1] C. Wang, A.S. Batsanov, M.R. Bryce and I. Sage, Org. Lett., **6** (13), 2181 -2184, 2004