Seminář odd. 26
Tenkých vrstev a nanostruktur

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TÉMA

Electron transport in molecular systems

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In this talk I will describe my recent work in the description of electron transport processes in organic molecular systems. The talk will focus on metal / single molecule / metal nanostructures, but I also mention some results in the field of organic photovoltaics on exciton dissociation.

The flow of current through single molecule circuits is very dependent on the junction electronic structure, which requires a description involving ab-initio methods. I will present results for several molecular junctions calculated using the DFT-NEGF formalism, where I will focus on two aspects: molecular linkers and quantum interference. Metal-molecule chemical linkers are used to anchor the molecule to the substrate and tip but greatly influence molecular conductance. We recently studied Au-C metal-molecule bonds and showed they result in very high calculated and measured conductance [1]. I will also address quantum interference in single molecule transport in a study of transmission through molecules that have two branches bound in parallel to the electrodes [2]. The calculated and measured conductance of these double backbone molecules can be more than twice (eg. ~3×) that of the single-backbone counterparts due to constructive quantum interference.

Finally I will describe my recent work in the field of organic photovoltaics, focusing on exciton dissociation in model donor-acceptor systems.

References:

[1] Z-L Cheng, R. Skouta, H. Vázquez, J. Widawsky, S. Schneebeli, M.S. Hybertsen, R.Breslow and L.Venkataraman, 'In situ formation of highly conducting covalent Au–C contacts for single-molecule junctions', Nature Nanotechnology 6 353 (2011).

[2] H. Vázquez, R. Skouta, S. Schneebeli, M. Kamenetska, R.Breslow, L. Venkataraman and M.S. Hybertsen, 'Probing the Conductance Superposition Law in Single Molecule Circuits with Parallel Paths', Nature Nanotechnology 7 663 (2012).

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