

Seminář odd. 26

Tenkých vrstev a nanostruktur

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TÉMA

Elastic and inelastic electron transport through alkane-based molecular junctions

Giuseppe Foti

Institute of Physics, Academy of Sciences of the Czech Republic

Molecular junctions formed by organic molecules bridging metallic electrodes represent nowadays an active field of research due to their interesting properties for both basic and applied science. Atomistic simulations provide a power tool for the prediction and comprehension of those properties. Among all computational techniques, density functional theory (DFT) in combination with the nonequilibrium Green's function formalism (NEGF) is one of the most mature and widely spread method for the study of the charge transport in nanoscale systems.

In this talk I will present the electronic and conduction properties of a series of alkane-based molecular junctions studied by means of first-principles calculations. In the first part I will focus on the process of band alignment between molecular and metal states as a function of the tilt angle of thiol- and amino-functionalized alkanes with respect to the electrode surface [1]. In the second part I will discuss some aspects related to the calculation and convergence of the inelastic electron tunneling spectrum (IETS) of alkanedithiolates in a periodic supercell approach [2]. Then I will show some examples of how IETS could be used to effectively identify highly conducting molecular junctions formed by alkanes anchored to gold electrodes through a covalent Au-C bond [3, 4].

Finally, in the context of inelastic processes in molecular junctions, I will briefly show a particular cooling mechanism for a one-level model system studied by means of the master equation approach.

[1] Foti G., Sánchez-Portal D., Arnau A., and Frederiksen T., J. Phys. Chem. C 117, 14272 (2013).

[2] Foti G., Sánchez-Portal D., Arnau A., and Frederiksen T., (submitted).

[3] Cheng, Z.-L., Skouta R., Vazquez H., Widawsky J. R., Schneebeli S., Chen W., Hybertsen M. S., Breslow R., Venkataraman, L., Nat. Nanotechnol. 6, 353-357 (2011).

[4] Foti G., Vázquez H., Sánchez-Portal D., Arnau A., and Frederiksen T., J. Phys. Chem. C 118, 27106-27112 (2014).