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Tenkých vrstev a nanostruktur

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TÉMA

Theoretical results in Single Molecule Transport

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The flow of current through metal-molecule-metal circuits depends, often delicately, on the details of the structural and electronic properties of the molecule and of the junction as a whole. In this talk I will present recent DFT-based theoretical results on single molecule transport focusing on achieving near ideal contact resistance through metal-molecule linker chemistry and on investigating the conductance superposition law at the single molecule scale. This work was carried out in close collaboration with STM break-junction experiments.

Trimethyltin (SnMe3)-terminated molecules result in direct Au-C covalent bonds between the molecular Carbon atoms and the Au electrodes as the SnMe3 groups are cleaved in situ at the junction. The resulting measured conductance for alkanes is ~100 times higher than with other linkers [1], and near-resonant transport is achieved for conjugated molecular junctions [2]. Theory can explain how Au-C links exhibit near ideal contact resistance.

I will also discuss the conductance superposition law in molecules that have two backbones bonded in parallel to the electrodes. The calculated and measured conductance of these double backbone molecules [3] can be more than twice (eg. ~3×) that of the single-backbone counterparts due to constructive quantum interference.

[1] Z.L. Cheng et al., Nature Nanotechnology 6, 353 (2011).
[2] W. Chen et al., J. Am. Chem. Soc. 133, 17160 (2011).
[3] H. Vazquez et al., Nature Nanotechnology 7, 663 (2012).

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