A model for inelastic transport through atomic surface wires

Serge Monturet

CEMES CNRS, 29 rue Jeanne Marvig, Toulouse, France
monturet@cemes.fr

When dealing with currents through molecules to probe either their electronic or vibrational structure, one can imagine two sorts of configurations: Firstly, a tip – molecule – surface experiment, corresponding to a “vertical” situation, where electrons are usually in the tunneling regime and secondly, a “horizontal” situation, as in the case of atomic surface wires connected to an adsorbed molecule. Regarding conductance, the latter case would rather qualify as a ballistic or pseudo-ballistic transport regime.

A quasi-1D conductor can be built using a hydrogen passivated silicon surface by desorbing H atoms in a row with the help of an STM tip. The row of dangling bonds play the role of an atomic-scale wire at the surface, and a current can flow through it. What is the maximum value of the current? Is the wire mechanically stable? What happens if the electrons heat it up? These questions all together indicate the need of calculating the electronic transport with interactions with the nuclei. To address them, I will present simple model, based on the mixed classical/quantum Ehrenfest approximation, capable of describing the dynamics of such a system.

Figures