# Vibronic effects in electron transport through atomic and molecular systems.

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Electron transport on the atomic scale is sometimes classified in two different regimes: tunnelling and ballistic. They correspond to the case of low-conductance because the electron has to tunnel through an isolating barrier, i.e. the vacuum gap in a scanning tunnelling microscope (STM) and the case of high conductance where electrical contact has been established. In the presence of vibrations, transport can be further classified by the strenght of the electron-vibration coupling: from weak interactions where at most the vibrator is excited once, to stronger coupling where the vibrator is multiply excited.

The spectroscopic analysis of vibrations induced on adsorbates on metallic surfaces with an STM [1] belongs to the cases of tunnelling in the presence of weak electron-phonon coupling. I will show that the simulation of inelastic electron tunnelling spectra is needed for determining the excited modes and identifying the measured species. Recently, we have been able to determine the product of an STM-induced reaction on benzene by simulating the spectra of the different possible products [2].

In the tunnelling regime, the strong electron-vibration coupling can be easily attained. In a very specific situation, we show that vibrations can eventually create electronic currents. This is the case of dangling-bond vibrations in a semiconducting surface. Indeed, the otherwise "state-in-the-gap" that is a dangling bond on a Si(111)$\sqrt{3}$x$\sqrt{3}R30°$-B surface, can become connected with the acceptor (boron, B) band via its large electron-vibration coupling. The role of the multiply excited vibration is to permit the electron flow between the tip of an STM and the bulk boron band [3]. I will present experimental and theoretical results on this system.

The high-conductance and weak electron-phonon coupling case corresponds to the ballistic regime. The electron current is not a tunnelling current, and the mean free path of electrons is much larger than the typical dimensions of the atomic objects. Recent experimental data have shown that it is possible to excite localized vibrations in mono atomic gold chains in this regime [4] akin to vibrational spectroscopy in the tunnelling regime. I will briefly review our theoretical work [5] that reveals the modes excited by the ballistic current, as well as the difference between the heating of atomic wires and the dynamics induced on molecules by the STM.

## References:

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