



DIRECTION DES SCIENCES DE LA MATIÈRE,  
INSTITUT RAYONNEMENT MATIÈRE DE SACLAY  
SERVICE DE PHYSIQUE ET DE CHIMIE DES SURFACES ET DES INTERFACES

# SEMINAIRE

Vendredi 26 octobre 2012 à 11h00  
Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

## A model for inelastic transport through atomic surface wires

**Serge Monturet**

Groupe Nanosciences, CEMES/CNRS,  
29 rue Jeanne Marvig, 31055 Toulouse, France.

(invité par Cyrille Barreteau)

*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 plays the role of an atomic-scale wire at the surface, and a current can flow through it [1]. What happens if the electrons heat it up? Calculating the electronic transport properties taking into account the interaction with the nuclei is a central question [2]. A time-dependent calculation is presented based on the mixed classical/quantum Ehrenfest approximation [3]. Treating the electron quantum mechanically and the oscillators classically, the ion dynamics will be discussed. One can also think of a model in which the vibrational degree of freedom is quantified and the electron is treated just in the same way as previously. In this case, it will be shown that the probability to excite the vibration is triggered by the motion of the electronic wave-packet propagating through the system. With the help of a simple model hamiltonian, it is shown that there is a condition to fulfill for the transition to occur [4].*

### References

- [1] R. Robles et al. accepted in *J. Phys.: Condens. Matter* and M. K'ep'en'ekian et al. submitted to *J. Phys.: Condens. Matter*.
- [2] S. Monturet and C. Joachim, *Theory of inelastic transport through atomic surface wires*, in *Advances in atom and single molecule machines*, Volume 2. Ed: C. Joachim (Springer Verlag) (2012) and F. Ample et al. *J. Phys.: Condens. Matter* 23, 125303 (2011).
- [3] A. P. Horsefield et al. *J. Phys.: Condens. Matter* 17, 4793 (2005).
- [4] S. Monturet and C. Joachim submitted to *Chem. Phys. Lett.*

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