



SEMINAIRE ISMO

Frederico D. Novaes

Institut de Ciència de Materials de Barcelona (CSIC)

Negative differential resistance in molecular devices explored with Transiesta.

Recent studies on molecular devices [1,2], using the Scanning Tunneling Microscope (STM) show a negative differential resistance (NDR). Ab-initio based transport calculations can be used to have an atomic level description of molecular junctions, helping to quantify the processes at work and to unravel the mechanisms of NDR in such systems.

We have used the Transiesta code [3] to simulate the I-V characteristics of fullerene molecules decoupled from a gold substrate by tetraphenyl adamantane molecules. We will compare our results to the ones experimentally obtained.

[1] Phys. Rev. Lett. **100**, 036807 (2008)

[2] Appl. Phys. Lett. **86**, 204102 (2005)

[3] Phys. Rev. B **65**, 165401 (2002)

* * * * *

Mardi 21 juin 2011 à 11 h 00

Bât 351 - 2^{ème} étage

Université Paris-Sud 91405 ORSAY Cedex