ELECTRONIC TRANSPORT IN NANOSTRUCTURES FROM FIRST PRINCIPLES

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An important factor in the development and success of silicon based microelectronics technology was the availability of reliable simulation tools to model the behavior of devices. This is clearly reflected in the fact that modeling is one of the key issues in the International Technology Roadmap Semiconductors. Going towards molecular or nanoscale electronics, the need of modeling and simulation is even greater, due to several factors. First, quantum effects determine the transport properties at this scale, and the need for simulation is therefore increased by the more complex behavior in the quantum world. Second, the structure and chemistry at the atomic level are of paramount importance in determining the properties of devices: at these sizes, the behavior of a device can change dramatically due to very small changes on its atomic structure and/or chemical bonding. Obviously, these effects can only be described properly within a method that takes explicitly into consideration the quantum mechanical electronic structure of the devices (including non-equilibrium effects due to the current flow), and that treat the device at the atomic level. The interplay between the two factors (current flow and atomic structure/chemistry) is also of great importance, and must be incorporated properly in the simulation tools.

I will describe our efforts to develop a method, TranSIESTA, that allows for first-principles quantum mechanical modeling of molecules and nanoscale systems under non-equilibrium conditions [1] . The method is based on the non-equilibrium Green's function technique, and is implemented into the SIESTA electronic structure package [2], in such a way that the density matrix of the system (and therefore the electronic structure) is calculated selfconsistently when the system is subject to an external bias. Therefore, the method incorporates the effect of the external bias (which maintains the non-equilibrium condition) on the chemistry of the device. I will also describe recent applications of the method to several problems related to transport in nanoscale systems like wires, nanotubos and molecules.

References:

[1] M. Brandbyge, J. L.- Mozos, P. Ordejón, J. Taylor and K. Stokbro, Phys. Rev. B, **65** (2002) 165401
[2] J. M. Soler, E. Artacho, J. Gale, A. García, J. Junquera, P. Ordejon, D. Sánchez-Portal, J. Phys. C.: Cond. Matt, **14** (2002) 2745
[3] http://www.uam.es/siesta