First-principles simulations of electronic transport with TranSIESTA

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Simulations of electronic transport properties based on first-principles (or *ab-initio*) methods can be crucial when investigating systems at the atomic-scale. Over the last decades, Density Functional Theory (DFT) has ben widely used to address problems at the atomistic level. Traditionally, however, for most of the DFT based implementations, there were two restrictions that limited the scope of systems that could be simulated: i) the use of periodic boundary conditions, and ii) the simulated system was considered to be in equilibrium. Green's Functions (GF) based methods were often used to handle the first of these issues[1] - for example in studies of single adsorbates on surfaces.

With the increasing miniaturization of electronic devices, one was often faced with a situation were the electronic transport was being controlled (determined) by a small constriction placed in contact with (comparatively) large electrodes, and were current would flow if a bias was applied between these electrodes (reservoirs). This non-equilibrium situation was modeled with the Non-Equilibrium Green's Functions (NEGF) formalism[2], first at a mesoscopic level, with no atomistic detail.

With the recent remarkable improvements in the experimental techniques, measurements of electronic transport through nano-sized constrictions – single molecules or atoms in the extreme cases - started to be reported. The modeling of such situations then demanded an atomic level description. The idea then was to extend DFT and couple it to the NEGF formalism. This DFT-NEGF methodology is nowadays widely used, since it combines the the power of DFT (accuracy at a reasonable computational cost), with the possibility of studying open systems (no periodicity imposed), possibly out of equilibrium.

In this talk I will describe the main aspects of the TranSIESTA[3] code, which is one of the first DFT-NEGF implementations, discussing its power and current limitations. Some *real life* examples will be discussed.

References

[1] – A. R. Williams *et al* ., *Phys. Rev. B* **26**, 5433 (82)

[2] – S. Datta, *Electron Transport in Mesoscopic Systems*, Cambridge University Press, Cambridge, 1995.

[3] – M. Brandbyge *et al.*, *Phys. Rev. B* **65**, 165401 (2002)