Study of the Influence of Localized Vibrational Modes in Charge Transport Properties at Nanoscale Systems

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In molecular and atomic devices the interaction between electrons and ionic vibrations has an important role in electronic transport. The electron-phonon coupling can cause the loss of the electron's phase coherence, the opening of new conductance channels and the suppression of purely elastic ones. From the technological viewpoint phonons might restrict the efficiency of electronic devices by energy dissipation, causing heating, power loss and instability.
The state of the art in electron transport calculations consists in combining *ab initio* calculations via Density Functional Theory (DFT) with Non-Equilibrium Green's Function formalism (NEGF). In order to include electron-phonon interactions, one needs in principle to include a self-energy scattering term in the open system Hamiltonian which takes into account the effect of the phonons over the electrons and vice versa. Nevertheless this term could be obtained approximately by perturbative methods. In the First Born Approximation one considers only the first order terms of the electronic Green's function expansion. In the Self-Consistent Born Approximation, the interaction self-energy is calculated with the perturbed electronic Green's function in a self-consistent way.
In this work we describe how to incorporate the electron-phonon interaction to the SMEAGOL program (*Spin and Molecular Electronics in Atomically Generated Orbital Landscapes*), an *ab initio* code for electronic transport based on the combination of DFT + NEGF. This provides a tool for calculating the transport properties of materials' specific system, particularly in molecular electronics. Preliminary results will be presented, showing the effects produced by considering the electron-phonon interaction in nanoscale devices.