ELECTRONIC CORRELATIONS AND INELASTIC SCATTERING IN TRANSPORT THROUGH MOLECULES

K. S. Thygesen[1], K. W. Jacobsen[1], I. S. Kristensen[1], A. Rubio[2]

[1]Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

[2]Departamento de Fisica de Materiales, Facultad de Quimicas, Centro Mixto CSIC-UPV/EHU, Universidad del Pais Vasco, 20018 San Sebastian, Spain.

In the "standard approach" to first-principles simulations of quantum transport in nano-scale junctions, the electrons are modelled as non-interacting particles moving in the effective potential obtained from a Density Functional Theory (DFT) calculation. While DFT, in principle, yields the exact groundstate energy of the interacting system, there is no guarantee that it provides a good decription of electrical current. In this talk I will discuss our recent work on including (i) inelastic electron-vibron scattering and (ii) electronic correlations in quantum transport calculations. In both cases (i) and (ii) we include the interactions as self-energies (first Born and GW approximations, respectively) evaluated self-consistently within the Keldysh non-equilibrium Green's function formalism. In one application, we find that inelastic scattering on the longitudinal (transverse) molecular vibrations of a metal-H_2-metal junction leads to negative (positive) steps in the conductance. In a second application, we investigate the role of electronic correlations in nonequilibrium transport using a generic two-level model of a molecular junction. In equilibrium, dynamic screening effects (image charge effects) lead to a characteristic renormalization of the quasi-particle (QP) HOMO-LUMO gap. As the bias is raised, the phase-space for QP scattering increases and this leads to significant reduction of the lifetime of the molecular levels. Both effects have a large impact on the IV curve of the model junction.

[1] D. Djukic et al. Phys Rev B **71**, 161402(R) (2005)

[2] K. S. Thygesen and A. Rubio, Phys. Rev. B **77**, 115333 (2008)

[3] K. S. Thygesen, Phys. Rev. Lett. **100**, 166804 (2008)

[4] K. S. Thygesen and A. Rubio, J. Chem. Phys. **126**, 091101 (2007)