THEORY OF ELECTRONIC TRANSPORT THROUGH SINGLE MOLECULE: EFFECTS OF ELECTRON-VIBRATION COUPLING

H. Ness,
CEA-Saclay, Service de Physique et Chimie des Surfaces et Interfaces,
DRECAM/DSM, Bat. 462, F-91191 Gif sur Yvette, France

E-Mail: hness@cea.fr

We describe how to treat the interaction between travelling electrons and localised or extended vibrational modes in molecular nanodevices [1]. We present a multichannel scattering technique which can be applied to calculate the transport properties for realistic systems, and show how
it is related to other methods (other scattering and non-equilibrium Green's functions techniques) [2]. We apply the technique to describe recent experiments on molecular junctions: the effects of the temperature on the conductance of molecular break-junctions are studied for a model system; we also show that it is necessary to go beyond the single-vibration mode analysis to understand the features observed in inelastic electron tunnelling spectroscopy [1]. Finally, we briefly discuss the effects of electron-vibration coupling in the presence of electron-electron interaction in single-molecule transistors [3].

[1] H. Ness, A.J. Fisher, PNAS 102, 8826 (2005).
[2] H. Ness, submitted.
[3] P. Cornaglia, D. Grempel, H. Ness, PRB 71, 075320 (2005).