Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab initio study of vibrational spectrum and electron-molecular vibration interaction in molecular electronic systems NIKOLAI SERGUEEV, DAN ROUBTSOV, HONG GUO, Department of Physics, McGill University — For the last few years it was realized that the electron-molecular vibration (e-mv) interaction has to be taken into account to predict transport properties of molecular electronic devices. For realistic calculations, however, the eigenmodes of molecular vibrations and the coupling constants in an e-mv interaction Hamiltonian have to be found from the first principles. We developed a technique to calculate eigenfrequencies of the molecular vibrations (a full spectrum) at both equilibrium and non-equilibrium conditions using the DFT within Keldysh Green's function formalism implemented into our McDCAL code. Using the obtained vibrational spectrum and the self-consistent Kohn-Sham Hamiltonian of the electrons, we can build the e-mv interaction Hamiltonian. By averaging this Hamiltonian over the scattering states of the total Kohn-Sham Hamiltonian, we obtain a dimensionless e-mv interaction strength (both elastic and inelastic ones), for each vibrational mode of the spectrum. These numbers tell us which molecular modes build strong inelastic channels in an electron tunneling through a molecule. As an example, we consider a dithiol-benzene molecule in a good covalent contact with two identical Al electrodes. In the vibrational spectrum of the dithiol-benzene in this device, we show which modes are important at different applied bias voltages.

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Date submitted: 03 Dec 2004 Electronic form version 1.4