MOLECULE - METAL CONTACTS: A FIRST PRINCIPLES ANALYSIS

Claudine Couture, Hong Guo
McGill University, Montreal, Canada
couturec@physics.mcgill.ca

The coupling between a molecule and metal contacts plays an important role in molecular scale devices. The strength of that coupling influences greatly the charge transport properties of such a system, although it has been difficult to experimentally control the configuration of the contacts and the coupling strength. In this work, we have theoretically calculated the molecule-contact coupling strength using density functional theory (DFT) within the nonequilibrium Green's functional framework (NEGF), for open device structures under voltage bias. Our NEGF-DFT ab initio technique evaluates the device Hamiltonian by DFT in which the density matrix is constructed via NEGF so that nonequilibrium physics of charge transport is accounted for. The molecule-contact coupling is then obtained by evaluating proper Dyson's equation via the surface Green's function method. We will present the theoretical formalism of this method and its associated numerical implementation, in addition to examples on molecular wires.