Theory and Modeling of Alternating and Transient Current in Molecular Scale Conductors

Hong Guo

Center for the Physics of Materials and Department of Physics, McGill University, Montreal, QC H3A 2T8 Canada

It has been a difficult problem to calculate transport properties of nano-scale conductors including all the atomic, chemical, and materials details from quantum mechanical first principles. Progress has been achieved in the past few years in this direction on *steady-state,* where an emerging technique is based on density functional theory (DFT) carried out within the Keldysh non-equilibrium Green's functions (NEGF). In this talk, I discuss an exact nonlinear response theory for time-dependent quantum transport far from equilibrium which can be used to analyze time dependent current flowing in nonelectronic devices under AC transport and transient regime. Our analysis is based on NEGF, and provides an exact analytical solution to the transport equations in the far from equilibrium, nonlinear response regime. The essential feature of our solution is that it does not rely on the commonly used wideband approximation where the coupling between device scattering region and leads is taken to be independent of energy. This way, our formalism can be used to analyze realistic system including atomic details. Examples will be given in this regard.

Work in collaboration with Joseph Maciejko, Eric Zhu and Jian Wang.