Electron transport with dissipation in nanoscale systems

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It is usually assumed that electron transport in molecular wires is ballistic and that scattering with phonons is only important to thermalize the electrons in the substrate far from the molecular contact. Here I discuss an alternative formulation in which both tunneling and dissipation are explicitly taken int account. In this approach electrons are accelerated by an external electric field, but coupling to a heat bath prevents the electrons from moving far out of equilibrium. Many-electron dynamics is treated within time-dependent current-density functional theory, while dissipative effects are treated phenomenologically by a master equation. The approach is well suited to numerical simulations and allows us to study steady state and dynamical phenomena. In particular, in the case of a simple double-barrier resonant tunneling structure, I discuss how dissipative effects and the approximations made in the master equation affect the calculated electric current.

This work has been done in collaboration with Roberto Car at Princeton University.