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Simple and accurate method for time-dependent transport along nanoscale junctions IGNACIO FRANCO, University of Rochester, THORSTEN HANSEN, University of Copenhagen, LIPING CHEN, University of Rochester —
A simple method that accurately captures the dynamics of metal-molecule-metal junctions under the influence of time-dependent driving forces is presented. In it, the metallic contacts are modeled explicitly as a discrete set of levels that are dynamically broadened via an artificial damping term in the equations of motion. The approximations that underlie the method are revealed via a derivation of the effective equations of motion within the framework of non-equilibrium Green's functions (NEGF) theory. As shown, the method applies to junctions that can be described by an effective independent-fermion Hamiltonian, admits arbitrary time dependence in the molecular Hamiltonian and is restricted to time-dependent voltages that are adiabatically slow. The method is trivial to computationally implement, has a well defined range where the results are independent of artificial model parameters, and is numerically shown to quantitatively reproduce the time-dependent transport characteristics of a model molecular junction driven by laser fields as described by an exact NEGF method. As such it constitutes an intuitive and technically accessible method to model time-dependent transport phenomena in molecular junctions that are driven by electric fields or fluctuating environments.

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