Electron transport in molecular electronics systems

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Abstract. We have coupled large-scale quantum electronic structure calculations with non-equilibrium Green function formulation for determining the quantum conductance on practical length scales. The combination of state-of-the-art quantum chemistry methods, efficient numerical algorithms, and high performance computing allows for realistic evaluation of properties at length scales that are routinely reached experimentally. Two illustrations of our method are presented. First, quantum chemical calculations using up to 10^4 basis functions are used to investigate the amphoteric doping of carbon nanotubes by encapsulation of organic molecules. As a second example of our method, we investigated the electron transport properties of a Si/organic-molecule/Si junction using a numerically optimized basis. In both cases, the efficiency of the numerical approach permits the inclusion of a large number of atoms and in turn allows for a realistic description of electronic processes governing transport at the nanoscale.

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