

Large scale quantum chemical evaluation of electronic transport properties at the nanoscale

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Present-day semiconductor devices are rapidly approaching their physical limits, prompting an increasing number of researchers across multiple disciplines to attempt to devise innovative ways for decreasing the size and increasing the performance of critical features in microelectronic circuits. One possible route is based on the idea of using molecules and molecular structures as functional electronic devices. In that respect, the description and optimization of novel devices for nanoelectronics call for the development of new theoretical, algorithmic and computational methods and techniques.

We have coupled large-scale quantum electronic structure calculations with a Green's function formulation for determining the quantum conductance at the nanoscale. The approach is based on an original scheme where quantum chemistry calculations on finite systems are recast to infinite, non-periodic (i.e., open) systems, thereby mimicking actual working devices. The full quantum-based calculations can be performed with up to 10,000 basis functions and allow for realistic evaluation of properties at length scales that are routinely reached experimentally.

In this talk, we will first introduce important features of quantum conductance and a number of notions associated with its applicability. The full method will then be illustrated for the case of amphoteric doping of carbon nanotubes. Results from our investigations suggest that the electronic structure of a carbon nanotube can be easily manipulated by encapsulating appropriate organic molecules and that charge transfer processes induced by encapsulated organic molecules lead to efficient n- and p-type doping of the carbon nanotube.

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