Quantum Transport Calculations through Molecules and Carbon Nanotubes

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Recently much effort has been focused to measure the transport properties of single molecules and carbon nanotubes (CNT) bridged between electrodes for the molecular electronics. Since it is still difficult to construct well-characterized nanometer-scale device system between electrodes, theoretical approaches based on the first-principles calculations become important to characterize the transport properties of such nanometer-scale devices.

Here we present our recent calculations for the transport properties of single molecules and carbon nanotubes (CNT) bridged between electrodes. We use two calculation methods.

One is the recursion-transfer-matrix (RTM) method, which is a reliable tool to calculate accurate scattering waves in plane-wave expansions. Combined with the NEGF method and density-functional formalism, we perform calculations of transport properties through single molecules and molecular wires between electrodes. Especially, we focus on the contact effects to electrodes on the transport.

The other is the time-dependent wave-packet diffusion method. Based on the linear-response Kubo formula with localized basis sets, we perform O(N) calculation for the transport of large systems (micron length). We apply this method for the carbon nanotube (CNT) transistors and show the results on the electron-phonon coupling, disorder, and contact effects on the conductance of CNT-FET.

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