Electron transport of nano-carbon materials

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We have investigated electron transport of nano-carbon materials at finite temperatures through the large scale simulation using high-end supercomputers. For our purpose, we have developed an electron transport simulation model, based on a non-equilibrium finite temperature Green's function. The advanced tight-binding, Hamiltonian and molecular dynamical approaches enable us to consider phonon mode effect on electron transport at finite temperatures.

Through oder (N) approach, we are able to simulate meso-scale transport phenomena with several ten thousands of carbon atoms. In addition to calculating fundamental transport coefficient, our method is able to give atomistic electron current for all atomic positions. From the atomistic point of view, we can more clearly understand the interesting behavior of electron transport as nanoscale carbon materials. Our results show that electron current properties of nano-carbon materials strongly depend on a way of attachment of electrodes to such materials. Moreover, a choice of carbon orbital, pi or sigma, which is connected to electrodes, has crucial influence on electron transport behaviors. As for carbon nanotube, grahene, and Macky crystal, we will introduce our progress of researches and our large-scale simulation experiences.