Atomistic nanoscale device modeling: charge and heat transport in large-scale systems

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First, I will briefly overview the standard approach for charge transport at nanoscale, based on the Density Functional Theory and single-particle Green Function method for coherent Landauer transport. Being about 15 years old and realized in the number of available atomistic codes, the standard approach is very successful in describing the coherent transport at nanoscale in low-dimensional and molecular materials and devices, also with complex geometries, many-terminal configurations and nonequilibrium states at finite voltages. However, extension of the theoretical and computational methods to more complex, large-scale, and interacting systems is still a challenge. I will present our recent results concerning the extended contacts [1]. We apply this approach to find a contact resistance of side CNT-metal contacts, transfer length in graphene-metal contacts and electronic properties of the diodes with CNT channel and asymmetric contacts (with the electrodes made of different metals). The other important developments are phonon transport and thermoelectric phenomena [2], and dephasing [3]. Finally, we discuss the realization of new quantum transport methods at nanoscale [4] in the DFTB+ code [5].

References

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