Multiscale modeling of optical and transport properties of nanostructures and low-dimensional materials

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Abstract

Computation methods including density-functional theory (DFT), tight-binding (TB) as well as effective bond-orbital model (EBOM), and k.p model for calculation of optical and transport properties of solids and nanostructures and low-dimensional materials (including quantum wires, quantum dots, and other low-dimensional materials) will be discussed. Transport properties of nanostructure junctions modeled by non-equilibrium Green function method in the Coulomb-blockade regime will also be presented. Examples include optical excitations of solids and nanostructures including the electron-hole interaction obtained within symmetry-adapted basis, time-dependent DFT calculations of optical excitations of semiconductor alloys, and tunneling current spectra as well as thermoelectric characteristics of coupled-quantum dot junctions.

A mixed basis approach based on density functional theory (DFT) is also employed for studying one- and two-dimensional systems such as carbon-dimer chain, carbon nanotube, graphene, graphene nanoribbon, semiconductor surfaces, and MoS2 sheets. The basis functions are taken to be plane waves for the periodic direction multiplied by B-spline functions in the non-periodic direction. B-splines are localized real-space functions, which are low-order polynomials, possessing easy treatment for derivatives. They are flexible, making the geometry optimization easy to implement. With this mixed basis set we can calculate the total energy of a finite-width slab or wire with finite cross-section directly without resorting to the supercell as in the conventional plane-wave based DFT code. One advantage of the mixed-basis code is the easy treatment of charged systems such as positively charged carbon-dimer chain. The spurious Coulomb interaction between the charged defect and its repeated images which appear in the supercell approach can thus be avoided.

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