Quantum Mechanics based Simulation for Nano-scale Materials

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ABSTRACT

Nanostructures can be found in diverse applications including faster and smaller electronic, biochemistry, biomedicine and renewable energy. When the materials reduce their size down to the nano-scale, many of the unusual and interesting properties appear. Quantum size confinement, ballistic electric transport, size tunable band-gap in semiconductor nanostructures, and shape-induced plasmonic modes in metallic nanostructures are some examples of the new physical phenomena that can be explored in these systems. These unique properties could not in general be predicted on the basis of those observed at macroscopic scales. The study of the consequences of these effects must rely on a quantum mechanics based theory that can provide accurate and reliable results, and has the predictive power. Such a theory is necessary to complement the experimental investigation of structures and properties of nano-structures and to pave the way for understanding, designing, and controlling these properties for functional molecular assemblies. In this talk, I will briefly introduce the basic theory of quantum mechanics simulation for nano-scale materials, followed by a brief introduction of the SCED-LCAO approach developed by the condensed matter theory group at the department of physics and astronomy, University of Louisville. Then, I will present some quantum mechanics based simulations for nano-scale materials, such as the carbon nanotubes and the SiC nanostructures.