Electronic structure calculation of low-dimensional systems

Numerical theoretical investigation of nanostructures presents a difficult task for computational science. Systems with reduced dimensionality lack translational periodicity in at least one direction and the calculation methods, designed to study bulk materials, are not always applicable. On the other hand, nanosized materials contain large number of atoms, making the use of modern quantum-chemical methods too expensive in terms of computational cost.

The tutorial presents some of the computational methods, widely used to study various nanostructures. This is accompanied with the application of these methods for the investigation of particular low-dimensional systems. The energy band features of few-layer III-VI (GaS, GaSe and InSe) structures are discussed. The variation of the electronic structure of these systems with the number of layers is explained in terms of the orbital composition of the energy bands. As an another modern task, the computational study of the atomic geometry and charge transfer of molecular and 1-d structures, encapsulated within single-walled carbon nanotubes is presented.