Multiscale Modeling of Nanomaterials

By

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Objective: This short tutorial course is designed to provide an introduction to multiscale modeling techniques for modern nanomaterials. The range and scope of the course will be apparent from the list of contents given below. We will also try to provide illustrative examples for hands-on experience during the tutorial. In Part A, we will provide and demonstrate some simple codes in ForTran and MathCad and their applications to graphene and other nanomaterials. For Part B, we will try to log on to MTU computer in USA and run a DFT code for a simple modeling problem. The course should be of interest to theory as well as experimental researchers, who want to familiarize themselves with the basics of multiscale modeling. It will prepare the theorists for learning more advanced techniques by further self-study. For experimental researchers, the course should also be useful because it will make them aware of the strength and limitations of multiscale modeling and its applicability to research problems. The necessary prerequisite for the course is graduate (M.Sc.) level knowledge of Solid State Physics, Quantum Mechanics, and Mathematical Physics.

Tentative list of contents

Part A: Classical Green's function methods (Three hours with one break)

1. Continuum and discrete atomistic models
2. Green's function as response function
3. Correspondence between continuum and lattice Green's functions
4. Interatomic potentials
5. Molecular dynamics and Green's function methods for discrete atomistic modeling of materials
6. Multiscale Green's functions
7. Bridging length scales
8. Bridging time scales
9. Application to graphene and other nanomaterials

Part B: *Ab initio* methods (Three hours with one break)

1. Molecular Electronics - Properties of interest at Nanoscale and role of quantum mechanics
2. First principles methods
3. Hartree Fock vs Density Functional Theory
4. Density Functional Theory - Basis sets, exchange and correlational functional forms
5. Conduction at nanoscale - Green's Function Approach
6. Device elements – Molecules
7. Spintronics – Molecules
8. Illustrative examples
9. Future directions