ELEC 542: Nanoscale Modelling and Simulations

Department of Electrical and Computer Engineering
The University of British Columbia

Overview

This course provides an extensive theoretical foundation for as well as hands-on introduction to several widely used methods for studying the properties of materials and structures, in particular at the nanoscale and mesoscale. The majority of the time is spent on quantum-mechanical methods: the first-principles approaches (starting from the Hartree-Fock theory and building up to Configuration Interaction and the Møller–Plesset Perturbation Theory) and, in particular, the Density Functional Theory, which are derived and discussed in detail. Semi-empirical methods such as Tight Binding and Molecular Dynamics are also covered, as well as strategies for modelling material properties (electronic, mechanical, optical, etc.). Practical activities include implementing some of the above theories in computer code, in addition to using established software (Gaussian, SIESTA, VASP, LAMMPS, etc.). Each student also works on a project of their choice using the methods discussed.

Mode of instruction

Every week, there will be pre-recorded videos to watch in prepartion for the lecture and in-class discussions. The course will be delivered fully in hybrid mode: The classes will be in person and also simultaneously broadcast online as well as recorded and made available for viewing later. Online attendees can participate in the discussions and ask questions at the same level as those present in person. Online office hours will also be available. It will thus be possible to take the course entirely remotely without any loss of quality.

(Note: If demand for in-person participation is low, the course may be delivered entirely online.)

Topics

- Introduction
  - Modelling quantum systems and phenomena
  - The many-body wave function and the Schrödinger equation
  - The Born-Oppenheimer approximation
  - Spin and the Pauli exclusion principle
  - Representation of functions
- Hartree-Fock theory
  - Hartree products and Slater determinants
  - The variation principle
  - The expectation value of the Hamiltonian with a single Slater-determinant
  - Lagrange's method of undetermined multipliers
  - Exchange interaction, the Fock operator, and the Hartree-Fock equations
- Interpretation of Hartree-Fock orbitals
  - Unitary transformations and the diagonalization of the Hartree-Fock equations
  - The Koopmans theorem and the significance of canonical Hartree-Fock orbitals

- Implementation of the Hartree-Fock equations
  - Basis functions and basis sets
  - The Roothaan equations
  - Mulliken population analysis
- Post-Hartree-Fock methods
  - Many-electron excitations
  - Basis set for many-electron wave functions
  - Configuration interaction
  - The Møller-Plesset perturbation theory
- The density functional theory (DFT)
  - Functional derivatives
  - The theorems of Hohenberg and Kohn
  - The Kohn-Sham method
  - Total energy in DFT, and the significance of Kohn-Sham orbitals
  - Correlation energy and exchange-correlation functionals
  - The connection between DFT and the Thomas-Fermi-Dirac and Hartree-Fock theories
  - Periodicity, the Bloch theorem, and band structure in DFT
  - Finite-temperature DFT
  - Time-dependent DFT
- Semi-empirical approach to studying electronic structure
  - Linear combination of atomic orbitals
  - The Hückel method
  - The Pariser-Parr-Pople method
  - The tight-binding method
- Semi-empirical approach to studying mechanical structure
  - Molecular mechanics and molecular dynamics
  - Force fields
  - Time propagation
  - Temperature, pressure, thermostats, and barostats

Textbook

Not required. All the material will be provided.

Useful references

- Modern quantum chemistry, A. Szabo and N. S. Ostlund
- Density functional theory of atoms and molecules, R. G. Parr and W. Yang

Additional reading (not required, but would provide complementary perspective)

- Quantum mechanics for scientists and engineers, D. A. B. Miller
- Elementary electronic structure, W. Harrison
- Relativistic quantum chemistry, K. G. Dyall K. Faegri, Jr.
- Theoretical materials science, A. Gonis
- Time-dependent density-functional theory: concepts and applications, C. A. Ullrich
- Molecular dynamics, Wm. G. Hoover

Grading scheme

- Assignments total: 50 points
- Final project (work accomplished, presentation, and report in the style of a Physical Review Letters paper): 50 points

Instructor

Alireza Nojeh, PhD, PEng
Professor, Department of Electrical and Computer Engineering
Principal Investigator, Quantum Matter Institute
The University of British Columbia
http://nanostructure.ece.ubc.ca/
https://qmi.ubc.ca/
alireza.nojeh@ubc.ca
604 827 4346