MS 508/EC 572: Computational Methods in Materials Science, Fall 2024

MW 10:10 pm-11:55 pm, KCB 102

This course will provide an introduction to computational materials science with a focus on electronic structure theory. The topics covered include tight binding theory, density functional theory, and many-body perturbation theory. Lectures provide the theoretical framework for understanding the computational methods; homework assignments and class project will involve computational projects performed on BU shared computing resources and NSF NanoHub.org.

Instructor: Sahar Sharifzadeh
Office Hours: M 1 pm - 2 pm, Tu 2 pm – 3 pm, PHO 535
Textbook: "Materials Modelling using Density Functional Theory: Properties and Predictions" by Feliciano Giustino (Oxford University Press, 2014)
Additional Resources:

- Modeling and Simulation Course: https://nanohub.org/courses/MSE697
- Learning the Unix environment: https://www.tutorialspoint.com/unix/index.htm
- Guide for Bash scripting: http://mywiki.wooledge.org/BashGuide/CommandsAndArguments

Prerequisite: EC/MS 577 or equivalent strongly encouraged
Grading:

- 40% Homework assignments
- 60% Class project

Class Project Details:
The class project is a computational project focused on a single scientific question, and is to be completed in teams. It will involve an end-of-semester presentation and brief summary report (2 pages). The expectation is that this project will be performed with scientific rigor and that every member of the team demonstrates contribution.

Academic conduct: Please note that all students are expected to follow BU's academic conduct code. For more information, see http://www.bu.edu/academics/policies/academic-conduct-code/

Tentative Syllabus

- Week 1: Introduction to computational materials science + crystal structures
- Week 2-3: Modeling electronic properties of materials: the many-body problem
  - Lectures 2-3: Review quantum mechanics and solid-state physics concepts
  - Lectures 4-5: The many-body problem in materials and the tight binding approximation
- Week 4-8: The electronic ground state: density functional theory (DFT)
  - Lecture 6: Brief overview of the theory
  - Lectures 7-8: Computational approximations (basis set, pseudopotential, functionals etc.)
  - Lectures 9-14: The ground state: structural and mechanical properties
  - Lectures 15-16: The electronic structure: charge density and bandstructure
- Week 9-10: The phonon normal modes: density functional perturbation theory (DFPT)
  - Lecture 17-18: DFPT theory
  - Lecture 19: Calculating the Raman spectrum
- Week 11+: Electronic excitations: random phase approximation (RPA); many-body perturbation theory (MBPT)
- Week 13-14: Course project presentations