PHYS 780 Quantum Mechanical Simulation of Condensed Matter - Syllabus

Course Description

Advanced computational course focusing on utilization of density-functional-theory (DFT) based quantum mechanical simulation for materials research. Introduces the fundamentals of density-functional-theory and key approximations as a power computational approach to condensed matter physics. By engaging state-of-the-art quantum-mechanical simulation software and its utility programs, students will have hands on computational exercises of calculating and understanding the electronic structure and bonding, and learn to accurately predict the physical properties of solids including phonon dispersion, Raman and IR spectroscopy, magnetism, superconductivity, ultra-fast dynamics.

Instructor

Prof. Howard Sheng

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Lectures

Tuesdays 4:30 - 7:10 PM, online with Blackboard Ultra Collaborate.

Course website

https://mymasonportal.gmu.edu/ultra/courses/_432844_1/cl/outline

Objectives

- Teach computational quantum mechanics and materials physics as is required to understand a particular method.
- Provide in-depth understanding of DFT methods, as implemented in popular software widely used in physics research.
- Familiarize the students with the Linux-HPC environment and teach how to install computational software and run parallel computational jobs.
- Be able to solve physical problems using DFT calculations, both in course work and in his/her future research.
- Understand the scope, possibilities and limitations of the simulation approaches. Evaluate the tools and their applicability to diverse physics problems.
- Keep abreast with the current research and development of DFT methods in the discipline of condensed matter physics.

Textbook

Teaching materials will be collected from different textbooks, published papers and online tutorials. There is no preferred textbook.

Suggested reference books:

- Materials Modelling Using Density Functional Theory: Properties and Predictions 1st Edition by Feliciano Giustino, Wiley.
- Quantum Chemistry, Third Edition by Jon P. Lowe and Kirk A. Peterson, Academic Press.
- Density Functional Theory: A Practical Introduction by David S. Sholl, Janice A. Steckel, Whiley (2009) https://onlinelibrary.wiley.com/doi/pdf/10.1002/9780470447710
- Electronic Structure: Basic Theory and Practical Methods: Basic Theory and Practical Density Functional Approaches by Richard M. Martin, Cambridge University Press (2004)
- Introduction to Solid State Physics, Eighth Edition by Charles Kittel, Wiley.

Prerequisite

There are not specific prerequisites, just permission of the instructor. Students are expected to have background in quantum mechanics and solid-state physics, and are expected to relatively quickly become comfortable with advanced concepts from mathematics and physics.

Homeworks and Projects

Each student will be responsible to cover the material in the textbook or lecture notes, do the assigned homework exercises, and complete a certain number of short computational projects. Project topics will be available to students as class progresses.

Software

VASP and WIEN2k.

Computers

Students will have access to Argo cluster running Scientific Linux. User accounts on the gmu argo cluster will be secured for this course.

User account:

Students need to request accounts from the link on this page: https://orc.gmu.edu/new-user-information/

Once they do, they'll get an email with the details for an new user tutorial for cluster users which they need to attend before they can start using the cluster. This is held regularly on Tuesdays at 10:00AM and

Thursdays at 4:00PM. The tutorial covers using SLURM on the cluster.

Office hours

I do not plan to hold regular office hours, but will have an open-door policy. Students are welcome to drop by my office any time. If you would like to make an appointment with me at a specific time, send emails to: hsheng@gmu.edu

Evaluation

- 80% acquired through four computational projects. Each project is worth 20%.
- 20% homework exercises and attendance.

Ethics

In this course, I expect students to be honest and truthful. Ethical violations include cheating on exams, plagiarism, unauthorized collaboration, alteration of graded assignments, forgery, falsification, lying, facilitating academic dishonesty, and unfair competition. More will be discussed on the first day of class.

Tentative Class Schedule

1. Introduction to DFT and key approximations used in DFT
2. Implementation of DFT in VASP
3. Self-consistent-field method and band-structure calculations
4. Tutorial on Wien2K
5. Phonon calculations and thermodynamics
6. Mechanical properties
7. Structural prediction with DFT
8. Raman and IR spectroscopy
9. Electric conductance and magnetism
10. Superconductivity *
11. Ultrafast electron dynamics *

(*optional)