DALHOUSIE UNIVERSITY

Computational Methods for Atomistic Simulation of Materials and Molecules

Department of Physics and Atmospheric Science

PHYC6601 Fall 2025

Dalhousie University acknowledges that we are in Mi'kma'ki, the ancestral and unceded territory of the Mi'kmaq People and pays respect to the Indigenous knowledges held by the Mi'kmaq People, and to the wisdom of their Elders past and present. The Mi'kmaq People signed Peace and Friendship Treaties with the Crown, and section 35 of the Constitution Act, 1982 recognizes and affirms Aboriginal and Treaty rights. We are all Treaty people.

Dalhousie University also acknowledges the histories, contributions, and legacies of African Nova Scotians, who have been here for over 400 years.

Instructor: Penghao Xiao *(E-Mail: pxiao@dal.ca; Office: Dunn 230)*

Lectures: *Wednesday 2:00-3:30 PM, Dunn 230 (bring your own laptop)*

Office hours: *by appointment, Dunn 230*

Course delivery: *In person*

Course Description

This course introduces computational methods for simulating materials and molecular systems at the atomic scale. Topics include electronic structure from density functional theory (DFT), geometry relaxation, diffusion/reaction barrier calculation, molecular dynamics, and kinetic Monte Carlo simulations. Applications span materials bulk properties and surface reactions, with an emphasis on linking atomistic processes to macroscopic observations.

Learning Objectives

The goal of this course is to help you run proper calculations to explain real-world observations. By the end of the course, students will be able to:

1. Construct appropriate computational models to represent experiments.
2. Perform simulations using suitable computational techniques.
3. Analyze, visualize, and present results in a clear and rigorous manner.
4. Interpret computational outcomes to provide insights into experimental findings.

Course Assessment

Assessment	Weight (% of final grade)	Date
Assignments	50%	Approximately biweekly
Final Project	50%	Report due by December 20
Total	100%	

Final Project: You will pick a topic to apply the computational methods learned. You will present your work to the class and write a report. Your final mark will be based on the presentation and the report. The report should be organized in five parts: introduction, method, results, conclusion and discussion, and appendix. Imagine it as a short paper to explain your project and findings.

Conversion of numerical grades to Final Letter Grades follows the Dalhousie Common Grade Scale

A+ (90-100)	**B+** (77-79)	**C+** (65-69)	**D** (50-54)
A (85-89)	**B** (73-76)	**C** (60-64)	**F** (<50)
A- (80-84)	**B-** (70-72)	**C-** (55-59)	

Course Policies on Missed or Late Academic Requirements

- Late assignments can be turned in, but a penalty mark (20% per day) will be deducted.
- Students may use the Student Declaration of Absence form for late assignments to avoid the late penalty. The form can be used 2 times in this course.

Course Policies related to Academic Integrity

You are encouraged to collaborate on assignments but not allowed to plagiarize.

Course Content

- Thermodynamics vs kinetics: the energy landscape perspective
- Basics of supercomputers and Linux (SSH, SBATCH job management, parallel computing)
- Thermodynamics: calculate energies with DFT
    - Input structures: periodic boundary condition for bulk, defects and molecules
    - Relax electrons (Energy cutoff of plain-wave basis set, k-points, pseudopotential, choice of functionals)
    - Relax ions (lattice parameters, atomic positions, convergence, steepest descent, restart from previous calculations)
    - Convex hull for different compositions
- Electronic structure analysis: to better understand the energetics.
    - Band structure and density of state (DOS)
    - Charge density analysis: Bader charge
    - Partial charge density in a specific energy range
- Kinetics: calculate reaction/diffusion barrier with the nudged elastic band method (NEB)
- Molecular dynamics/Monte Carlo (Al liquid, Al adatom diffusion on (111) surface, diffusivity)
- Analysis of vibrational frequencies and modes, if time permits

DALHOUSIE UNIVERSITY

University Policies and Statements

Recognition of Mi'kmaq Territory

Dalhousie University would like to acknowledge that the University is on Traditional Mi'kmaq Territory. The Elders in Residence program provides students with access to First Nations elders for guidance, counsel, and support. Visit or e-mail the Indigenous Student Centre at 1321 Edward St or elders@dal.ca. Additional information regarding the Indigenous Student Centre can be found at: https://www.dal.ca/campus_life/communities/indigenous.html

Internationalization

At Dalhousie, 'thinking and acting globally' enhances the quality and impact of education, supporting learning that is "interdisciplinary, cross-cultural, global in reach, and orientated toward solving problems that extend across national borders." Additional internationalization information can be found at: https://www.dal.ca/about-dal/internationalization.html

Academic Integrity

At Dalhousie University, we are guided in all our work by the values of academic integrity: honesty, trust, fairness, responsibility, and respect. As a student, you are required to demonstrate these values in all the work you do. The University provides policies and procedures that every member of the university community is required to follow to ensure academic integrity. Additional academic integrity information can be found at: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Student Accessibility Centre is Dalhousie's centre of expertise for matters related to student accessibility and accommodation. If there are aspects of the design, instruction, and/or experiences within this course (online or in-person) that result in barriers to your inclusion, please contact the Student Accessibility Centre (https://www.dal.ca/campus_life/academic-support/accessibility.html) for all courses offered by Dalhousie with the exception of Truro. For courses offered by the Faculty of Agriculture, please contact the Student Success Centre in Truro (https://www.dal.ca/about-dal/agricultural-campus/student-success-centre.html)

Conduct in the Classroom – Culture of Respect

Substantial and constructive dialogue on challenging issues is an important part of academic inquiry and exchange. It requires willingness to listen and tolerance of opposing points of view. Consideration of individual differences and alternative viewpoints is required of all class members, towards each other, towards instructors, and towards guest speakers. While expressions of differing perspectives are welcome and encouraged, the words and language used should remain within acceptable bounds of civility and respect.

Diversity and Inclusion – Culture of Respect

Every person at Dalhousie has a right to be respected and safe. We believe inclusiveness is fundamental to education. We stand for equality. Dalhousie is strengthened in our diversity. We

are a respectful and inclusive community. We are committed to being a place where everyone feels welcome and supported, which is why our Strategic Direction prioritizes fostering a culture of diversity and inclusiveness (Strategic Priority 5.2). Additional diversity and inclusion information can be found at: http://www.dal.ca/cultureofrespect.html

Student Code of Conduct

Everyone at Dalhousie is expected to treat others with dignity and respect. The Code of Student Conduct allows Dalhousie to take disciplinary action if students don't follow this community expectation. When appropriate, violations of the code can be resolved in a reasonable and informal manner - perhaps through a restorative justice process. If an informal resolution can't be reached, or would be inappropriate, procedures exist for formal dispute resolution. The full Code of Student Conduct can be found at: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

Fair Dealing Policy

The Dalhousie University Fair Dealing Policy provides guidance for the limited use of copyright protected material without the risk of infringement and without having to seek the permission of copyright owners. It is intended to provide a balance between the rights of creators and the rights of users at Dalhousie. Additional information regarding the Fair Dealing Policy can be found at: https://www.dal.ca/dept/university_secretariat/policies/academic/fair-dealing-policy-.html

Originality Checking Software

The course instructor may use Dalhousie's approved originality checking software and Google to check the originality of any work submitted for credit, in accordance with the Student Submission of Assignments and Use of Originality Checking Software Policy. Students are free, without penalty of grade, to choose an alternative method of attesting to the authenticity of their work and must inform the instructor no later than the last day to add/drop classes of their intent to choose an alternate method. Additional information regarding Originality Checking Software can be found at: https://www.dal.ca/about/leadership-governance/academic-integrity/faculty-resources/ouriginal-plagiarism-detection.html

Student Use of Course Materials

Course materials are designed for use as part of this course at Dalhousie University and are the property of the instructor unless otherwise stated. Third party copyrighted materials (such as books, journal articles, music, videos, etc.) have either been licensed for use in this course or fall under an exception or limitation in Canadian Copyright law. Copying this course material for distribution (e.g. uploading to a commercial third-party website) may lead to a violation of Copyright law.