

**Faculty of Science Course Syllabus**  
**Department of *Chemistry***

*CHEM6363*

*Electronic Structure Theory of Solids*

*Winter 2021*

**Instructor(s):** Josef Zwanziger, [jzwanzig@dal.ca](mailto:jzwanzig@dal.ca). Office hours by appointment, through Microsoft Teams. Reach me via e-mail.

**Lectures:** Delivered asynchronously as screen-capture videos, served through Brightspace. As this is a half course, but will last all term, I anticipate one upload per week.

**Tutorials:** As lectures will be delivered asynchronously, there will be one tutorial per week at a time to be agreed upon by the class. Tutorials will be held through Teams.

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### **Course Description**

The electronic structure and properties of solids will be explored through use of a modern open-source density function theory code, ABINIT.

### **Course Objectives/Learning Outcomes**

Basic understanding of the electronic structure of solids, and response functions such as phonons, dielectric, and elasticity. Ability to use a modern DFT code, and to understand how to check its outputs and convergence.

### **Course Materials**

- REQUIRED: access to a current version of ABINIT, preferably 9.2.2 or later
- Online: [www.abinit.org](http://www.abinit.org), [www.pseudo-dojo.org](http://www.pseudo-dojo.org)
- Useful reference texts include R. M. Martin, *Electronic Structure*, Cambridge 2004
- Much of this course will be served through the CHEM 6363 page at Brightspace.

**Course Assessment**

Assignments                      Roughly weekly, online assignments of calculations and tutorials using ABINIT, with a report submitted.                      50%

Final Project                      Each student will develop their own final calculation project in consultation with Dr. Zwanziger, to be submitted by the end of exam period. 50%

**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**

Collaboration: As all assignments are on-line, each student will submit his/her own work. For homework assignments and the final projects, discussion amongst the students is permitted and encouraged.

**Course Content**

Most of [www.abinit.org/tutorial](http://www.abinit.org/tutorial)

## University Policies and Statements

**This course is governed by the academic rules and regulations set forth in the University Calendar and by Senate**

### **Missed or Late Academic Requirements due to Student Absence**

As per Senate decision instructors may not require medical notes of students who must miss an academic requirement, **including the final exam**, for courses offered during fall or winter 2020-21 (until April 30, 2021). Information on regular policy, including the use of the Student Declaration of Absence can be found here: [https://www.dal.ca/dept/university\\_secretariat/policies/academic/missed-or-late-academic-requirements-due-to-student-absence.html](https://www.dal.ca/dept/university_secretariat/policies/academic/missed-or-late-academic-requirements-due-to-student-absence.html).

### **Academic Integrity**

At Dalhousie University, we are guided in all of our work by the values of academic integrity: honesty, trust, fairness, responsibility and respect (The Center for Academic Integrity, Duke University, 1999). As a student, you are required to demonstrate these values in all of 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.

**Information:** [https://www.dal.ca/dept/university\\_secretariat/academic-integrity.html](https://www.dal.ca/dept/university_secretariat/academic-integrity.html)

### **Accessibility**

The Advising and Access Services Centre is Dalhousie's centre of expertise for student accessibility and accommodation. The advising team works with students who request accommodation as a result of a disability, religious obligation, or any barrier related to any other characteristic protected under Human Rights legislation (Canada and Nova Scotia).

**Information:** [https://www.dal.ca/campus\\_life/academic-support/accessibility.html](https://www.dal.ca/campus_life/academic-support/accessibility.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.

**Code:** [https://www.dal.ca/dept/university\\_secretariat/policies/student-life/code-of-student-conduct.html](https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html)

### **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

**Statement:** <http://www.dal.ca/cultureofrespect.html>

### **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 (1321 Edward St) ([elders@dal.ca](mailto:elders@dal.ca)).

**Information:** [https://www.dal.ca/campus\\_life/communities/indigenous.html](https://www.dal.ca/campus_life/communities/indigenous.html)

### **Important Dates** in the Academic Year (including add/drop dates)

[https://www.dal.ca/academics/important\\_dates.html](https://www.dal.ca/academics/important_dates.html)

### **University Grading Practices**

[https://www.dal.ca/dept/university\\_secretariat/policies/academic/grading-practices-policy.html](https://www.dal.ca/dept/university_secretariat/policies/academic/grading-practices-policy.html)

## **Student Resources and Support**

## Advising

**General Advising** [https://www.dal.ca/campus\\_life/academic-support/advising.html](https://www.dal.ca/campus_life/academic-support/advising.html)

**Science Program Advisors:** <https://www.dal.ca/faculty/science/current-students/academic-advising.html>

**Indigenous Student Centre:** [https://www.dal.ca/campus\\_life/communities/indigenous.html](https://www.dal.ca/campus_life/communities/indigenous.html)

**Black Students Advising Centre:** [https://www.dal.ca/campus\\_life/communities/black-student-advising.html](https://www.dal.ca/campus_life/communities/black-student-advising.html)

**International Centre:** [https://www.dal.ca/campus\\_life/international-centre/current-students.html](https://www.dal.ca/campus_life/international-centre/current-students.html)

## Academic supports

**Library:** <https://libraries.dal.ca/>

**Writing Centre:** [https://www.dal.ca/campus\\_life/academic-support/writing-and-study-skills.html](https://www.dal.ca/campus_life/academic-support/writing-and-study-skills.html)

**Studying for Success:** [https://www.dal.ca/campus\\_life/academic-support/study-skills-and-tutoring.html](https://www.dal.ca/campus_life/academic-support/study-skills-and-tutoring.html)

**Copyright Office:** <https://libraries.dal.ca/services/copyright-office.html>

**Fair Dealing Guidelines** <https://libraries.dal.ca/services/copyright-office/fair-dealing.html>

## Other supports and services

**Student Health & Wellness Centre:** [https://www.dal.ca/campus\\_life/health-and-wellness/services-support/student-health-and-wellness.html](https://www.dal.ca/campus_life/health-and-wellness/services-support/student-health-and-wellness.html)

**Student Advocacy:** <https://dsu.ca/dsas>

**Ombudsperson:** [https://www.dal.ca/campus\\_life/safety-respect/student-rights-and-responsibilities/where-to-get-help/ombudsperson.html](https://www.dal.ca/campus_life/safety-respect/student-rights-and-responsibilities/where-to-get-help/ombudsperson.html)

## Safety

**Biosafety:** <https://www.dal.ca/dept/safety/programs-services/biosafety.html>

**Chemical Safety:** <https://www.dal.ca/dept/safety/programs-services/chemical-safety.html>

**Radiation Safety:** <https://www.dal.ca/dept/safety/programs-services/radiation-safety.html>

**Scent-Free Program:** <https://www.dal.ca/dept/safety/programs-services/occupational-safety/scent-free.html>