

**Faculty of Science Course Syllabus**  
**Department of Chemistry**  
**CHEM 6363**  
***Electronic Structure Theory of Solids***  
***Winter Term 2018***

**Instructor(s):** Josef Zwanziger [jzwanzig@dal.ca](mailto:jzwanzig@dal.ca) Chemistry 326

**Lectures:** T 10:05-11:25 Chemistry 540

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### Course Description

Electronic structure of solids, with emphasis on density functional theory. The pseudopotential approximation will be emphasized, together with computation of properties such as phonons and elasticity.

### Course Prerequisites

Permission of instructor.

### Course Objectives/Learning Outcomes

Understanding of approximations made in density functional theory treatment of electronic structure in solids; facility for computing solid-state properties with a DFT code.

### Course Materials

None required; recommended: R. M. Martin, *Electronic Structure* (Cambridge).

### Course Assessment

Component	Weight (% of final grade)	Date
<i>Assignments</i>	50%	Weekly problem sets due in class
<i>Project</i>	50%	April 20

### Other course requirements

Must pass final project (70% or better) in order to pass class (note that passing a graduate-level course means B- or above).

### 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

No late homework accepted.

### Course Content

Date	Topic
Jan 9	Total energy: Kohn-Sham DFT, planewaves, pseudopotentials
Jan 16	Band structure: k points
Jan 23	Forces and stresses: geometry optimization
Jan 30	Projector-augmented Wave method (PAW)
Feb 6	At the nucleus: field gradients and Moessbauer
Feb 13	Density functional perturbation theory (DFPT): electric fields
Feb 27	Phonons and elastic properties
Mar 5	Phonons and elastic properties continued
Mar 12	Spin degrees of freedom
Mar 19	Polarization
Mar 26	Optics in the IPA
Apr 3	Many-body effects: GW and BSE
Apr 20	Project due

## University Policies and Statements

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

### 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 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**

**Research Lab Safety** [https://www.dal.ca/content/dam/dalhousie/pdf/dept/safety/lab\\_policy\\_manual\\_2007.pdf](https://www.dal.ca/content/dam/dalhousie/pdf/dept/safety/lab_policy_manual_2007.pdf)

**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>