

**Faculty of Science Course Syllabus**  
**Department of Chemistry**  
**CHEM 4301/5301**  
**Theory of Chemical Bonding**  
**Winter 2020**

**Instructor:** Dr. Erin R. Johnson, erin.johnson@dal.ca, Chemistry Building Room 530

**Lectures:** Mondays, Wednesdays, and Fridays, 2:35–3:25 pm, Chemistry Building Room 223

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### **Course Description**

This course develops molecular-orbital theory from both qualitative and quantitative perspectives. Topics include the basic principles of the LCAO (Linear Combination of Atomic Orbitals) method, qualitative understanding of molecular orbitals in simple molecules, and orbital symmetries, through to state-of-the-art techniques for computational prediction of molecular properties.

### **Course Prerequisites**

A grade of C- or better in CHEM 3301: Quantum Mechanics and Chemical Bonding.

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

At the conclusion of the course, students will be expected to:

- explain chemical bonding in terms of quantum-mechanical concepts,
- use molecular-orbital theory to predict or explain chemical properties,
- perform quantum-chemical calculations of molecular properties using the Gaussian electronic-structure program.

### **Course Material**

There is no required textbook for this course. “Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian” by Foresman and Frisch, is very strongly recommended for the computational component.

### **Course Assessment**

The course grade will be based on a combination of assignments and the final exam:

Component	Weight (% of final grade)	Date
Assignments	50%	Alternate Fridays by 4:30 pm.
Final Exam	50%	To be scheduled.

A minimum grade of 50% on the final exam is required in order to pass the course. In the event that the final-exam mark is higher than the sum of the assignment marks, then the final course grade will be determined solely based on the exam.

There will be a total of six assignments that will be given biweekly and will be due on Fridays before 4:30 pm. In the event that there is a statutory holiday or weather-related closure on the Friday when an assignment would be due, an extension to the following Monday will be granted to all students. The initial four assignments will be based on molecular-orbital theory, while the final two assignments will use the Gaussian electronic-structure program, which is available on the computers in the Chemistry resource center.

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

Late assignments will not be accepted and will be assigned a mark of zero, unless students have a legitimate excuse.

In the event that you are sick and cannot write the final exam as scheduled, you must email me to let me known **before** the exam starts. You must also supply a doctor's note within 48 hours of the end of the exam. You will only be excused from the exam and allowed to write a make-up exam if both these criteria are met. The make-up exam must be written before the end of the exam period.

With respect to the computational assignments, students are expected to perform all calculations independently and should save their input and output files on a memory stick. They may be asked to produce these files in the event of any suspected incidents of plagiarism.

Use of cellular phones during lectures is strictly prohibited; phones must be turned off before the start of the lecture.

## Course Content

Topics to be covered include:

- Atomic orbitals
- The variational principle
- Molecular orbitals for simple diatomics
- Molecular orbitals for polyatomics
- Hückel molecular-orbital theory

- Hartree-Fock theory
- Gaussian basis sets
- Configuration interaction
- Perturbation theory
- Density-functional theory

## 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**

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>