Faculty of Science Course Syllabus
Department of Chemistry
CHEM 4301/5301
Theory of Chemical Bonding
Winter 2023

Instructor: Dr. Erin R. Johnson, erin.johnson@dal.ca

Lectures: Mondays, Wednesdays, and Fridays, 12:35–1:25 pm in Room 540 of the Chemistry Building. For the computational component to be covered during the final 3 weeks of term, synchronous lectures will be held online using Zoom. Links will be provided to the class by email. Students are expected to have a working microphone and webcam for discussion.

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 or an equivalent course in quantum mechanics.

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 6:00 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.

The final exam will be held during the exam period on a date agreed upon by all students using a doodle poll. The exam will be distributed by email and students will have a period of six hours in which to submit their solutions by return email. These can either be typed solutions, or a photo or scan of handwritten solutions. If a student is ill, they must contact the instructor prior to the start of the exam. In this case, they will be able to write a make-up exam on a later date agreed upon by both the student and instructor. This date will fall during the exam period, unless the student is still unable to write due to an extended illness. Students must complete the exam independently, although the course notes, any textbooks, or other static online resources (such as wikipedia) are permitted. Evidence of collusion between students (such as identical solutions), posting exam questions in online forums, or using cheating websites (such as chegg), will result in a mark of zero and failure of the course.

There will be a total of six assignments that will be given biweekly, which will be due on Fridays before 6:00 pm. The solutions should be submitted to the instructor by email. Late submission of the assignments will result in a mark of zero, unless the student has a legitimate excuse, such as illness. In this case, they will be granted an extension of a suitable length, to be agreed upon by the student and instructor.

The initial four assignments will be based on molecular-orbital theory, while the final two assignments will use the Gaussian electronic-structure program. To use this software, students will be given access to a Linux server used by the Johnson group. They will be expected to connect to this server remotely from their home computer. Guidance on connecting to and using the server will be provided through a series of tutorials. Use of Gaussian will be covered in class time. It is very strongly recommended that students install the free Avogadro program (https://avogadro.cc/) on their home computers to visualize molecular structures. Students are expected to perform all Gaussian calculations independently and should save their input and output files on the Linux server. Students must have unique input and output files. Copying files from another student will result in a mark of zero on the related assignment.

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 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

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

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

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).

Information: 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

University Grading Practices

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
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
Black Advising Centre: https://www.dal.ca/campus_life/communities/black-student-advising.html
International Centre: 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
Studying for Success: 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
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

Safety

Lab Safety: 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