

Faculty of Science Course Syllabus
Department of Chemistry
CHEM 6353
Density-Functional Theory
Fall 2020

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

Lectures: Tuesdays 1:35-4:25 pm, for the first 6 weeks of term. Synchronous lectures will be held online using google hangouts. Links will be provided by email a few minutes prior to the start of each lecture. Students are expected to have a working microphone and webcam for discussion and presentations.

Course Description

The fundamental principles of density-functional theory (DFT) will be developed, from the Hohenberg-Kohn-Sham theorems to the construction of modern exchange-correlation functionals via the exchange-correlation “hole” concept.

Course Prerequisites

CHEM 4301/5301 or permission of the instructor.

Course Objectives/Learning Outcomes

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

- explain key concepts in density-functional theory,
- perform derivations involving density functionals,
- be able to select an appropriate density functional for a given problem.

Course Material

There is no required textbook for this course. Students will be expected to download and read relevant journal articles.

Course Assessment

The course grade will be based on a combination of an assigned problem set and an online presentation.

Component	Weight (% of final grade)	Date
Problem Set	50%	Due Thursday, October 15, by 11:59 pm
Presentation	50%	Tuesdays, October 6 and 13, during lecture times

The problem set will be given to students during the first week of class. The solutions should be submitted to the instructor by email, no later than 11:59 pm on Thursday, October 15. Late submission of the problem set will result in a mark of zero, unless the student has a legitimate excuse, such as extended illness. In this case, they will be granted an extension of a suitable length, to be agreed upon by the student and instructor. If the student cannot present on their scheduled date and have a legitimate excuse, for example due to illness or technology malfunction, they will be permitted an extension, to present the following week with no penalty.

The presentation will be given on a topic of the student's choice in the field of density-functional theory. All proposed topics must be approved by the instructor in the first two weeks of class. It is strongly recommended that students pick a topic that is related to their thesis project. The student should then prepare an in-depth lecture on their topic of choice, summarising the theory or findings from the original literature. The presentation will be given via google hangouts during the regular lecture time and should be between 30-40 minutes in length. It will be followed by questions and discussion from the audience. The presentation will be assessed based on clarity of explanations, depth of understanding, and ability to answer questions.

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)		

As this is a graduate course, a grade of B- or above is required to pass.

Course Content

Topics to be covered include:

- Kohn-Sham theory
- Properties of exchange and correlation holes
- The local spin-density approximation
- Generalized gradient approximations
- Hybrid functionals
- Delocalization error

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 the 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

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 wel-

come 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>