

Faculty of Science Course Syllabus
Department of Chemistry
CHEM 6353
Density-Functional Theory
Winter 2018

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

Lectures: Mondays 1:35-4:25 pm, January-February, Chemistry Building Room 540

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 in-class presentation.

Component	Weight (% of final grade)	Date
Assignment	50%	Friday, February 16, by 4:30 pm
Presentation	50%	Monday, February 12, in class

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 doctoral 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 can be given using either the chalkboard or slides and should be roughly 30 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)		

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

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>