Obsolete web version – see the course Brightspace Shell for current information

CHEM 3102 (Winter 2026)

Methods of Computational Chemistry

Course Instructor: Christopher Rowley

Email: [redacted]

Student Hours: **By appointment**

Office: Please make arrangements in advance to meet with the instructor

Class Times: Wed and Fri, 11:35 - 12:55, [redacted]

Prerequisites: CHEM 3101

Department/Unit: Chemistry

Course Format

This course's lectures and midterms will be delivered in person. The quizzes are administered online through Brightspace. Assignments will be submitted through Brightspace.

Required Text: None. Some of the course material is available freely through Wikibooks: https://en.wikibooks.org/wiki/Molecular_Simulation. Useful but optional texts are listed in Available Materials.

Course Materials

Lecture slides in PDF format are available in on the Brightspace shell.

CHEM3102A Methods: Computational Chem (LEC)

Students are not required to purchase textbooks or other learning materials for this course.

Communication

You may communicate with Chris through Carleton email ([redacted]).

Evaluation

Component	Weight
written assignments	25
midterms	25
wikibook	5
online quizzes	10
final exam	35

Quizzes

There will be an online quiz for each set of lecture notes. They must be completed by the date posted on Brightspace. You should study material before attempting the quizzes.

Midterms

There will be two midterm exams, each worth 12.5% of the final grade.

If you do not complete the a midterm exam, its weight will be automatically added to your final exam grade.

If your final exam grade is higher than any midterm exam, your grade exam grade will automatically replace your midterm grade.

The dates of the midterms will be:

[redacted]
[redacted]

Wikibook Project

You will contribute to the course wikibook https://en.wikibooks.org/wiki/Molecular_Simulation. Your entry will be worth 5% of your final grade and is due [redacted].

Your assigned question and the details of the assignment will be assigned during the term.

Assignments

There will be four written assignments. They must be submitted electronically on Brightspace. They can either be handwritten or typed, but must be in PDF format. The evaluation of your assignments will be completed through Brightspace.

The assignments will be posted at least two weeks in advance of the due dates. Notices of extensions will be posted on Brightspace. You are allowed to discuss the theory and strategy for solving these problems with your classmates; however, you must submit a unique assignment. Copying a solution is a serious form of academic misconduct. You may not use external sources that provide answers to questions, although you are encouraged to meet with the instructor if you are stuck on an assignment problem.

The tentative due dates for the assignments are:

Assignment 1	[redacted]
Assignment 2	
Assignment 3	
Assignment 4	

These assignment due dates may need to be rescheduled due to closures, weather cancellations, etc. Notices of changes to the due dates will be posted to Brightspace.

Course Format

The course will be delivered through in person lectures. Some of the course content is also available as narrated videos of these notes.

Additional Material

Part of the course content is available through the course Wikibook:

https://en.wikibooks.org/wiki/Molecular_Simulation

If you wish to make use of additional resources, there are several books in the library that include the material covered in this course:

- Tuckerman, M. Statistical Mechanics: Theory and Molecular Simulation
- https://ocul-crl.primo.exlibrisgroup.com/permalink/01OCUL_CRL/1gorbd6/alma991022687891705153
- McQuarrie, D. A., Statistical Mechanics, University Science Books, 2000, QC 174.8 M3
- https://ocul-crl.primo.exlibrisgroup.com/permalink/01OCUL_CRL/1gorbd6/alma991008833869705153
- Israelachvili, J. N. Intermolecular and Surface Forces, Academic Press, 2011
- https://ocul-crl.primo.exlibrisgroup.com/permalink/01OCUL_CRL/1gorbd6/alma991022630466305153
- Allen, M. P., Computer Simulation of Liquids. Clarendon Press, 1987. QC 145.2 A43 1987
- https://ocul-crl.primo.exlibrisgroup.com/permalink/01OCUL_CRL/1gorbd6/alma991022680767505153

You are not required or expected to purchase any text for this course.

Topics Covered and Learning Outcomes

Quantum chemistry	H_2^+ and chemical bonding
	Hartree–Fock theory
	Basis sets
	Methods for electron correlation
	Density functional theory
	Practical Calculations: Basis sets, potential ener structures, prediction of reaction rates
Intermolecular forces	Coulomb's law
	Charge-charge interactions
	Multipole expansion of electrostatic interactions
	Induced polarization
	Pauli repulsion
	Orientational averaging
Classical statistical thermodynamics	Thermodynamic ensembles
	Classical partition functions

	Configurational integrals
	Expectation value and the connection to classica
Molecular Simulation	Monte Carlo
	Molecular Dynamics
	Radial distribution functions and the structure o
Chemoinformatics and Machine Learning in Chemistry	ML concepts and definitions
	Regression methods (linear regression, random
	Classifier methods

Intended Student Learning Outcomes

At the end of CHEM 3102, students will be able to:

- Understand the postulates and general principles of quantum mechanics as they pertain to chemical bonding
- Understand and apply electronic structure methods in modelling chemical reactions and bonding
- Understand intermolecular interactions both conceptually and qualitatively
- Understand simulation algorithms including Monte Carlo, molecular dynamics
- Understand machine learning in chemistry, including

This contributes to the learning outcomes for the B.Sc. Chemistry program:

- 3 Demonstrates competency in theoretical and practical aspects of organic, inorganic, physical and analytical chemistry.
- 4 Integrates theoretical and practical knowledge of subdisciplines of chemistry to solve complex chemistry problems.

- 14 Practices meta-cognition and applies learned knowledge to new situations.

Late and Missed Work Policies

Late Work

Late assignments will not be accepted and will be awarded a grade of zero.

Any request for an academic consideration should first be made to the instructor. Considerations may be considered through the academic considerations form process.

Missed Work

Assignments that are not submitted will be awarded a grade of zero.

Any short-term request for an academic consideration should first be made to the instructor. Considerations may be considered through the academic considerations form process.

Long-term (> 5 days): Insert statement about course-related policy for longer-term accommodation.

Learning Material(s) and Other Course/Lab-Related Resources

None

Academic Accommodations and Regulations

Carleton is committed to providing academic accessibility for all individuals. You may need special arrangements to meet your academic obligations during the term. The accommodation request processes are outlined on the Academic Accommodations website (https://students.carleton.ca/course-outline/).

ChatGPT/Generative AI usage

As our understanding of the uses of AI and its relationship to student work and academic integrity continue to evolve, students are required to discuss their use of AI in any circumstance not described here with the course instructor to ensure it supports the learning goals for the course.

Statement on Academic Integrity

Students are expected to uphold the values of academic integrity, which include fairness, honesty, trust, and responsibility. Examples of actions that that compromise these values include but are not limited to plagiarism, accessing unauthorized sites for assignments or tests, unauthorized collaboration on assignments or exams, and using artificial intelligence tools such as ChatGPT when your assessment instructions say it is not permitted.

Misconduct in scholarly activity will not be tolerated and will result in consequences as outlined in Carleton University's Academic Integrity Policy. A list of standard sanctions in the Faculty of Science can be found here.

Additional details about this process can be found on the Faculty of Science Academic Integrity website.

Students are expected to familiarize themselves with and abide by Carleton University's Academic Integrity Policy.

Student Rights & Responsibilities

Students are expected to act responsibly and engage respectfully with other students and members of the Carleton and the broader community. See the 7 Rights and Responsibilities Policy for details regarding the expectations of non-academic behaviour of students. Those who participate with another student in the commission of an infraction of this Policy will also be held liable for their actions.