

# CHEM 3102 (Winter)

## Methods of Computational Chemistry

**Course Instructor:** Christopher Rowley

**Email:** [christopherrowley@cunet.carleton.ca](mailto:christopherrowley@cunet.carleton.ca)

**Student Hours:** By appointment

**Office Location:** 6304 Health Science Building. (Note: this office is not accessible without keycard access - Please make arrangements in advance to meet with the instructor)

**Class Location:** Please check Carleton Central for class locations.

**Class Times:** Wed and Fri, 11:35 - 12:55

**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](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.

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Recordings of the lecture material also available on this page:

<https://www.rowleygroup.net/chem3102videos>

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

### Communication

You may communicate with Chris through Carleton email (ChristopherRowley@cunet.carleton.ca).

## Evaluation

Component	Weight
written assignments	30
midterms	25
wikibook	5
online quizzes	10
final exam	30

## 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:

February 7
March 21

## Wikibook Project

You will contribute to the course wikibook

[https://en.wikibooks.org/wiki/Molecular\\_Simulation](https://en.wikibooks.org/wiki/Molecular_Simulation). Your entry will be worth 5% of your final grade and is due March 15.

Your assigned question and the details of the assignment are described on this [page](#).

## 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	January 27
Assignment 2	February 24
Assignment 3	March 10
Assignment 4	April 8

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](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](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](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](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](https://ocul-crl.primo.exlibrisgroup.com/permalink/01OCUL_CRL/1gorbd6/alma991022680767505153)

## Topics Covered and Learning Outcomes

Quantum chemistry	H <sub>2</sub> <sup>+</sup> and chemical bonding
	Hartree–Fock theory
	Basis sets
	Methods for electron correlation
	Density functional theory
	Practical Calculations: Basis sets, potential energy surfaces, geometry optimization, transition state 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 classical thermodynamics
Molecular Simulation	Monte Carlo
	Molecular Dynamics
	Radial distribution functions and the structure of liquids
Chemoinformatics and Machine Learning in Chemistry	ML concepts and definitions
	Regression methods (linear regression, random forests, and neural networks)
	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.

### Missed Work

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

## 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.

### Academic Integrity

Students are expected to uphold the values of academic integrity, which include fairness, honesty, trust, and responsibility. Examples of actions 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.

## **Release of Grades**

Standing in a course is determined by the course instructor subject to the approval of the Faculty Dean. This means that grades submitted by the instructor may be subject to revision. No grades are final until they have been approved by the Dean.

## **Statement on Student Mental Health**

As a student you may experience a range of mental health challenges that significantly impact your academic success and overall well-being. If you need help, please speak to someone. There are numerous resources available both on- and off-campus to support you. For more information, please consult <https://wellness.carleton.ca/>

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