

CHEM 3102 - Methods of Computational Chemistry

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

Instructor: Christopher N. Rowley (ChristopherRowley@cunet.carleton.ca)

Prerequisites: CHEM 3101

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.

Meeting Date: Jan 9, 2024 to Apr 9, 2024 Days: Tuesday-Thursday Time: 2:35 PM - 3:55 PM
Building: Richcraft Hall Room: 1201

Course Materials

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

CHEM3102A Methods: Computational Chem (LEC) Winter 2024

Recordings of the lecture material also available on this page:

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

Communication

You may communicate with Chris through Carleton email (ChristopherRowley@cunet.carleton.ca). You will also be able to communicate with Chris and other members of the class through the online messaging system, Slack. To join the Slack group for this course, use the following link:

https://join.slack.com/t/slack-ub36845/shared_invite/zt-10zflipc2-gLXOFgFTM8YUeXSZwb1tMw

The URL to access the slack channel is <https://chem3102-2022.slack.com/>

A demonstration on how to use Slack is available here:

<https://youtu.be/CkZjL3WcWnI?si=JkQoA6Jg3vG0QRiT>

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 the recorded lectures and online course notes before attempting the quizzes.

Midterms

There will be two midterm examples, 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 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 1
March 14

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 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 26
Assignment 2	February 23
Assignment 3	March 8
Assignment 4	April 5

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

Syllabus

1. Quantum chemistry
 1. H_2^+ and chemical bonding
2. Intermolecular forces
 1. Coulomb's law
 2. Charge-charge interactions
 3. Multipole expansion of electrostatic interactions
 4. Induced polarization
 5. Pauli repulsion
 6. Orientational averaging
3. Classical statistical thermodynamics
 1. Thermodynamic ensembles
 2. Classical partition functions
 3. Configurational integrals
 4. Expectation value and the connection to classical thermodynamics
4. Molecular simulation
 1. Metropolis Monte Carlo
 2. Molecular dynamics
 3. Radial distribution functions
 4. Thermostats and barostats
 5. Transport properties
 6. Free energy methods
 1. Free energy perturbation
 2. Thermodynamic integration
5. ~~Solvation free energies~~
6. Free energy surfaces
7. ~~Ab initio molecular dynamics, QM/MM, and coarse grain models~~

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 the helium atom and electron spin
- Understand intermolecular interactions both conceptually and qualitatively
- Understand simulation algorithms including Monte Carlo, molecular dynamics, free energy perturbation, and thermodynamic integration

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.

Standard University Outline Items

Self Declaration Form

For any medical issue that requires an accommodation to a course requirement, you may submit a [Medical self-declaration form](#) as sufficient documentation. An alternative mode of assessment will be assigned by the instructor.

Approval 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.

Academic Accommodation

You may need special arrangements to meet your academic obligations during the term. For an accommodation request the processes are as follows:

Pregnancy obligation: write to me with any requests for academic accommodation during the first two weeks of class, or as soon as possible after the need for accommodation is known to exist. For accommodation regarding a formally-scheduled final exam, you must complete the [Pregnancy Accommodation Form](#).

Religious obligation: write to me with any requests for academic accommodation during the first two weeks of class, or as soon as possible after the need for accommodation is known to exist. For more details [click here](#).

Academic Accommodations for Students with Disabilities: The Paul Menton Centre for Students with Disabilities (PMC) provides services to students with Learning Disabilities (LD), psychiatric/mental health disabilities, Attention Deficit Hyperactivity Disorder (ADHD), Autism Spectrum Disorders (ASD), chronic medical conditions, and impairments in mobility, hearing, and vision. If you have a disability requiring academic accommodations in this course, please contact PMC at 613-520-6608 or pmc@carleton.ca for a formal evaluation. If you are already registered with the PMC, contact your PMC coordinator to send me your Letter of Accommodation at the beginning of the term, and no later than two weeks before the first in- class scheduled test or exam requiring accommodation (if applicable). After requesting accommodation from PMC, meet with me to ensure accommodation arrangements are made. Please consult the PMC website for the deadline to request accommodations for the formally- scheduled exam (if applicable).

Survivors of Sexual Violence

As a community, Carleton University is committed to maintaining a positive learning, working and living environment where sexual violence will not be tolerated, and where survivors are supported through academic accommodations as per Carleton's Sexual Violence Policy. For more information about the services available at the university and to obtain information about sexual violence and/or support, visit: <https://carleton.ca/equity/sexual-assault-support-services>

Accommodation for Student Activities

Carleton University recognizes the substantial benefits, both to the individual student and for the university, that result from a student participating in activities beyond the classroom experience. Reasonable accommodation will be provided to students who compete or perform at the national or international level. Write to me with any requests for academic accommodation during the first two weeks of class, or as soon as possible after the need for accommodation is known to exist. <https://carleton.ca/senate/wp-content/uploads/Accommodation-for-Student-Activities-1.pdf>

COVID

It is important to remember that COVID is still present in Ottawa. The situation can change at any time and the risks of new variants and outbreaks are very real. There are a number of actions you can take to lower your risk and the risk you pose to those around you including being vaccinated, wearing a mask, staying home when you're sick, washing your hands and maintaining proper respiratory and cough etiquette. Feeling sick? Remaining vigilant and not attending work or school when sick or with symptoms is critically important. If you feel ill or exhibit COVID-19 symptoms do not come to class or campus. If you feel ill or exhibit symptoms while on campus or in class, please leave campus immediately. In all situations, you must follow Carleton's symptom reporting protocols.