

Chemistry 4424B Molecular Structure and Simulation Winter 2026

Course Outline

1. Course Information

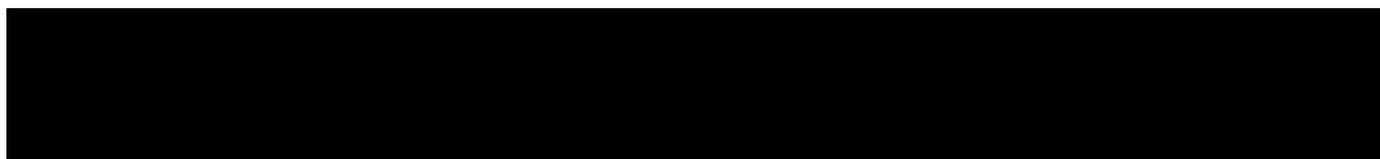
Course Information



Prerequisite(s): Chemistry 2284B or the former Chemistry 3374A/B or Physics 3200A/B.

Unless you have either the prerequisites for this course or written special permission from the Department of Chemistry to enroll in it, you may be removed and withdrawn from this course in accordance with university policy. This may be done after the add/drop deadline of the academic term, and the course will be marked as withdrawn (WDN) on your academic record. This decision may not be appealed.

2. Instructor Information



The office hours can be in-person or in-zoom.

3. Course Syllabus, Schedule, Delivery Mode

Course Description: Exposition of modern computational methods used in chemistry, biological modelling, and materials research. Topics include molecular quantum mechanics, molecular dynamics, and elements of statistical and machine-learning techniques.

Course Topics

- Number representation in a computer (binary system, machine epsilon, ASCII files, errors due to finite representation in the computer) and errors in the number operations. Relations to simulation software;
- Key methods of electrostatics including Poisson equation and multipole expansion. Introduction to Intermolecular forces. Introduction to MAPLE.
- *Relation of Statistical Mechanics to Simulations*. Postulates of statistical mechanics, ensembles, time and ensemble average. Computation of thermodynamic quantities.
- *Molecular Dynamics and Computation of Structure and Dynamical Properties*. Molecular modelling, convergence and reproducibility of the computations, sources of errors.
- *Use of Simulation Methods for Different System Sizes and Time Scales*. Key concepts of a variety of simulation methods – quantum, molecular, coarse-grained models, large-scale modelling using Lattice-Boltzmann and Dissipative Particle Dynamics, continuum modelling.
- *Solvation and Free Energy*.
- *Reaction Rates*. Rare events and umbrella sampling.
- *Quantum Chemistry*. One electron Shroedinger equation; Slater determinant and electron densities. Variational principle. Self-consistent field methods: Hartree, Hartree-Fock (HF) & Hartree-Fock-Roothaan method.
- *Electron Correlation*. Basis sets in quantum chemistry, including Gaussian, Slater functions and plane waves. Post-HF methods: Perturbation methods. Basics of the density functional theory & Hohenberg-Kohn theorems.
- *Potential energy surfaces*.
- *Basics of Machine Learning*.

Learning Outcomes

1. Knowledge of Methods: Obtain knowledge on computational methods used in molecular and quantum chemistry modelling. Be able to select the appropriate computational method depending on the system size, time scale and phenomena to be examined.
2. Communication: Be able to prepare logical and concise written reports via training in tests and assignments.
3. Awareness of Knowledge Limits: Recognize assumptions and limitations in the computational models and their possible impact on the results by training on case studies, lectures, assignments, tests. Develop critical thinking in the usage of computational methods and be able to assess these methods in the scientific literature.

4. Autonomy and Professional Capacity: (i) Be able to work productively and collaboratively individually and as a team member by solving problems with other students. (ii) Evaluate the potential impact of computational chemistry may have in society, health, and environment.

4. Course Materials

All course material will be posted to OWL: <https://westernu.brightspace.com/>

Textbook and Other Learning Materials

Resources for molecular simulations

- Required: Instructor's lecture notes and assigned reading posted on owl.
- Required: "Computer Simulation of Liquids" by M. P. Allen and D. J. Tildesley. (Oxford University Press, 2nd Ed.). Excellent and complete book for molecular simulations. One of the most rigorous ones in the field of molecular modelling. The book is found online at the UWO library free of charge.
- Optional: "Statistical Mechanics: Theory and Molecular Simulation" by M. E. Tuckerman (Oxford University Press, 1st Ed.). Advanced book, suitable for the graduate level. The book is found online at the UWO library free of charge.
- Optional: "Statistical Mechanics" by D. McQuarrie (University Science Book). This is an advanced and complete book on statistical mechanics suitable for upper year undergraduate students and graduate students who are interested in physical chemistry, statistical mechanics, and the origin of simulation methods.

Resources for quantum chemistry methods

- Required: Instructor's lecture notes and assigned reading posted on owl.
- Optional: "Exploring Chemistry with Electronic Structure Methods" by J. B. Foresman and A. Frisch (3rd ed., Gaussian, Inc., Wallingford, CT, 2015).
- Optional: "Quantum Chemistry" by D. A. McQuarrie (University Science Books, Sausalito, CA, 2008, 2nd Ed.)

Students are responsible for checking the course OWL site (<https://westernu.brightspace.com/>) regularly for news and updates. This is the primary method by which information will be disseminated to all students in the class.

If students need assistance with the course OWL site, they can seek support on the [OWL Brightspace Help](#) page. Alternatively, they can contact the Western Technology Services Helpdesk. They can be contacted by phone at 519-661-3800 or ext. 83800.

5. Methods of Evaluation

Grading Scheme and Assessment Dates

The overall course grade will be calculated as listed below:

Assignments (5)	25%
Midterm Tests (2)	20% Mon., February 9 (in class, open book); March 11 (in class, open book)
Computational Project	15%
Final Exam	40% Date to be determined by the registrar. Open book exam.

Dates for midterm make-up exams: Feb. 11, 3-3:45 pm (location TBA); March 13, 3-3:45 pm (location TBA). In the open book exams, you are allowed to bring your notes, the instructor's notes or any other book you think that it is helpful. You can use this material via your laptop during the exam. However, AI tools, and searches in google or other search engines are not permitted.

Assignment	Date released	Due Date
1	Jan 12	Jan 21
2	Jan 23	Feb 2
3	Feb 9	Feb 23
4	Feb 25	March 6
5	March 16	March 23

- **Information about the Project:** The selection of the assigned project will be discussed with the instructor. The project will involve an essay and an oral presentation.
- **Essay:** The essay length will be up to 8 double-spaced pages including a list of references. The essay is worth 9% of the final grade. **Deadline: April 3, 2026.** The essay can be submitted earlier, any time before the deadline. The essay will be submitted on an owl assignment.
- **Use of Turnitin:** All required papers may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for the detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (<http://www.turnitin.com>).
- **Oral presentation:** The oral presentation is worth 6% of the final grade. The oral presentation will have a duration of 10 min (plus/minus 1 min), followed by 3 min of questions from the peers and the instructor. The oral presentation will be marked by the instructor based on a rubric prepared by the instructor. The oral presentations will take place in the last week of lectures. Detailed schedule will be posted.

Use of Generative AI Tools

Generative AI tools (e.g., ChatGPT, Copilot, Gemini) are prohibited in their usage for any assignment, test, examination, essay, project, presentations.

General information about missed coursework

Students must familiarize themselves with the *University Policy on Academic Consideration – Undergraduate Students in First Entry Programs*, posted on the Academic Calendar:

https://uwo.ca/univsec/pdf/academic_policies/appeals/academic_consideration_Sep24.pdf

This policy does not apply to requests for Academic Consideration submitted for **attempted or completed work**, whether online or in person.

The policy also does not apply to students experiencing longer-term impacts on their academic responsibilities. These students should consult [Accessible Education](#).

For procedures on how to submit Academic Consideration requests, please see the information posted on the Office of the Registrar's webpage: https://registrar.uwo.ca/academics/academic_considerations/
All requests for Academic Consideration must be made within 48 hours after the assessment date or submission deadline.

All Academic Consideration requests must include supporting documentation; however, recognizing that formal documentation may not be available in some extenuating circumstances, the policy allows students to make one Academic Consideration request **without supporting documentation** in this course. However, the following assessments are excluded from this and, therefore, always require formal supporting documentation:

- Examinations scheduled during official examination periods (Defined by policy)
- Midterms (Defined by policy)

When a student *mistakenly* submits their one allowed Academic Consideration request **without supporting documentation** for the assessments listed above or those in the **Coursework with Assessment Flexibility** section below, the request cannot be recalled and reapplied. This privilege is forfeited.

Evaluation Scheme for Missed Assessments

Make-up exams: If a student misses a midterm exam, a make-up exam may be provided upon a recommendation from academic counseling, a few days after the scheduling of the regular exam. If the make-up date is still not met because of a valid reason also approved by the Academic Counselling Office, then the weight of the missed exam, will be transferred to the final exam.

When a student misses the Final Exam and their Academic Consideration has been granted, they will be allowed to write the Special Examination (the name given by the University to a makeup Final Exam). See the Academic Calendar for details (under [Special Examinations](#)), especially for those who miss multiple final exams within one examination period.

Essential Learning Requirements

Even when Academic Considerations are granted for missed coursework, the following are deemed essential to earn a passing grade.

- one midterm exam,
- the final exam,
- the computational project and provide an essay,
- 3 out of the 5 assignments

Students who fail to meet any of these requirements will receive a course grade of not greater than 40% even if the calculated grade is higher. For students with academic consideration or accommodation for any of the essential assessments, the only remedy against an F grade would be to apply for Incomplete

Standing (a grade of INC) by submitting a written request to the Dean of the Faculty of Registration. If Incomplete Standing is granted, the student will be able to complete the missed items the next time the course is offered. In this case the maximum course load may be reduced during the term in which they complete their course requirements.

A student who is unable to sit in the Final Exam must apply for permission to write a Special Final Examination (SPC Exam).

Coursework with Assessment Flexibility

By policy, instructors may deny Academic Consideration requests for the following assessments with built-in flexibility:

Deadline with a No-Late-Penalty Period

Assignments. Students are expected to submit each of the assignments by the deadline listed. Should extenuating circumstances arise, students do not need to request Academic Consideration and they are permitted to submit their assignment up to 72 hours past the deadline without a late penalty.

Should students submit their assessment beyond 72 hours past the deadline, a late penalty of 10% per day will be applied up to 5 days. After 5 days, a grade of zero will be applied.

Academic Consideration requests may be granted only for extenuating circumstances that started before the deadline and lasted longer than the No-Late-Penalty Period (48 or 72 hours).

For a first not-submitted assignment, you do not need to provide any documentation to anyone but, if you wish to be excused you must send a written request for consideration to the instructor before the due date. The value of the assignment will be added to the final exam. If two or more assignments are not submitted, then formal documentation must be submitted to the academic counsellor. If the reason is approved by the academic counsellor, the value of the assignments will be added to the final exam.

If either the **oral presentation or essay** due dates are missed by a student due to a valid reason, the instructor can offer accommodation for a different date of the oral presentation up to April 9 which is the last day of classes or/and an extension of up to seven days of the due date of the essay. If despite the accommodation for the oral presentation, it is still not delivered for a valid reason, the value of the oral presentation will be added to the final examination.

6. Additional Statements

6.1 Religious Accommodation

When a recognized religious holiday or observance conflicts with an examination, test, or other scheduled academic obligation, students must request accommodation via the University's Student Absence Portal (SAP). This request should identify the conflict and specify which course component(s) (e.g. test, midterm, exam) are affected.

Students are encouraged to submit the SAP request as early as possible, but no later than two weeks before any examination, or one week before any mid-term test or quiz, to allow sufficient time for adjustment.

The SAP request serves as official notification to both the course instructor and the Academic Advising Office, in accordance with University policy:
https://www.uwo.ca/univsec/pdf/academic_policies/appeals/accommodation_religious.pdf

The Faculty of Science considers religious accommodations as scheduling conflicts. Instructors should provide either a make-up exam or an earlier sitting of the same exam to accommodate the student.

For more information on recognized religious holidays, please visit the Diversity Calendar posted on the Equity, Diversity & Inclusion website - <https://www.edi.uwo.ca>

6.2 Academic Accommodation Policies

Students with disabilities are encouraged to contact Accessible Education, which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. The policy on Academic Accommodation for Students with Disabilities can be found at:

https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Accommodation_disabilities.pdf.

6.3 General Academic Policies

The website for Registrar Services is <https://www.registrar.uwo.ca/>.

Use of @uwo.ca email: In accordance with policy, https://www.uwo.ca/univsec/pdf/policies_procedures/section1/mapp113.pdf, the centrally administered e-mail account provided to students will be considered the individual's official university email address. It is the responsibility of the account holder to ensure that emails received from the University at their official university address are attended to in a timely manner.

Requests for Relief (formerly known as "appeals")

Policy on Request for Relief from Academic Decision:

https://uwo.ca/univsec/pdf/academic_policies/appeals/requests_for_relief_from_academic_decisions.pdf

Procedures on Request for Relief from Academic Decision (Undergraduate):

https://uwo.ca/univsec/pdf/academic_policies/appeals/undergrad_requests_for_relief_procedure.pdf

All requests for relief based on medical, compassionate, or extenuating circumstances should be directed to the Dean's Office of the student's Home Faculty: <https://www.uwo.ca/sci/advising/procedures/appeals/index.html>. In cases involving allegedly inaccurate or unfair marks or grades, the issue must be raised with the instructor as soon as possible and no later than three (3) weeks from the date the mark or grade was issued. If the student is dissatisfied with the instructor's decision, or does not receive a decision, a written request for relief must be submitted to the Department Chair via the Chemistry Help Portal, also no later than three (3) weeks from the date the mark or grade was issued.

6.4 Scholastic Offences

Policy on Scholastic Offences:
https://uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_offences.pdf

Procedures on Scholastic Offences (Undergraduate):

https://uwo.ca/univsec/pdf/academic_policies/appeals/undergrad_scholastic_offence_procedure.pdf

Use of Electronic Devices During Assessments

In courses offered by the Faculty of Science, the possession of unauthorized electronic devices during any in-person assessment (such as tests, midterms, and final examinations) is strictly prohibited. This includes, but is not limited to: mobile phones, smart watches, smart glasses, and wireless earbuds or headphones. **Unless explicitly stated otherwise in advance by the instructor, the presence of any such device at your desk, on your person, or within reach during an assessment will be treated as a *scholastic offence*, even if the device is not in use.** Only devices expressly permitted by the instructor (e.g., non-programmable calculators) may be brought into the assessment room. It is your responsibility to review and comply with these expectations.

Use of Generative AI Tools

Unless otherwise stated, the use of generative AI tools (e.g., ChatGPT, Microsoft Copilot, Google Gemini, or similar platforms) is **not permitted** in the completion of any course assessments, including but not limited to: assignments, lab reports, presentations, tests, and final examinations. Using such tools for content generation, code writing, problem solving, translation, or summarization—when not explicitly allowed—will be treated as a **scholastic offence**. If the use of generative AI is permitted for a particular assessment, the conditions of use will be specified by the instructor in advance. If no such permission is granted, students must assume that use is prohibited. It is your responsibility to seek clarification before using any AI tools in academic work.

All required papers may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for the detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (<http://www.turnitin.com>).

6.5 Support Services

Please visit the Science & Basic Medical Sciences Academic Advising webpage for information on adding/dropping courses, academic considerations for absences, requests for relief, exam conflicts, and many other academic-related matters: <https://www.uwo.ca/sci/counselling/>.

Students who are in emotional/mental distress should refer to Mental Health@Western (<https://uwo.ca/health/>) for a complete list of options about how to obtain help.

Western is committed to reducing incidents of gender-based and sexual violence (GBSV) and providing compassionate support to anyone who has gone through these traumatic events. If you have experienced GBSV (either recently or in the past), you will find information about support services for survivors, including emergency contacts, at:

https://www.uwo.ca/health/student_support/survivor_support/get-help.html.

To connect with a case manager or set up an appointment, please contact support@uwo.ca.

Please contact the course instructor if you require lecture or printed material in an alternate format or if any other arrangements can make this course more accessible to you. If you have any questions regarding accommodations, you may also wish to contact Accessible Education at

http://academicsupport.uwo.ca/accessible_education/index.html

Learning-skills counsellors at Learning Development and Success (<https://learning.uwo.ca>) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Additional student-run support services are offered by the USC, <https://westernusc.ca/services/>.

Important Academic Dates (Jan 2026 – April 2026)

Jan. 5 Classes resume

Jan. 8 First day December SPC Exams can be held (On or after the 1st Thursday in January following the beginning of classes)

Jan. 13 Last day to add a Winter 12-week course

Jan. 30 Last day to withdraw from a Fall/Winter 24-week course without academic penalty

Feb. 14–22 Spring Reading Week (including Family Day, Saturday to Sunday on the following week)

Mar. 30 Last day to withdraw from a Winter 12-week course without academic penalty

Apr. 3 Good Friday (no classes)

Apr. 9 Last day of classes in the Winter term

Apr. 10-11 Study Days

Apr. 12-30 April examination period