

WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 4424 – Molecular Structure and Simulation

COURSE OUTLINE 2024

Welcome to CHEM 4424B!

Course Information

Prerequisites and anti-requisites

Antirequisite(s): the former Chemistry 4444A/B, the former Chemistry 4474A/B.

Brief 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.

Contingency plan for instruction

Although the intent is for this course to be delivered in person, should any university-declared emergency require some or all of the course to be delivered online, either synchronously or asynchronously, the course will adapt accordingly. The grading scheme will **not** change. Any assessments affected will be conducted online as determined by the course instructor.

For accommodation due to illness or other serious reasons see section on “Accommodation and Accessibility”.

Course Syllabus

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.

Textbooks & Readings

- Lecture notes, assigned reading from textbooks & assignments posted on OWL.

Resources for molecular simulations

- "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 one in the field of molecular modelling.
- "Statistical Mechanics: Theory and Molecular Simulation" by M. E. Tuckerman (Oxford University Press, 1st Ed.). Advanced book, suitable for the graduate level.
- "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

- "Exploring Chemistry with Electronic Structure Methods" by J. B. Foresman and A. Frisch (3rd ed., Gaussian, Inc., Wallingford, CT, 2015).
- "Quantum Chemistry" by D. A. McQuarrie (University Science Books, Sausalito, CA, 2008, 2nd Ed.)

Course website

- All course material will be posted to OWL: <http://owl.uwo.ca>. This is the primary method by which information will be disseminated to all students in the class. Students are responsible to check OWL (<http://owl.uwo.ca>) on a regular basis for news and updates.

If students need assistance, they can seek support on the OWL Help page. Alternatively, they can contact the Western Technology Services Helpdesk. They can be contacted by phone at 519-661-3800 or ext. 83800.

Follow chemistry on Twitter: **@WesternuChem** and join the conversation.

Course Evaluation

- **5 Assignments 30%**
- **A short computational project written up in an essay (9%) and presentation (6%). Total 15%**
- **Two in-class tests (open book) 10% each**
- **Final exam (open book) 35%**

- **To pass the course**, you must obtain a minimum of 50% in the average of the midterms, assignments, project and final. **Obtaining a good average grade in the midterms and assignments is not sufficient to pass the course. The final exam MUST be written.** The minimal requirement to pass the course if there are repeated excused absences approved by the Academic Counsellor is that the student must write at least one midterm exam, the final exam, do the computational project and provide an essay and submit 2 out of the 5 assignments. The weight of the other missed midterm, of the oral presentation, and of the assignments will be transferred to the final exam. A student who is unable to submit the required minimum number of assignments, tests, and projects for medical or compassionate reasons, and who wishes to complete the missed work, will need 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. A student who is unable to sit in the Final Exam must apply for permission to write a Special Final Examination (SPC Exam).

Tentative Lecture Schedule

In the schedule that follows, the dates of midterms and posting of assignments and due dates are firm. The schedule of lecture material is **TENTATIVE**. The instructor reserves the right to re-arrange the order of the sub-topics if it is necessary for the flow of the course.

Week 1 [Jan.8 -12] : *Introduction*. Key methods of electrostatics including Poisson equation and multipole expansion. Intermolecular forces. Introduction to MAPLE. 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.

Week 2 [Jan 15-19] : *Relation of Statistical Mechanics to Simulations*. Relation of statistical mechanics to simulations, which is another name for computational statistical mechanics. Postulates of statistical mechanics required to be satisfied in simulations and Boltzmann statistics. Time and ensemble average. Computation of thermodynamic quantities. Introduction to GROMACS or NAMD and visualization package VMD.

Week 3 [Jan 22-26] *Molecular Dynamics and Computation of Structure and Dynamical Properties*. Molecular modelling – Basic molecular dynamics methods, integrators, thermostats. Computation of radial distribution functions and diffusion coefficients. Langevin equation and diffusion coefficient. Correction terms to the diffusion coefficient. Convergence and reproducibility of the computations. Sources of errors.

Week 4 [Jan 28-Feb 2] **Midterm 1 on Feb. 1st (in-class, duration 45 min). Make-up exam: Wed. Feb. 7, at 4:00 pm. Location TBA.** *Use of Simulation Methods for Different System Sizes and Time Scales*. Selecting the appropriate simulation method depending on the problem at hand. The map of computational methods in relation to system size 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 that aim to account for hydrodynamic interactions, and continuum modelling.

Week 5 [Feb 5-9] *Solvation and Free Energy*. Key elements of explicit, implicit solvent models. Born model of solvation. Explicit and implicit protein solvation. Free energy computational methods.

Week 6 [Feb 12-16] *Reaction Rates*. Rare events and umbrella sampling. Reaction coordinates, transition states of chemical reactions in solution and conformational changes of macromolecules such as proteins.

Week 7 [Feb 19-23] *Reading week*

Week 8 [Feb 26-Mar 1] *Quantum Chemistry - Fundamentals*. One electron Shroedinger equation; Slater determinant and electron densities. Variational principle. Self-consistent field methods: Hartree, Hartree-Fock (HF) & Hartree-Fock-Roothaan method.

Week 9 [Mar 4-8] *Symmetry in Quantum Chemistry*. Symmetry of molecules, orbitals, and electronic wave functions. Irreducible representations. Character tables. Symmetry labels. Molecular term symbols.

Week 10 [Mar 11-15] **Midterm 2 on March 12 (in-class, duration 45 min). Make-up exam: March 18 at 4:00 pm. Location TBA.** *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. Configuration interaction and other methods that account for electron correlation.

Week 11 [Mar 18-22] *Potential energy surfaces*. Born-Oppenheimer approximation; Potential energy surfaces; Molecular geometry optimization; Stationary points: intermediates and transition states.

Week 12 [Mar 25-29] *Machine Learning*. Basics of Machine Learning.

Week 13 [April 1 – 5] Complete topics that have not finished in the previous lectures. Students' presentations.

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 9 double-spaced pages including a list of references. The essay is worth 9% of the final grade. **Deadline: April 15, 2024.** 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 will worth 6% of the final grade. The oral presentation will have a duration of 12 min (plus/minus 1 min), followed by 4 min of questions from the peers and the instructor. The oral presentation will be marked by the instructor and peers based on a rubric prepared by the instructor. The final grade of the oral presentation will be estimated by a weighted average of the grade of the instructor that will carry a weight of 65% and the average of the grades from the peers that will weigh 35%. The oral presentations will take place in the last week of lectures. Detailed schedule will be posted.

Accommodation and Accessibility

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

Student Absences

If you are unable to meet a course requirement due to illness or other serious circumstances, please follow the procedures below.

Assessments worth less than 10% of the overall course grade:

The assessments that are worth less than 10% are the individual assignments, essay and oral presentation. If there is a valid reason (e.g. illness, compassionate leave, varsity competitions, religious day) for missing the due date of an **assignment** the instructor can offer an extension of the due date (without providing documentation) up to seven days (including weekends).

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. See also the next paragraph for “Assessments worth 10% or more of the overall course grade”.

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 30 which is the end of the exam period 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. The computational project and essay are among the minimum requirements for passing the course. If the computational project and essay cannot be completed for a valid reason by the end of the examination period, which is April 30th, the student can 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.

Assessments worth 10% or more of the overall course grade:

For missed work worth 10% or more of the final course grade, you must provide valid medical or supporting documentation to the Academic Counselling Office of your Faculty of Registration as soon as possible.

For further information, please consult the University’s medical illness policy at https://www.uwo.ca/univsec/pdf/academic_policies/appeals/accommodation_medical.pdf.

The Student Medical Certificate is available at https://www.uwo.ca/univsec/pdf/academic_policies/appeals/medicalform.pdf

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.

Absences from Final Examinations

If you miss the Final Exam, please contact the Academic Counselling office of your Faculty of Registration as soon as you are able to do so. They will assess your eligibility to write the Special Examination (the name given by the University to a makeup Final Exam).

You may also be eligible to write the Special Exam if you are in a “Multiple Exam Situation” (e.g., more than 2 exams in 23-hour period, more than 3 exams in a 47-hour period).

If a student fails to write a scheduled Special Examination, the date of the next Special Examination (if granted) normally will be the scheduled date for the final exam the next time this course is offered. The maximum course load for that term will be reduced by the credit of the course(s) for which the final examination has been deferred. See the Academic Calendar for details (under [Special Examinations](#)).

Accessible Education

- 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.
- 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. You may also wish to contact Accessible Education at http://academicsupport.uwo.ca/accessible_education/index.html if you have any questions regarding accommodations.

Religious Accommodation

When a course requirement conflicts with a religious holiday that requires an absence from the University or prohibits certain activities, students should request accommodation for their absence in writing at least two weeks prior to the holiday to the course instructor and/or the Academic Counselling office of their Faculty of Registration. Please consult University's list of recognized religious holidays (updated annually) at

<https://multiculturalcalendar.com/ecal/index.php?s=c-univwo>.

Academic Policies

The website for **Registrarial Services** is <http://www.registrar.uwo.ca>.

E-mailing: In accordance with policy, <http://www.uwo.ca/its/identity/activatenonstudent.html>, the centrally administered e-mail account provided to students will be considered the individual's official university e-mail address. It is the responsibility of the account holder to ensure that e-mail sent by the University to his/her/their official university address is attended to in a timely manner.

Electronic devices: Only basic scientific calculators are permitted on tests and exams. All other electronic devices (cell phones, laptops, tablets, cameras, etc.) are prohibited. Students found in possession of prohibited devices will receive a mark of ZERO for the entire test or exam.

Scholastic offences: Scholastic offences, including plagiarism, are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site: http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf.

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>).

Code of Conduct: Students are reminded of the University's Code of Conduct found on the university website. To maintain a high standard of learning environment in our classrooms, those who are disruptive, rude, or show unacceptable behavior, either to the instructor, or the other students, will be asked to leave.

Support Services

Managing academics and well-being: Western University is committed to a thriving campus as we deliver our courses in the mixed model of both virtual and face-to-face formats. We encourage you to check out the Digital Student Experience

website to manage your academics and well-being:
<https://www.uwo.ca/se/digital/>.

Learning-skills Services: Learning-skills counsellors at the Student Development Centre (<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.

Emotional/mental distress services: 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 and providing compassionate support to anyone who has gone through these traumatic events. If you have experienced sexual or gender-based violence (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.

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