

WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 9654S - Advanced Methods in Molecular Simulations
Quarter Graduate Course 2025
January 6 - February 14, 2025

COURSE OUTLINE

Instructor Information

Instructor Dr. Styliani Conostas, ChB 071 (Lower ground floor in the Chemistry Building)

Delivery mode In-person

Schedule and place TBA

Time period of the course January 6, 2025 - February 14, 2025

Office hours By appointment

Brief Course Description

The course presents advanced molecular simulation topics that include methods of electrostatics, rare event dynamics, free energy calculations. The software NAMD/VMD will be used in practicing with the methods.

Prerequisites

No prerequisites in terms of courses. Fundamental knowledge of molecular simulations would be helpful for progressing in the course. If there is a gap of basic knowledge in simulations, still one may catch up if they put some additional effort. Review of simulation basics will be provided in the class. The students would need to bring a laptop with them in class.

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.

Use of Generative Artificial Intelligence (AI)

Generative Artificial Intelligence (AI) is not permitted in the assignment and essay preparations, as well as during the open-book exam. SGPS provides Provisional Guidance for the use of Generative AI in Graduate Studies at:

https://grad.uwo.ca/about_us/policies_procedures_regulations/ai.html

Course Learning Outcomes

Breadth and Depth of Knowledge: Be able to describe the fundamental principles of molecular simulations and apply these principles in modelling of chemical and biochemical systems such as solutions, stability of proteins and nucleic acids.

Application of Knowledge: Be able to apply the knowledge to predict and rationalize the physical and chemical properties of chemical and biochemical systems and to critically use computer simulation methods.

Communication: Be able to prepare logical and concise written reports via training in assignments and essay.

Awareness of Knowledge Limits: Recognize assumptions and limitations in the scientific models and their possible impact on computational results by training on case studies, lectures, assignments, essay.

Autonomy and Professional Capacity: (i) Be able to work productively and collaboratively individually and as a team member. (ii) Communicate the results to peers and instructor by preparing and presenting an essay.

Material

Material presented in the class and assigned reading. Suggested textbooks:

1. "Computer Simulation of Liquids" by M. P. Allen and D. J. Tildesley, 3rd Edition.
2. "Understanding Molecular Simulation" by D. Frenkel and B. Smit, 3rd Edition.
3. "Statistical Mechanics: Theory and Molecular Simulation" by M. E. Tuckerman (Oxford University Press, 1st Ed.). Advanced book, suitable for the graduate level.
4. "Introduction to Electrodynamics" by David J. Griffiths, 4th Edition

Course website

All course material will be posted in the OWL Brightspace.

This is the primary method by which information will be disseminated to all students in the class. Students are responsible to check the OWL Brightspace 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.

Course evaluation

- 3 assignments ($3 \times 10\% =$) 30 % of the final mark;
- Midterm (open-book) (30 %);
- Project (40 % of the final mark).

Assignments One of the assignments will be done in a team and two others individually.

Midterm Exam 1.5-hour open-book exam. Usage of books, instructor's notes or student's note is allowed during the exam. Searching of answers in the internet and usage of AI during the exam is not permitted. The format of the exam will be short-answers.

- **Project selection:** The project will be in the field of molecular modeling and simulations. Its selection will be discussed with the instructor. The project may be within the interests of the student. The instructor may also suggest or assign projects. The completion of the project includes a written essay and a 15 min (± 1 min) in-class presentation followed by a 5 min question period. The questions will be asked by the peers and the instructor. The essay and oral presentation are worth, 20 % each. Evaluation rubrics and instructions for preparation of the essay and the oral presentation will be provided by the instructor.
- **Essay:** The essay length will be up to 9 double-spaced pages and not less than 7 pages, and in addition to the main body it should include a list of references, with no less than five primary references and without an upper limit. The essay is worth 20% of the final grade. Submission deadline: Feb. 14, by 11:55 pm. The essay can also be submitted earlier, any time before the deadline. The essay can be submitted electronically as a WORD document or as a hard copy.
- **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 20% of the final grade. The oral presentation will have a duration of 15 min (plus/minus 1 min), followed by 5 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 70% and the average of the grades from the peers that will weigh 30%. The oral presentations will take place in the last week of lectures. Detailed schedule will be posted.

Requirements to pass the course To pass the course, you must obtain a minimum of 50% in the average of assignments, midterm and project. Obtaining a good average grade in the assignments and midterm is not sufficient to pass the course. The minimum requirement to pass the course is one assignment, the midterm exam and the project preparation.

Tentative Lecture Topics

1. Review of simulation methods; Usage of NAMD/VMD.
2. Review of electrostatics that apply in chemistry and biochemistry: Coulomb's law, electric field, potential, Gauss's law, energy of electrostatic systems, self-energy, Laplace equation, Poisson equation, Numerical solution of Poisson equation, implicit solvent, solution of the Poisson-Boltzmann equation.
3. Intermolecular interactions and force-fields.
4. Methods of Electrostatics used in simulations: Ewald summation, Particle-Mesh Ewald method, Multi-level summation methods. Comparison of methods; Use of "star"-shaped droplets as a sensitive test of electrostatic interactions in molecular software.
5. Electrical double layer.
6. Rough energy landscapes.
7. Collective variables, reaction coordinates and transition state theory of a chemical reaction in solution.
8. Statistical methods of rare events. Umbrella sampling.
9. Free energy calculation methods; Alchemical transformations.

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 that are worth 10%

The assignments are the only components of the course, which are worth 10% each. If a student cannot meet the assignment due date for a legitimate reason, the instructor in consultation with the student may provide an alternate due date. No medical documentation is required.

Assessments that are worth more than 10%

For missed work worth more than 10% 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 project component of the course.

Missed essay due date and presentation due date: The instructor in consultation with the student may provide an alternate due date or a different presentation date.

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](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://academicupport.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 and a laptop are permitted on tests and exams. All other electronic devices (cell phones, 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.

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>).

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 HealthWestern (<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>

Social Media

Twitter - Follow us @westernuchem

Facebook - www.facebook.com/ChemistryatWestern

Important academic dates for Winter 2025

- Jan. 6 Classes resume
- Jan. 9 First day December SPC Exams can be held (On or after the 1st Thursday in January following the beginning of classes)
- Jan. 14 Last day to add a second-term half course or drop a course without showing WDN
- Feb. 17 – 21 Spring Reading Week (including Family Day)

- Mar. 30 Last day to withdraw from a second-term half course without academic penalty
- Apr. 4 Last day of classes in the Winter term
- Apr. 5-6 Study Days
- Apr. 7-30 April examination period
- Apr. 18, 20 Good Friday and Easter Sunday
- May 7 First day April SPC Exams can be held (On or after the 5th business day in May following the April exam period)