WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 4424 ς Molecular Structure and Simulation

COURSE OUTLINE 2024

# 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



in the midterms

Week 1 [Jan.8 -12] : 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, 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 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.

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] . 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] . 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]

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

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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 docum0 GBTf1 0 0 1 433.37 267.94841(u)-8(m)6(0 GBTf1 0 0 1 433.37 267.94841(u)-8(m)6(0 GB

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,

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-