

The University of Western Ontario
Department of Chemistry

Chemistry 4424B

MOLECULAR STRUCTURE AND SIMULATION

Winter 2025

Course Information

Instructor:

[REDACTED]
[REDACTED]
[REDACTED]

Lectures:

[REDACTED]
[REDACTED]

Office hours (for administrative matters): by appointment

Course web site: <https://westernu.brightspace.com>

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

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

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

Recommended texts:

1. I. N. Levine, *Quantum Chemistry*, 7th ed., Pearson–Prentice Hall, 2013. Cost: \$67 on Amazon.ca
2. R. Y. Prasad and Pranita, *Computational Quantum Chemistry*, 2nd ed., CRC Press, Boca Raton, 2023. Available online at Western Libraries.
3. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, 2nd ed., Oxford University Press, Oxford, 2017. Available online at Western Libraries.

Learning Outcomes

1. Understand the key principles and concepts of molecular structure and simulation;
2. Recognize the capabilities and limitations of various computational methods;
3. Learn how to calculate molecular structure and properties and properties of bulk matter;
4. Model chemical processes using computational software packages;
5. Know how to choose an appropriate methodology for molecular simulation and present computational findings in scientific reports.

Course Topics

1. *Principles of quantum mechanics.* How quantum mechanics explains chemistry. Schrödinger equation and molecular structure prediction.
2. *Quantitative molecular orbital theory.* Hartree–Fock self-consistent field method. Calculation of molecular orbitals and orbital energies.
3. *Molecular quantum mechanics.* Quantum-mechanical methods beyond molecular orbital theory. Configuration interaction, perturbation theory, coupled-cluster theory, and other post-Hartree–Fock techniques. Model chemistries.
4. *Density-functional methods.* The Kohn–Sham scheme. Exchange and correlation functionals. Empirical and nonempirical density-functional approximations. Popular density functionals (B3LYP, PBE, etc.), their origin, and scope of applicability.
5. *Principles of equilibrium statistical mechanics.* Statistical ensembles. Computation of mechanical and thermodynamical properties of matter for systems of independent molecules.
6. *Computational thermochemistry.* Potential energy surfaces and vibrational analysis. Reaction intermediates and transition states.
7. *Molecular simulations.* Applications of statistical mechanics to systems of interacting molecules (liquids, mesoscopic systems, diffusion). Molecular dynamics and Monte Carlo methods.
8. *Principles of machine learning.* Elements of machine-learning techniques and their applications in chemistry.

Evaluation

Assignments (6 in total)	30%	
Test 1 (open book)	10%	Thursday, February 6, in class
Test 2 (open book)	10%	Thursday, March 13, in class
Mini-project in computational chemistry	10%	
Final Exam (closed book)	40%	To be scheduled by the Registrar (3 hours)

Policies

Late assignments. Late submissions will be accepted within 24 hours after the due date without penalty, but will be rejected afterwards. Students with applicable accommodations recommended by Accessible Education can request a longer one-time deadline extension. This extension cannot exceed 7 days after the regular due date because graded assignments will normally be returned by that time. Students with disability accommodations who ask for a longer extension will be excused instead and the weight of the missed work will be transferred to the Final Exam.

Missed assignments. There are no make-up assignments. If you miss an assignment and are granted academic consideration, the weight of the missed assignment will be transferred to the Final Exam.

Missed tests. There are no make-up tests. If you miss a test and are granted academic consideration, the weight of the missed test will be transferred to the Final Exam.

Missed final exam. If you miss the Final Exam, contact the Academic Counselling office of your Faculty of Registration as soon as possible. They will assess your eligibility to write the Special Examination.

Use of electronic devices. Only basic scientific calculators are permitted on all tests and exams. All other electronic devices (cell phones, laptops, tablets, cameras, etc.) are prohibited.

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. [Link](#)

Scholastic offences. Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence. [Link](#)