

Chemistry 3300G
COMPUTER METHODS IN CHEMISTRY

Winter 2023

Course Information

Instructor:	Viktor N. Staroverov E-mail: vstarove@uwo.ca Office: ChB 063
Teaching Assistant:	Ivan Bosko
Lectures:	Monday, Wednesday, Friday, 10:30 am–11:30 am, ChB 9
Labs:	See the dates below, 6:00 pm, SSC 1000
Office hours:	By appointment (administrative matters)
Course web site:	https://owl.uwo.ca/portal
Prerequisites:	Chemistry 2272F, 2281G, 2283G, 2384B

Description: An introduction to computer methods and tools used in all branches of chemistry. Topics include molecular structure visualization, calculation of molecular structure and properties, analysis of reaction mechanisms using potential energy surfaces, simulation of molecular spectra, numerical methods, data processing, and symbolic computation software.

Course Topics

1. *Molecular visualization.* How to specify molecular structure on a computer. Z-matrices and internal coordinates. Introduction to WebMO.
2. *Mathematical techniques in chemistry.* Elements of linear algebra and their chemical applications. Statistical data analysis, least squares fitting.
3. *General-purpose scientific software.* Introduction to symbolic computation software. Using MAPLE to evaluate integrals, solve differential equations, plot functions, etc.
4. *Molecular orbital theory.* One- and many-electron Schrödinger equations. Hartree–Fock self-consistent field method. Atomic and molecular orbitals. Basis sets. Calculation of molecular orbital diagrams. Visualization of molecular orbitals. Frontier orbitals and chemical reactivity.
5. *Potential energy surfaces.* Potential energy surface (PES) functions. Geometry optimization. Normal modes of vibration. Reaction pathways, intermediates, and transition states. Thermochemistry and chemical kinetics from PES.
6. *Molecular mechanics and molecular dynamics methods.* Modeling the PES by molecular mechanics methods. Force fields. Molecular dynamics simulations.
7. *Wave-function and density-functional methods.* Post-Hartree–Fock and semi-empirical methods. Density-functional techniques. Model chemistries and their use for computing PES. Performance and limitations of various *ab initio* techniques.
8. *Calculation of molecular properties and spectra.* Dipole moments, electrostatic potential, atomic charges, bond orders. Simulation of IR, Raman, and UV-vis spectra.

Expected Learning Outcomes

- Recognize the utility of computer tools in chemistry research
- Understand the basic theoretical principles of molecular structure calculations
- Visualize, build, and manipulate molecular structures on a computer
- Understand the origin and meaning of molecular orbitals
- Know how to use the *Gaussian* program to predict the most stable structures of molecules, calculate reaction enthalpies and Gibbs energies, simulate vibrational spectra, correlate electronic structure with chemical properties
- Be able to perform basic operations of calculus and linear algebra using *Maple*
- Be able to perform least-squares fitting and regression analysis of data using *Excel*
- Be aware of the capabilities and limitations of computational chemistry techniques

Course materials: There is no required text. All course materials (lecture notes, lab manuals, etc.) will be distributed via the course website.

Recommended textbook: E. G. Lewars, *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*, 2nd ed., Springer, Dordrecht, 2011, ISBN 978-90-481-3862-3. Online access is available through the Western Library Catalogue.

Evaluation: The course grade will be determined as a weighted average of the following components:

Computer labs (6)	30% (5% each)	See the schedule below
Assignments (4)	16% (4% each)	See the schedule below
Midterm test	14%	Wednesday, March 1 (50 min, in class, written answers)
Final exam	40%	To be scheduled by the Registrar (3 hours, written answers)

Conditions required to pass the course: The labs, assignments, and exams are essential components of the course. You must submit at least 4 of the 6 labs reports, at least 2 of the 4 assignments, and write the Final Exam. Students who fail to meet any of these requirements without a proper excuse for the missed work will receive a course grade of not greater than 40%, even if the calculated grade is higher. A student who is unable to submit the required minimum number of lab reports and assignments 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 write the Final Exam must apply for permission to write a Special Final Examination (SPC Exam).

Lab Schedule (Mondays)

#	Lab Date	Report Due Date
1	January 23	January 30
2	January 30	February 6
3	February 6	February 13
4	March 6	March 13
5	March 13	March 20
6	March 20	March 27

* Due on OWL by 6:00 pm as PDF files

Assignment Schedule (Wednesdays)

#	Assignment Posted	Due Date
1	January 25	February 1
2	February 8	February 15
3	March 8	March 15
4	March 22	March 29

*Due in class as paper copies

Policies

Student absences and missed work. Students who are unable to meet their academic responsibilities due to medical or compassionate reasons may submit a request for academic consideration. For each missed piece of work **worth 10% or more** of the total course grade, you must apply for such consideration by providing valid medical or supporting documentation to the Academic Counselling Office of your Faculty of Registration. For each missed or late piece of work **worth less than 10%** of the total course grade (i.e., a lab report or assignment), you do not need to provide medical documentation or contact the Academic Counselling Office, but you must send a written explanation of your absence to the instructor within 48 hours of the due date to be excused. Note that *all* accommodations for missed work, regardless of who grants them, are subject to the *Conditions required to pass the course*.

Accommodation for students with disabilities. Students with disabilities are encouraged to contact Accessible Education, which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. In cases where a student misses a piece of work for reasons related to the disability on file with Accessible Education, the student should request accommodation by contacting Accessible Education instead of the Academic Counselling Office.

Missed lab reports. There are no make-up labs. If you fail to submit a lab report and are granted accommodation, the weight of the missed lab will be transferred to the Final Exam.

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

Missed midterm test. If you miss a midterm test and are granted accommodation, a make-up test will be offered. If you miss the make-up midterm test and are excused as well, the weight of the midterm 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. 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).

Late assignments and lab reports. Late submissions will be accepted within 24 hours after the due date (see page 2) 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 and lab reports will normally be returned by that time. Students with disability accommodations who ask for a longer extension will be excused instead, subject to the *Conditions required to pass the course*.

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.

Scholastic offences. The University will take all appropriate measures to promote academic integrity and deal appropriately with scholastic offences. For definitions of what constitutes a scholastic offence, see http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf

Support services. Detailed information on academic considerations for absences, religious accommodation, exam conflicts, appeals, and other academic matters may be found on the Science & Basic Medical Sciences Academic Counselling webpage: <https://www.uwo.ca/sci/counselling>. Students who are in emotional/mental distress should refer to Mental Health@Western (<https://uwo.ca/health>) for help.