Chemistry 3300B
COMPUTER METHODS IN CHEMISTRY
Winter 2024

Course Information

Instructor: Viktor N. Staroverov

[redacted]

Lectures: [redacted]

Tutorials: [redacted]

Office hours: [redacted]

Course web site: `https://owl.uwo.ca/portal`

Prerequisites: Chemistry 1301A/B, Chemistry 1302A/B, and any 1.0 courses at the 1000 level or higher from Calculus, Applied Mathematics or Mathematics, with no mark less than 60%. Integrated Science 1001X with a minimum mark of 60% may be used as a substitute for (Chemistry 1302A/B and Calculus 1301A/B).

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. Curve fitting, basic statistical data analysis.
3. *General-purpose scientific software.* Introduction to MAPLE. Use of MAPLE as a calculator for evaluating derivatives and integrals, solving differential equations, and other mathematical tasks.
4. *Computational chemistry*. Principles of molecular structure theory. Separation of electronic and nuclear motions. Classical and wavefunction-based models.
5. *Calculation of molecular orbitals*. Atomic and molecular orbitals and orbital energies. Visualization of molecular orbitals. Frontier orbitals and chemical reactivity.
6. *Potential energy surfaces.* Potential energy curves and surfaces. Local and global minima. Normal modes of vibration. Reaction pathways, intermediates, and transition states. Computational studies of reaction mechanisms.
7. *Molecular mechanics methods*. Ball-and-stick models of molecules and force fields.
8. *Wavefunction-based and density-functional methods.* Methods beyond molecular orbital theory. Introduction to density-functional techniques.
9. *Computational prediction of molecular properties*. Simulation of IR, Raman, and UV-vis spectra. Calculation of dipole moments, atomic charges, bond orders.

Expected Learning Outcomes

- Recognize the utility of computer tools in chemistry research
- Understand the basic theoretical principles of molecular structure calculations
- Visualize, build, and manage 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, 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:

Tutorials	30% (5% each)
Quizzes*	16% (4% each)
Midterm test	14% (in class on Wednesday, February 28)
Final exam	40%

***Quizzes.** Each quiz consists of a problem similar to one of the problems of the preceding take-home assignment. *Assignments* will be posted according to the schedule below but will not be collected or marked. Students are encouraged to bring and use their worked-out assignments to answer quizzes.

Conditions required to pass the course: The tutorials, quizzes, tests, and exams are essential components of the course. You must submit at least 4 of the 6 tutorial write-ups, write at least 2 of the 4 quizzes, and write the Final Exam. Students who fail to meet any of these requirements without a proper excuse will receive a course grade of not greater than 40%, even if the calculated grade is higher. A student who is unable to meet this requirement 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 the INC grade is granted, the student will be able to complete the missed items the next time the course is offered.

Tutorial Schedule (Tuesdays)

#	*Tutorial Date*	*Write-up Due Date*
1	January 23	January 30
2	January 30	February 6
3	February 6	February 13
4	March 5	March 12
5	March 12	March 19
6	March 19	March 26

* Due on OWL by 1:30 pm

Assignment/Quiz Schedule

#	*Assignment Posted*	*Quiz*
1	January 24	January 31
2	February 7	February 14
3	March 15	March 22
4	March 29	April 5

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 tutorial write-up or quiz), you do not need to provide any documentation to anyone but, if you wish to be excused, you must send a written explanation of your absence to the instructor within 48 hours of the due date. Note that *all* considerations and accommodations for missed work 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 tutorial write-ups. There are no make-up tutorials. If you fail to submit a tutorial write-up and are excused, the weight of the missed tutorial will be transferred to the Final Exam.

Missed quizzes. There are no make-up quizzes. If you miss a quiz and are excused, the weight of the missed quiz will be transferred to the Final Exam.

Missed midterm test. If you miss the midterm test and are excused, 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.

Late tutorial write-ups. 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 tutorial write-ups 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. Students found in possession of prohibited devices will receive a mark of ZERO for the entire test or exam.

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.

Date: January 4, 2024