

A. General Information

- Course: CHEM 431 and CHEM 631, *Computational Chemistry for Chemists and Biochemists*, 3 credits, Winter 2017.
- Time and place: Wednesdays, 18:00-20:30, CC-425.
- Instructor: Dr. Gilles H. Peslherbe, Professor, Department of Chemistry & Biochemistry, Faculty of Arts & Science, Concordia University.
- Office location: SP-275.19.
- Telephone: 514-848-2424 ext. 3335
- E-mail: Gilles.Peslherbe@Concordia.CA
- Website: access from <http://moodle.concordia.ca/moodle>.
- Office Hours: by appointment (e-mail preferred).

B. Course Description

- This course presents the concepts, tools, and techniques of modern computational chemistry, and provides a very broad overview of the various fields of application across chemistry and biochemistry. The course is divided into two parts: 1) Molecular structure, which covers molecular mechanics and elementary electronic structure theory of atoms and molecules; and 2) Chemical reactivity, which covers applications of quantum chemistry and molecular dynamics techniques to studies of chemical reactions. The applications discussed include organic molecules and their reactions, peptides and proteins, drug design, DNA, polymers, inorganics and materials. The course includes a practical component where students acquire hands-on experience with commonly used computational chemistry software. Lectures and laboratory..
- Prerequisite: CHEM 234, 241, 333 or permission of the Department.
- **Virtual laboratory component:** it will consist of a set of tutorials to be performed as homework. Access to a standard computer with Web browsing capabilities is required. Students with no access to such equipment should make arrangements with the Instructor to access a University computer at specific times.
- Detailed outline:

INTRODUCTION TO COMPUTATIONAL CHEMISTRY

1. EXPLORING POTENTIAL ENERGY SURFACES

- 1.1. The importance of minimum energy structures
- 1.2. Local optimization techniques
- 1.3. Global optimization techniques
- 1.4. Characterization of stationary points

2. MOLECULAR STRUCTURE -- PART I: MOLECULAR MECHANICS

- 2.1. Force field
- 2.2. General considerations
- 2.3. Organics
- 2.4. Biological applications
- 2.5. Inorganics
- 2.6. Force fields: advantages and limitations

3. MOLECULAR STRUCTURE - PART II: ELECTRONIC STRUCTURE THEORY

- 3.1. Molecular orbital (MO) self-consistent-field (SCF) method
- 3.2. Atomic basis sets Resource
- 3.3. Hartree-Fock (HF) theory Resource
- 3.4. Semiempirical MO-SCF methods Resource
- 3.5. Electronic correlation Resource
- 3.6. Density-functional theory (DFT)
- 3.7. Configuration interaction (CI)
- 3.8. Many-body perturbation theory
- 3.9. Coupled cluster (CC) theory

4. CHEMICAL REACTIVITY AND THERMODYNAMICS

- 4.1. Reaction mechanisms
- 4.2. Reaction kinetics and thermochemistry

5. SIMULATIONS OF FINITE-TEMPERATURE SYSTEMS AND DYNAMICS

- 5.1. Monte Carlo (MC) simulations
- 5.2. Molecular Dynamics (MD) simulations
- 5.3. Periodic systems: solids and liquids
- 5.4. The classical trajectory approach to reaction dynamics
- 5.5. Quantum dynamics

C. Objectives

In this course, you will learn the foundations of computational chemistry, and you will be expected to 1) understand and remember its basic concepts and 2) be able to apply them to solve practical problems. CHEM 631 students will also be expected to understand and remember advanced concepts and mathematical models. Only basic knowledge of computers, chemistry & biochemistry and physics is required.

D. Schedule

- Lab Exam, during class time, April 5, 2017 (location TBA).
- Final Exam, during exam period, April 19 – May 2, 2017 (SGW).

E. Course Materials: Suggested Readings / Relevant Books

Molecular Mechanics, Burkert and Allinger (ACS, Washington, 1982).

Molecular Mechanics Across Chemistry, Rappé and Casewit (U. Science Books, Sausalito, CA, 1997).

Quantum Chemistry, Levine (Prentice Hall, Englewood Cliffs, NJ, 1991).

Exploring Chemistry with Electronic Structure Methods, Foresman and Frisch (Gaussian Inc., 1996).

Computer Simulation of Liquids, Allen and Tildesley (Oxford University Press, New York, 1989).

Chemical Kinetics and Dynamics, Steinfeld, Francisco and Hase (Prentice Hall, Englewood Cliffs, NJ, 1989).

F. Grading / Evaluation

- Grades will be based on 4 homework assignments (55% total), a computer lab exam (15%) and a final exam (30%). The schedule of assignments will be posted on the course website. Late assignments might not be accepted or penalties might apply for late assignments.
- Grading scales:

	CHEM 431	CHEM 631
90 - 100 %	A+	A+
85 - 90 %	A	A
80 - 85 %	A-	A-
77 - 80 %	B+	B+
73 - 77 %	B	B
70 - 73 %	B-	B-
67 - 70 %	C+	C
63 - 67 %	C	
60 - 63 %	C-	
57 - 60 %	D+	F
53 - 57 %	D	
50 - 53 %	D-	
0 - 50 %	F	

G. Rights and Responsibilities

Plagiarism:

The most common offense under the Academic Code of Conduct is plagiarism which the Code defines as **"the presentation of the work of another person as one's own or without proper acknowledgement."**

This could be material copied word for word from books, journals, internet sites, professor's course notes, etc. It could be material that is paraphrased but closely resembles the original source. It could be the work of a fellow student, for example, an answer on a quiz, data for a lab report, a paper or assignment completed by another student. It might be a paper purchased through one of the many available sources. Plagiarism does not refer to words alone - it can also refer to copying images, graphs, tables, and ideas. "Presentation" is not limited to written work. It also includes oral presentations, computer assignments and artistic works. Finally, if you translate the work of another person into French or English and do not cite the source, this is also plagiarism.

In Simple Words:

DO NOT COPY, PARAPHRASE OR TRANSLATE ANYTHING FROM ANYWHERE WITHOUT SAYING FROM WHERE YOU OBTAINED IT!

(Source: The Academic Integrity Website: <http://provost.concordia.ca/academicintegrity/plagiarism/>)

Plagiarism and other forms of academic dishonesty:

The academic code of conduct can be found in section 17.10 of the academic calendar (<http://www.concordia.ca/academics/undergraduate/calendar/current/17-10.html>). Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. The Department of Chemistry and Biochemistry offers a seminar on the academic conduct code and the appropriate use of information sources which aims to clarify what practices will be considered unacceptable with regards to work submitted for grading in Chemistry and Biochemistry courses. Attendance at this seminar is highly recommended and represents a clear and fair opportunity to learn what our faculty regards as academic misconduct. Failure to take part in this learning opportunity and thus ignorance of these regulations is no excuse and will not result in a reduced sanction in any case where academic misconduct is observed. This short seminar (1 hour) will be held at the following times (note that late-comers will not be admitted):

Date	Time	Place
Monday, Jan. 23	16:45-17:45	HC-155
Monday, Jan. 23	20:45-21:45	HC-155
Tuesday, Jan. 24	16:45-17:45	CC-308
Wednesday, Jan. 25	16:45-17:45	HC-155
Wednesday, Jan. 25	20:45-21:45	SP-S110
Thursday, Jan. 26	16:45-17:45	HC-155
Friday, Jan. 27	16:45-17:45	CC-310

As space for each of the seminars is limited by the room size, please sign up to your preferred time. Sign up sheets are available outside SP 201.01 (Departmental office).

In the event of extraordinary circumstances beyond the University's control, the content and/or evaluation scheme in this course is subject to change.

IMPROVING STUDENTS' ACADEMIC EXPERIENCE

LIST OF AVAILABLE SERVICES

- **Ms. Hilary Scuffell, Academic Advisor, Chemistry & Biochemistry**
- **Concordia Counselling and Development** offers career services, psychological services, student learning services, etc.
<http://cdev.concordia.ca/>
- **The Concordia Library Citation and Style Guides:**
<http://library.concordia.ca/help/howto/citations.html>
- **Advocacy and Support Services**
<http://supportservices.concordia.ca/>
- **Student Transition Centre**
<http://stc.concordia.ca/>
- **New Student Program**
<http://newstudent.concordia.ca/>
- **Access Centre for Students with Disabilities**
<http://supportservices.concordia.ca/disabilities/>
- **Student Success Centre**
<http://studentsuccess.concordia.ca/>
- **The Academic Integrity Website**
<http://provost.concordia.ca/academicintegrity/>
- **Financial Aid & Awards**
<http://web2.concordia.ca/financialaid/>
- **Health Services**
<http://www-health.concordia.ca/>

