CHEM 431 / 631

Computational Chemistry

for Chemists and Biochemists

A. General Information

- Course: CHEM 431 and CHEM 631, *Computational Chemistry for Chemists and Biochemists*, 3 credits, Winter 2023.
- Time and place: Wednesdays, 18:00-20:45, CC-405.
- 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: Wednesdays, 13:15-14:45, or 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 computer software. Lectures and laboratory.
- Prerequisite: CHEM 234, 241, 333 or 335, 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. Semiempirical MO-SCF methods
3.3. Atomic basis sets
3.4. Hartree-Fock (HF) theory
3.5. Electronic correlation
3.6. Density-functional theory (DFT)
3.7. Configuration interaction (CI)
3.8 Many-body perturbation theory
3.9. Coupled cluster (CC) theory
3.10. Excited states

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

6. ADVANCED TOPICS (TBA)

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. Exam Schedule

- Lab Exam, during class time, April 12, 2023.
- Final Exam, during class time, April 5, 2023.

E. Course Materials: Suggested Readings / Relevant Books

Introduction to Computational Chemistry, Jensen (Wiley, 2017). Available electronically from the library.

Molecular Mechanics Across Chemistry, Rappé and Casewit (U. Science Books, 1997).
Quantum Chemistry, Levine (Prentice Hall, 1991).
Computer Simulation of Liquids, Allen and Tildesley (Oxford University Press, 1989).
Chemical Kinetics and Dynamics, Steinfeld, Francisco and Hase (Prentice Hall, 1989).

F. Grading / Evaluation

- Grades will be based on 4 homework assignments, a computer lab exam, a final exam and an advanced topic presentation. ***The schedule of assignments (and tutorials) will be posted on the course website***. Late assignments might not be accepted or penalties might apply for late assignments.

	CHEM 431	CHEM 631
Assignments	55%	45%
Lab Exam	15%	10%
Final Exam	30%	30%
Presentation		15%

- 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	

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