Chemistry 395/435: Computational Chemistry (Spring 2021)
Department of Chemistry and Biochemistry, Loyola University Chicago

Instructor:	Dr. Pengfei Li
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Lectures:	Monday and Wednesday 5:30-6:45 PM (CST), online
Office Hours:	Friday 4:30-5:30 PM (CST) or by appointment, online

Please see the Sakai site for up-to-date information and posts.

Course Prerequisites: CHEM 302 or 305 for undergraduate students. No prerequisites for graduate students. If you have not completed these course prerequisites, you may be administratively dropped from the class. Please discuss this with the instructor immediately!

Required Textbook: "Essentials of Computational Chemistry", 2nd edition, by Christopher J. Cramer, John Wiley & Sons Ltd 2004, ISBN-10: 0470091827; ISBN-13: 9780470091821.

Suggested Textbooks (not exhaustive): *Computational Chemistry:* "Introduction to Computational Chemistry" F. Jensen.; "Molecular Modelling: Principles and Applications" A. Leach; "Molecular Modelling for Beginners" A. Hinchliffe. *Quantum Mechanics:* "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory" A. Szabo and N. S. Ostlund; "A Chemists Guide to Density Functional Theory" W. Koch and M. C. Holthausen. *Molecular Simulations:* "Molecular Modeling and Simulation" T. Schlick; "The Art of Molecular Dynamics Simulation" D. Rapaport.

Required Software: Zoom.

Class Preparation: In order to understand the material presented during lectures, it is important to come to the class with good background knowledge. This can be achieved by previewing the relevant material in the textbook, reviewing appropriate material from calculus, physics, and physical chemistry classes. Knowledge of basic quantum mechanics and statistical mechanics is expected. Access to a laptop or desktop is required. A basic understanding of LINUX or UNIX is expected as well. For a quick study of LINUX or UNIX system, one can follow this tutorial: http://www.ee.surrey.ac.uk/Teaching/Unix/.

Course Overview: Computational chemistry is a chemistry discipline that uses theoretical and computational methods to study chemical processes. This class aims to enable the students to understand different methods in computational chemistry, apply them to investigate chemical and biochemical systems, and interpret the results. During the lectures, we will cover fundamental methods in computational chemistry, such as the Hartree-Fock, density functional theory, and molecular dynamics methods. Moreover, we will have hands-on practices through labs and projects. In these labs and projects, students will use the Gaussian (https://gaussian.com/) program and/or the AMBER software package (https://ambermd.org/) to perform relevant calculations and simulations. A tentative schedule is shown at the end of this syllabus. Your attendance at lectures and labs is expected.

Computer accounts: The class will use the education allocation of the XSEDE platform (https://www.xsede.org/). Both Gaussian and AMBER are available from the allocation granted. For using this allocation, students need to have access to the internet through their computers. In order to visualize the structures, students need to install GaussView (https://gaussian.com/gaussview6/, which program has been bought by the Department of Chemistry and Biochemistry) and VMD (https://www.ks.uiuc.edu/Research/vmd/, which is free of charge) on their computers.

Course Structure and Online Class Specifics: There are two 75-minute classes (Monday and Wednesday) per week. There will be lectures, labs, and project reports during class time. You will work in small groups (1-4 people) on projects, with the goal of applying computational chemistry to investigate chemical and biochemical problems. The lectures and labs will be delivered through the "Zoom" tool on Sakai and will be recorded in keeping with the statement shown below. The office hours will be accessed by the "Office Hours" tool on Sakai. Again, it is highly recommended that you read (and think about) the related contents in the textbook before each lecture, and ask relevant questions during the lectures and office hours. Materials from the course, including the exam problems, cannot be shared outside the course without the instructor's written permission.

Recording of Zoom Class Meetings: In this class software will be used to record live class discussions. As a student in this class, your participation in live class discussions will be recorded. These recordings will be made available only to students enrolled in the class, to assist those who cannot attend the live session or to serve as a resource for those who would like to review content that was presented. All recordings will become unavailable to students in the class when the course has concluded. *Students will be required to turn on their cameras at the start of class. Students who have a need to participate via audio only must reach out to me to request audio participation only without the video camera enabled.* The use of all video recordings will be in keeping with the University Privacy Statement shown below.

Privacy Statement: Assuring privacy among faculty and students engaged in online and face-to-face instructional activities helps promote open and robust conversations and mitigates concerns that comments made within the context of the class will be shared beyond the classroom. As such, recordings of instructional activities occurring in online or face-to-face classes may be used solely for internal class purposes by the faculty member and students registered for the course, and only during the period in which the course is offered. Students will be informed of such recordings by a statement in the syllabus for the course in which they will be recorded. Instructors who wish to make subsequent use of recordings that include student activity may do so only with informed written consent of the students involved or if all student activity is removed from the recording. Recordings including student activity that have been initiated by the instructor may be retained by the instructor only for individual use.

Projects: Students will work in small groups (each has 1-4 students) to carry out projects. When working as a group, each member should contribute to the study. The computational investigation should provide insights into chemical or biochemical systems. Finally, each group should provide a written project report and a project presentation. These projects will involve quantum chemistry calculations and/or molecular dynamics simulations. The quantum chemistry calculations will be performed by using the Gaussian program. The molecular dynamics simulations will be performed by using the AMBER software package. Other software may be used according to the goals of the specific projects. The general project plan is: (1) Set up project teams; (2) Select a computational project; (3) Execute the project; (4) Analyze the results; (5) Present and write-up the project.

Exam: There will be one take-home exam. The take-home exam will be distributed before the project presentations, and students will have two weeks to finish the take-home exam. If a student disagrees with her/his score for the exam, she/he must request re-grading ***within one week*** from the day he/she received the graded exam. Additional time will not be granted, even if you start late. There will be no make-up exams given.

Grade Components: In the end, the class score will be calculated based on the following components:

Participation:	60%
Written Report:	10%
Presentation:	10%
Take-home exam:	20%

Finally, the class score will be rounded to the nearest integer, and then the course grade will be determined based on the class score through the following scale:

Scale	Grade
85 ≤ score	A
80 ≤ score < 85	A-

75 ≤ score < 80	B+
70 ≤ score < 75	B
65 ≤ score < 70	B-
60 ≤ score < 65	C+
55 ≤ score < 60	C
50 ≤ score < 55	C-
score < 50	D

Ethical Considerations:

a. Academic integrity: All students in this course are expected to have read and to abide by the demanding standard of personal honesty, drafted by the College of Arts and Sciences, which can be viewed at:

http://www.luc.edu/cas/advising/academicintegritystatement/

> A basic mission of a university is to search for and to communicate the truth as it is honestly perceived. A genuine learning community cannot exist unless this demanding standard is a fundamental tenet of the intellectual life of the community. Students of Loyola University Chicago are expected to know, to respect, and to practice this standard of personal honesty.
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> Academic dishonesty can take several forms, including, but not limited to cheating, plagiarism, copying another student's work, and submitting false documents.

Any instance of dishonesty (including those detailed on the website provided above or in this syllabus) will be reported to The Chair of The Department of Chemistry and Biochemistry who will decide what the next steps may be.

b. Exam: Students will not collaborate on any exams. Only those materials and devices permitted by the instructor may be used to assist in examinations. Students will not represent the work of others as their own. Any student caught cheating during an exam will be reported to the Dean's office and will receive zero points for the given exam. The Chair of the Department of Chemistry and Biochemistry will also be notified and will decide what the next steps may be. Please be honest with your work.

Loyola University Absence Policy for Students in Co-Curricular Activities Students: missing classes while representing Loyola University Chicago in an official capacity (e.g. intercollegiate athletics, debate team, model government organization) shall be allowed by the faculty member of record to make up any assignments and to receive notes or other written information distributed in the missed classes. Students should discuss with faculty the potential consequences of missing lectures and the ways in which they can be remedied. Students must provide their instructors with proper documentation (develop standard form on web) describing the reason for and date of the absence. This documentation must be signed by an appropriate faculty or staff member, and it must be provided as far in advance of the absence as possible. It is the responsibility of the student to make up any assignments. If the student misses an examination, the instructor is required to give the student the opportunity to take the examination at another time. (https://www.luc.edu/athleteadvising/attendance.shtml).

Student Accommodations: The Student Accessibility Center (formerly known as Services for Students with Disabilities), Sullivan Center (773-508-3700), www.luc.edu/sac, has the mission "to serve students with documented disabilities by creating and fostering an accessible learning environment," including "support[ing] faculty, staff, and administrators on matters such as ADA and Section 504 compliance, as it relates to individuals with disabilities." Please direct all questions concerning accommodations of disabilities to the Student Accessibility Center. Academic accommodations afforded to students require documentation and review. The Student Accessibility Center will issue accommodation letters for registered students to present to their instructors: accommodations are not active until students present these letters to their instructors. If students' accommodations involve attendance or deadlines, instructors and students will jointly complete and execute an Agreement Form articulating their terms. See https://www.luc.edu/sac/faculty/facilitatingaccommodations/ for guidance about implementing various kinds of accommodations in a way that is appropriate to your class. The Student Accessibility Center stands ready to work with you.

Accommodations for Religious Reasons: If you have observances of religious holidays that will cause you to miss class or otherwise effect your performance in the class you must alert the instructor ***within 10 calendar days of the first class meeting of the semester*** to request special accommodations, which will be handled on a case by case basis.

Course Repeat Rule: Effective with the Fall 2017 semester, students are allowed only THREE attempts to pass Chemistry courses with a C- or better grade. The three attempts include withdrawals (W). After the second attempt, the student must secure approval for a third attempt. Students must come to the Chemistry Department, fill out a permission to register form or print it from the Department of Chemistry and Biochemistry website: http://www.luc.edu/chemistry/forms/ and personally meet and obtain a signature from either the Undergraduate Program Director, Assistant Chairperson, or Chairperson in Chemistry. A copy of this form is then taken to your Academic Advisor in Sullivan to secure final permission for the attempt.

The Loyola COVID-19 Website: https://www.luc.edu/coronavirus/

The Return to Campus Website: https://www.luc.edu/returntocampus/

Student Services at Loyola Online: https://www.luc.edu/online/resources/index.html

- Student Complaint Procedure: https://www.luc.edu/online/resources/student-grievances/
- Technology Support, including Sakai, Zoom, and LOCUS: https://www.luc.edu/online/resources/technology/
- Academic Services, including the Center for Tutoring and Academic Excellence, and the Writing Center: https://www.luc.edu/online/resources/academicservices/
- Student Support Services, including the Student Accessibility Center, and the Wellness Center: https://www.luc.edu/online/resources/studentsupportservices/

Tentative Schedule*

Week	Dates	Topics
1	Wednesday Jan 20	Introduction of computational chemistry, syllabus
2	Monday Jan 25	Review of key concepts from math
	Wednesday Jan 27	The Born-Oppenheimer approximation, potential energy surfaces
3	Monday Feb 1	Foundations of the molecular orbital theory
	Wednesday Feb 3	Slater determinants, the Hartree-Fock (HF) method
4	Monday Feb 8	
	Wednesday Feb 10	***First Spring Break, no class***
5	Monday Feb 15	The Hartree-Fock method
	Wednesday Feb 17	Basis sets, semi-empirical methods
6	Monday Feb 22	*Lab 1: XSEDE accounts, Linux/Unix, and GaussView*
	Wednesday Feb 24	Geometry optimization, ground state properties
7	Monday Mar 1	*Lab 2: Using the HF method to investigate a reaction in gas phase*
	Wednesday Mar 3	Electron correlation, the configuration interaction method
8	Monday Mar 8	***Second Spring Break, no class***
	Wednesday Mar 10	The many-body perturbation theory, open-shell calculations
9	Monday Mar 15	Fundamentals of density functional theory (DFT)
	Wednesday Mar 17	Exchange-correlation functionals
10	Monday Mar 22	Solvent models
	Wednesday Mar 24	*Lab 3: Using DFT to study a reaction in solvent*
11	Monday Mar 29	Excited states
	Wednesday Mar 31	*Lab 4: Using DFT to calculate molecular spectra*
12	Monday Apr 5	Force fields, the QM/MM method
	Wednesday Apr 7	The Docking, molecular dynamics (MD), and Monte Carlo methods
13	Monday Apr 12	Free energy methods in molecular simulations
	Wednesday Apr 14	*Lab 5: Use MD to study a protein-ligand system*
14	Monday Apr 19	*Project presentations*
	Wednesday Apr 21	*Project presentations*
15	Monday Apr 26	*Project presentations*
	Wednesday Apr 28	*Project presentations*

*The instructor reserves the right to make changes to the schedule.