Advanced Topics in Physical Chemistry:

Computational Chemistry

CHE 466A08

3 credit hours

Department of Chemistry – Illinois State University

COURSE SYLLABUS

Spring 2022

INSTRUCTOR

Instructor:	Dr. Jean M. Standard
email:	standard@ilstu.edu
Phone:	309-xxx-xxxx
Office hours:	By appointment

COURSE PREREQUISITES

One semester of Physical Chemistry (CHE 360 or 362 or equivalent) or consent of instructor required.

CATALOG DESCRIPTION

Applications of the principles of physical chemistry to modeling molecular structures, properties, and reactivity using modern software packages.

COURSE OVERVIEW

Computational Chemistry provides an overview of techniques employed for modeling molecular structures, properties, and chemical reactivity, including classical molecular and quantum mechanics methods. The selection of appropriate techniques for solving a variety of chemical problems using common computational chemistry software packages will be emphasized. The focus of the course also will include the analysis, visualization, and interpretation of results from calculations employing the various computational methods. No prior computing experience is necessary.

STUDENT OUTCOMES

Upon successful completion of this course, students will be able to:

- Use common computational chemistry software packages to build and visualize molecular systems.
- Select appropriate computational methods for the simulation of various types of molecular systems.
- Carry out molecular simulations using computational chemistry software packages and analyze and interpret the results.

TOPICAL OUTLINE

	Topic	Chapter
I.	**Introduction to Computational Chemistry**	1
	A. What is computational chemistry?	
	B. Computational chemistry examples	
	C. History of scientific computing in chemistry	
II.	**Potential Energy Surfaces**	2
	A. Born-Oppenheimer approximation	
	B. Molecular potential energy functions	
	C. Stationary points	
	D. Energy minimization	
III.	**Molecular Mechanics**	3
	A. Force fields	
	B. Parameterization	
	C. Strain energies	
	D. Molecular mechanics examples	
IV.	**Conformation Searching**	notes
	A. Systematic methods	
	B. Monte Carlo methods	
	C. Molecular Dynamics methods	
	D. Conformation searching examples	
V.	**Molecular Orbital Methods**	4, 5
	A. Quantum mechanics background	
	B. Hartree-Fock equations	
	C. Basis sets	
	D. Electron correlation	
VI.	**Additional Quantum-based Methods**	6, 7
	A. Semi-empirical methods	
	B. Density functional theory	
VII.	**Molecular Orbital Applications**	5, 7, 8
	A. Thermochemistry	
	B. IR spectroscopy	
	C. NMR spectroscopy	
	D. Reaction paths	
	E. Solvent effects	
	F. Biomolecular systems	
VIII.	**Advanced Methods and Applications**	
	(time permitting)	

TENTATIVE SCHEDULE OF LECTURES / ASSIGNMENTS / EXAMS

Week of	Lectures / Quizzes	Reading	Assignments / Exams
Jan. 9 (Week 1)	Regular Lectures 1 & 2 / Quizzes 1& 2 Hands-on Lecture 1	Ch. 1	
Jan. 16 (Week 2)	**M. L. King Day – Monday, January 17** Regular Lecture 3 / Quiz 3 Hands-on Lecture 2	Ch. 2	**Assignment 1**
Jan. 23 (Week 3)	Regular Lectures 4 & 5 / Quizzes 4 & 5 Hands-on Lecture 3	Ch. 2	
Jan. 30 (Week 4)	Regular Lectures 6 & 7 / Quizzes 6 & 7 Hands-on Lecture 4	Ch. 3	**Assignment 2**
Feb. 6 (Week 5)	Regular Lectures 8 & 9 / Quizzes 8 & 9 Hands-on Lecture 5	Ch. 3	
Feb. 13 (Week 6)	Regular Lectures 10 & 11 / Quizzes 10 & 11 Hands-on Lecture 6	Ch. 3	**Assignment 3**
Feb. 20 (Week 7)	Regular Lectures 12 & 13 / Quizzes 12 & 13 Hands-on Lecture 7	notes	
Feb. 27 (Week 8)	Regular Lectures 14 & 15 / Quizzes 14 & 15	notes	**EXAM 1**
Mar. 6	**SPRING BREAK**		
Mar. 13 (Week 9)	Regular Lectures 16 & 17 / Quizzes 16 & 17 Hands-on Lecture 8	Ch. 4	**Assignment 4**
Mar. 20 (Week 10)	Regular Lectures 18 & 19 / Quizzes 18 & 19 Hands-on Lecture 9	Ch. 5	
Mar. 27 (Week 11)	Regular Lectures 20 & 21 / Quizzes 20 & 21 Hands-on Lecture 10	Ch. 5	**Assignment 5**
Apr. 3 (Week 12)	Regular Lectures 22 & 23 / Quizzes 22 & 23 Hands-on Lecture 11	Ch. 6	
Apr. 10 (Week 13)	Regular Lectures 24 & 25 / Quizzes 24 & 25 Hands-on Lecture 12	Ch. 7	**Assignment 6**
Apr. 17 (Week 14)	Regular Lectures 26 & 27 / Quizzes 26 & 27 Hands-on Lecture 13	Ch. 7	
Apr. 24 (Week 15)	Regular Lectures 28 & 29 / Quizzes 28 & 29 Review and Course Summary	Ch. 8	
May 1 (Week 16)	**FINAL EXAM WEEK**		**EXAM 2**

TEXTBOOK AND OTHER READINGS

The required textbook is: *Computational Chemistry*, 2nd ed., Errol G. Lewars, Springer, New York, NY 2011 (ISBN: 978-90-481-3860-9).

In addition to the required text, a number of journal articles and other readings related to the course topics will be provided throughout the semester.

REQUIRED STUDENT TASKS / ASSIGNMENTS

The course includes lectures, readings, quizzes, assignments, and exams. Each week will include three lectures, with the exception of weeks with exams or holidays: two of the lectures will cover theoretical background and applications (referred to as "regular" lectures), while the third lecture will involve demonstrations of the computational chemistry software packages employed in the class (referred to as "hands-on" lectures).

Quizzes:

A quiz will be given following the end of each regular lecture for a total of 29 during the semester. The quizzes will cover key aspects of the material covered in the lectures and are worth 4 points each. The lowest four quiz scores will be dropped in determining the overall quiz grade for the semseter.

Assignments:

Six assignments worth 50 points each will be distributed during the semester. The assignemtns will involve using the computational chemistry software packages introduced in class to investigate molecular systems. These assignments also will include questions related to assigned reading and literature studies as well as calculations connected to the theoretical background and practical aspects of the computational techniques.

Exams:

Two exams worth 150 points each will be administered during the semester. The exams will include questions related to the lecture material, assigned reading, theoretical background, computational methods, and assignments.

DUE DATES

The deadline for quizzes is the end of each week. For example, the deadline for completion of Quizzes 1 and 2 is 11:59 PM CST on Saturday of Week 1. At that point the quizzes for the week will close in ReggieNet and the answer keys will be posted. No late quizzes will be accepted.

The due date for each assignment is 10 days after it is made available. Each assignment will be made available at noon CST on Friday (see schedule for specific dates). The assignment is then due at noon 10 days later (on a Monday). No late assignments will be accepted.

The due date for each exam is **three** hours after the exam is downloaded. The completed exam must be uploaded to ReggieNet or sent via email and received by the course instructor within three hours of the timestamp for the download from ReggieNet.

If a student has a legitimate and verifiable reason for missing a deadline, a make-up assignment may be arranged at the instructor's discretion. Such reasons may include, but are not limited to, serious illness, hospitalization, death in the immediate family, and participation in officially-sanctioned university events. Please contact the instructor in advance if possible to discuss alternate arrangements.

GRADING

Grades will be assigned based upon achievement on quizzes, assignments, and exams. The overall course grades will be based on the following point totals:

Quizzes (best 25 @ 4 points each):	100
Assignments (6 @ 50 points each):	300
Exams (2 @ 150 points each):	300
Total Points:	**700**

The final grade will be calculated as a percentage of the total number of points. The grading scale is: A: 90–100%, B: 80–89%, C: 70–79%, D: 60–69%, and F: 59% and below.

COURSE POLICIES

COURSE WEB SITE

This course will employ the ReggieNet web site for access to all course materials and grades: https://reggienet.illinoisstate.edu/.

OFFICE HOURS

Since most course participants will be located off campus, traditional office hours will be replaced by email discussions. Students also may seek assistance through the online discussion forums for the course in ReggieNet or request a Zoom meeting with the instructor.

HARDWARE AND SOFTWARE REQUIREMENTS

In order to participate in this online course, it is important that you have access to the following hardware and software:

- personal computer (Mac, PC, or Linux) with access to the internet
- web browser (Chrome, Firefox, Safari, etc.)
- email
- word processing software (Microsoft Office 365 is available to all ISU students, although it is not required. See https://ithelp.illinoisstate.edu/knowledge/728-logging-in-to-office-365/ for information about access.)
- spreadsheet software (Excel in Office 365 or any other spreadsheet package is acceptable.)

TECHNOLOGY SUPPORT

Support for technology issues related to your university login ID (ULID) or account, ISU email, ReggieNet, Microsoft Office software, or other campus-related technology issue is available through the IT Help center: https://ithelp.illinoisstate.edu/. For specific questions related to the course materials or the computational chemistry software you will be accessing for this class, contact the instructor via email (the IT Help center will not be able to assist).

ACADEMIC HONESTY

All students are expected to adhere to the Illinois State University Code of Student Conduct, a copy of which can be found at https://deanofstudents.illinoisstate.edu/conduct/code/. Violations of this code may result in the instructor penalizing the student with a loss of points. The exact amount deducted is at the discretion of the instructor and will vary depending on the severity of the infraction and whether it is a repeat offense or not.

STUDENT ACCESS AND ACCOMMODATION SERVICES

Any student needing to arrange a reasonable accommodation for a documented disability and/or medical/mental health condition should contact Student Access and Accommodation Services at 350 Fell Hall, (309) 438-5853, or visit the website at StudentAccess.IllinoisState.edu.