Course Syllabus – Spring 2023

Course Information

Course	CHEM 5311-CHEM4311
Title	Classical Simulations for Biological and Condensed Systems
Term	Spring 2023
Days & Times	Tuesdays and Thursdays, 4:00-5:15 PM
Location	Brazos Lab (FO 1.206C)

Professor Contact Information

Professor	Dr. Hedieh Torabifard
Office Phone	972-883-4686
Email Address	hedieh.torabifard@utdallas.edu
Office Location	BE 3.312
Office Hours	Tuesdays and Thursdays, 3:00-4:00 PM

TA Contact Information

TA Information Kira Mills, kira.mills@utdallas.edu

Course Pre-requisites, Co-requisites, and/or Other Restrictions

Prerequisites for undergraduate students: CHEM 3361 or BIOL 3361, CHEM 3321 and CHEM 3322

Course Description

This course will focus on the application of the classical simulations to investigate and understand bio-related problems. The topics covered in this class include force field development, molecular dynamics (MD) simulations, free energy methods, and hybrid quantum mechanics and molecular mechanics (QM/MM) simulations.

Student Learning Objectives/Outcomes

The course will provide the foundations for the application of computational simulations based on physical concepts to investigate and understand biological and chemical systems at the molecular level. The topics covered will involve material from various areas of computational biochemistry, with emphasis on classical mechanics and its application. While the mathematics will not be onerous, students should have a working understanding of quantum and classical mechanics, as well as linear algebra and calculus. At the completion of the course the students will:

1) Learn different types of force field and the principles for force field development. This section involves performing molecular simulations with Quantum Mechanics methods.
2) Learn different Molecular Mechanics methods including all atom molecular dynamics simulations, free energy methods, and hybrid QM/MM.
3) Become familiar with high performance computing (HPC) environments, and Linux OS.
4) Perform MD simulations and related analyses.
5) Deduce molecular properties from simulations
6) Develop a project that involves MD simulations of biological or chemical systems.

7) Write a 1-2-page scientific proposal for the developed project (Grad students only).
8) Write a 3-5-page report for the results of the project (Grad students only).
9) Give a 25 (20)-minute talk for the project that follows a 5-minute Q/A for grad students (undergrads students).

Suggested Textbooks and Materials

"Introduction to Computational Chemistry" Frank Jensen
"Essential of Computational Chemistry, Theories and Models" Christopher Cramer

Grading Policy for graduate students
For graduate students: The course grade will be based on one midterm (20% each), computational assignments (20%), and a research project (60%). The 60% of the research project involves a 1-2-page research proposal (20%), a 25-minute presentation (20%), and a 3-5-page report for the research project. You need to develop a project and submit a proposal and a final report of your findings by the scheduled deadline. The presentations will be in the last week of class.

A+	96-100	B+	81-85	C+	66-70
A	91-95	B	76-80	C	61-65
A-	86-90	B-	71-75	F	<61

Grading Policy for undergraduate students
For undergraduate students: The course grade will be based on one midterm (35% each), computational assignments (30%), and a research project (35%). You need to select and discuss a project with Prof. Torabifard by the scheduled deadline. For the research project, you need to give a 20-minute presentation to the class in the last week of class.

A+	96-100	B+	81-85	C+	66-70	D+	51-55
A	91-95	B	76-80	C	61-65	D	46-50
A-	86-90	B-	71-75	C-	56-60	F	< 46

Course & Instructor Policies

1. **No late assignments will be accepted.**

2. **<u>The mid-term exam must be taken, will be comprehensive and cannot be replaced by any other grade.</u> There will be no makeup exams.**

3. The project will be individual. If you are involved in research, your research project in this class maybe used to complement your research.

4. The project could be related to any chemistry or biochemistry relevant topic. You should start thinking about your research project as early as possible and discuss it with Prof. Torabifard. You are welcome to ask for support and guidance as required for the development of the proposal for your project, and as you carry out the simulations and analysis of your results.

5. **Assignments will be due on the date and time specified in the schedule**. Assignments must be turned in digitally by email to TA. Assignments turned in after the deadline will not receive any credit. Deadline extensions may be given for exceptional cases or for

religious observance or accepted, documented reason (e.g. documented illness). Excused extensions should be arranged prior to the due date.

6. **Attendance** and **participation** will be necessary for you to completely achieve the course goals.

7. All students who take mid-term exam at StudentAccessAbility must schedule their exams at the times given in the syllabus.

8. Mid-term exam is a strictly an individual assessment. For tests/exams, students may only use pen/pencil, paper, and basic calculators to work problems. No external aids such as notes, formula notecards, lectures, books, or the internet should be used. If the use of any external aids is detected, the students will receive zero for the given exam/tests.

9. **No extra credit assignments will be given.**

10. If you wish to submit **an exam for re-grading** because you believe you lost points unfairly, you must do so within **one week of receiving your test. For the final exam, you must request it within 24 hours of receiving your raw grade on eLearning.** Your entire exam will be re-graded, not just the exact problem you pointed out. No exception will be allowed.

11. Class notes will be posted on eLearning/Teams.

12. It is expected that students will abide by the academic integrity requirements as stated in the student code of conduct. Turn your cell phone, iPod, etc. off during class time. Use of these devices during class is disrespectful to your classmates and Professor. Any person using these devices without explicit request from the instructor during class will have points deducted off her/his final grade.

13. Learning is a two–way street, therefore, I will ask you for feedback throughout the course. I will take your feedback seriously and work hard to incorporate your ideas on how to improve the course.

- **Assignments & Academic Calendar:** This is a tentative calendar. The changes will be announced on eLearning.

	Lecture	Workshop				
Week	Tue	Thr	Lecture	Workshop	Assignments	Deadlines
Week 1	1/17	1/19	Introduction to COMP-	Set up account on Europa/Google Colab/ WebMO		
Week 2	1/24	1/26	Force Field	Assignment 1		
Week 3	1/31	2/2	Classical Mechanics	Assignment 1-2	Assignment 1 due on 2/2	
Week 4	2/7	2/9	Classical Mechanics	Assignment 2		
Week 5	2/14	2/16	Quantum Mechanics	Assignment 3	Assignment 2 due on 2/16	
Week 6	2/21	2/23	Input preparation: Proteins	Assignment 4	Assignment 3 due on 2/23	
Week 7	2/28	3/2	Protein simulation	Assignment 5	Assignment 4 due on 3/2	
Week 8	3/7	3/9	Analysis of Protein Simulation	Assignment 6	Assignment 5 due on 3/9	Project selection for undergrads only-schedule a meeting with Dr. Hedi
Week 9	3/14	3/16	Spring break	Spring break	Spring break	Spring break
Week 10	3/21	3/23	Midterm and Project Selection	Assignment 6	--	Midterm (All students) on 3/21 Project Proposal Due on 3/23 (Grad only)
Week 11	3/28	3/30	Input preparation, simulation, and analyses: condensed phase	Assignment 6	Assignment 6 due on 3/30	
Week 12	4/4	4/6	Sampling Approach	Assignment 7	--	
Week 13	4/11	4/13	Free Energy Methods	Assignment 7	Assignment 7 due on 4/13	
Week 14	4/18	4/20	Hybrid QM/MM	Help with the final project	--	
Week 15	4/25	4/27	Help with the final project	Help with the final project		
Week 16	5/2	5/4	Presentations of term project (All students)	Presentations of term project (All students)		Report Due on 5/4 (Grad students only)

Class Materials

The instructor may provide class materials that will be made available to all students registered for this class as they are intended to supplement the classroom experience. These materials may be downloaded during the course, however, these materials are for registered students' use only. Classroom materials may not be reproduced or shared with those not in class, or uploaded to other online environments except to implement an approved Office of Student AccessAbility accommodation. Failure to comply with these University requirements is a violation of the Student Code of Conduct.

Class Attendance

The University's attendance policy requirement is that individual faculty set their course attendance requirements. Regular and punctual class attendance is expected. Students who fail to attend class regularly are inviting scholastic difficulty. In some courses, instructors may have special attendance requirements; these should be made known to students during the first week of classes. Faculty have the discretion to set an attendance policy for their in-person meetings, but the absences due to COVID-19 cannot be counted against a quarantined student.

Class Participation

Regular class participation is expected regardless of course modality. Students who fail to participate in class regularly are inviting scholastic difficulty. A portion of the grade for this course is directly tied to your participation in this class. It also includes engaging in group or other activities during class that solicit your feedback on homework assignments, readings, or materials covered in the lectures (and/or labs). Class participation is documented by faculty. Successful participation is defined as consistently adhering to University requirements, as presented in this syllabus. Failure to comply with these University requirements is a violation of the Student Code of Conduct.

Class Recordings

Students are expected to follow appropriate University policies and maintain the security of passwords used to access recorded lectures. Unless the Office of Student AccessAbility has approved the student to record the instruction, students are expressly prohibited from recording any part of this course. Recordings may not be published, reproduced, or shared with those not in the class, or uploaded to other online environments except to implement an approved Office of Student AccessAbility accommodation. Failure to comply with these University requirements is a violation of the Student Code of Conduct.

NOTE: if the instructor records any part of the course, then the instructor will need to add the following syllabus statement:

The instructor may record meetings of this course. These recordings will be made available to all students registered for this class if the intent is to supplement the classroom experience. If the instructor or a UTD school/department/office plans any other uses for the recordings, consent of the students identifiable in the recordings is required prior to such use unless an exception is allowed by law.

Classroom Citizenship

See class participation, class recording, and student code of conduct sections.

Comet Creed

This creed was voted on by the UT Dallas student body in 2014. It is a standard that Comets choose to live by and encourage others to do the same:

"As a Comet, I pledge honesty, integrity, and service in all that I do."

Academic Support Resources
The information contained in the following link lists the University's academic support resources for all students.

Please see http://go.utdallas.edu/academic-support-resources.

UT Dallas Syllabus Policies and Procedures
The information contained in the following link constitutes the University's policies and procedures segment of the course syllabus. Please review the catalog sections regarding the credit/no credit or pass/fail grading option and withdrawal from class.

Please go to http://go.utdallas.edu/syllabus-policies for these policies.

The descriptions and timelines contained in this syllabus are subject to change at the discretion of the Professor.