

Computational Chemistry – CHM 6586 Syllabus

CHM 6586, **Fall 2024**, Monday 9:35 am – 10:25 am, Wednesday 8:30 am – 10:25 am

Room: Weil 408A. Lectures scheduled for synchronous delivery on Canvas

Instructor: Mingjie Liu, mliu@chem.ufl.edu, Office: LEI 240C;

Course Description. This class will cover different aspects of computational chemistry tools from quantum mechanical calculations to classical molecular dynamics simulations.

Course Coverage. Basic of quantum mechanics, HF theory, density functional theory, approximations, QM packages (Gaussian, Quantum Espresso), MD packages (LAMMPS, Amber)

Course Goals. • Understand when, which and how to use computational tools to gain insights into chemical systems.

- Gain a basic understanding on how to run QM calculations on molecules and materials.
- Gain a basic understanding of how to run classical mechanics tools for MD simulations.
- Understand and analyze the results from computational chemistry.
- An introduction to software packages for computational chemistry.
- Hands-on exercises using Gaussian, Quantum Espresso, LAMPPS, and Amber.

Tentative Schedule of Classes:

Date	Topic (lecture)	Topic (lab)	Homework
Aug 26	Introduction to the course	Install software (windows, mac, linux)	
Aug 28	Basic of QM	HiPerGator Orientation (tentative)	
Sep 2	Holiday		
Sep 4	Structure generation and visualization; File transfer to HiPerGator, structure generation		HW1
Sep 9	Intro basis sets with HF		
Sep 11	Basis sets test single point H2O (Gaussian) (Lab 1)		
Sep 16	Post HF (electron correlation)		
Sep 18	Exchange-Correlation functionals test (Gaussian) (Lab 2)		
Sep 23	Intro to DFT & DFT functionals		
Sep 25	Geometry optimization (Gaussian) (Lab 3)		
Sep 30	Geometry optimization		
Oct 2	Vibration, HOMO-LUMO visualization (Gaussian and Gaussian View) (Lab 4)		HW2
Oct 7	Frequency and spectroscopic properties		
Oct 9	Transition State and Frequency (Gaussian) (Lab 5)		
Oct 14	Open shell, thermodynamic properties		
Oct 16	Spectra (IR, NMR) and Reaction energy (Gaussian) (Lab 6)		
Oct 21	Solid state physics-Intro and surface science		
Oct 23	Surface Adsorption of molecules (QE) (Lab 7)		
Oct 28	Band structure of solid-state materials		
Oct 30	Band structure of Si (QE) (Lab 8)		
Nov 4	Molecular Dynamics-Intro		
Nov 6	LAMMPS-1 (Lab 9)		HW3
Nov 11	Holiday		
Nov 13	LAMMPS-2 (Lab 10)		
Nov 18	QM/MM, solvation		
Nov 20	Intro to Quantum Computing & Student Presentation (1, 2)		
Nov 25	Thanksgiving Holiday		
Nov 27	Thanksgiving Holiday		
Dec 2	Student Presentation (3, 4)		
Dec 4	Student Presentation (5, 6, 7, 8, 9)		

Recommended Textbooks:

Exploring Chemistry with Electronic Structure Methods 3rd Edition by J. B. Foresman and Æ. Frisch

Molecular Modeling: Principles and Applications 2nd Edition by A. R. Leach

Essentials of Computational Chemistry: Theories and Models 2nd Edition by C. J. Cramer

Canvas Website. All students will have access to the Canvas website: <https://ufl.instructure.com/>

You will login with your Gatorlink account username and password. This is where you will find general class information, important news, office hours, handouts, class notes, and keys. This is also where you will be able to find out your point totals and histograms.

Class Requirements (for graduate level):

- 1) Three homework (10 points each = 30 points)
 - 2) Ten lab exercise (5 points each = 50 points)
 - 3) Final project & presentation (15 points)
 - 4) Attendance and in-class participants (5 points)
- = 100 points total**

Class Requirements (for undergraduate level):

- 1) Three homework (10 points each = 30 points)
 - 2) Ten lab exercise (5 points each = 50 points)
 - 3) Attendance and in-class participants (20 points)
- = 100 points total**
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Homework (In-Class Lab). Homework (In-Class Lab report) due date is posted on the class calendar. Late homework (if it is turned in on the same day, but after the deadline) will have a 20% deduction on the grade. The day after, the solutions will be posted, and no more homework will be accepted for grading.

Final Projects. Graduate Students will use the techniques they have acquired to simulate their systems of interest and prepare a report.

Presentation. The final projects results will be presented at the end of the semester with 15min + 5min Q&A.

Grading. Grades will be curved based on points earned out of 100.

85-100	A
75-85	B+
65-75	B
60-65	B-
< 60	C

Assignment Regrading. If you have a question concerning the grading of an assignment, you may submit the entire assignment for complete regrading. The assignment must be submitted for regrading by the next class meeting after the date the assignment was returned to the class.

Office Hours. Wednesday 1-3 pm, LEI 240C by email appointment.

TA Office Hours. TBD

Accommodations for students with disabilities. Students requesting classroom accommodation must first register with the Dean of Students Office. The Dean of Students Office will provide documentation to the student who must then provide this documentation to the instructor when requesting accommodation.

Course Evaluations. "Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/students/>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via <https://ufl.bluer.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>."

UF Honor Code: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

On all work submitted for credit by students at the university, the following pledge is either required or implied: **"On my honor, I have neither given nor received unauthorized aid in doing this assignment."** "The university requires all members of its community to be honest in all endeavors. A fundamental principle is that the whole process of learning and pursuit of knowledge is diminished by cheating, plagiarism and other acts of academic dishonesty. In addition, every dishonest act in the academic environment affects other students adversely, from the skewing of the grading curve to giving unfair advantage for honors or for professional or graduate school admission. Therefore, the university will take

severe action against dishonest students. Similarly, measures will be taken against faculty, staff and administrators who practice dishonest or demeaning behavior.”

Cheating and Plagiarism. Cheating and/or plagiarism will not be tolerated. The minimum penalty will be an automatic zero on the assignment in question. Suspension from the University may also result. Do not risk it. It is not worth it. Plagiarism consists of passing off as one’s own the ideas, words, writings, etc. that belong to someone else. You are committing plagiarism if you copy the work of another person and turn it in as your own, even if you have that person’s permission. See: <https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>

Copyright Notice. All handouts used in this course are copyrighted and may not be copied without my expressly granted permission. “Handouts” include all materials generated for this class, which include but are not limited to syllabi, quizzes, exams, problems, in-class materials, lecture note templates, lecture notes, review sheets, problem sets, or other materials. Tutors and tutoring services are expressly forbidden from copying any or all of these materials, unless you pay me two million U.S. dollars. Only students currently enrolled in the class may make a single copy of this material for their personal use.

Counseling. The University of Florida provides counseling services for students, staff, and faculty.

U Matter, We Care: If you or someone you know is in distress, please contact umatter@ufl.edu, 352-392-1575, or visit U Matter, We Care website to refer or report a concern and a team member will reach out to the student in distress.

Counseling and Wellness Center: Visit the Counseling and Wellness Center website or call 352-392-1575 for information on crisis services as well as non-crisis services.

Student Health Care Center: Call 352-392-1161 for 24/7 information to help you find the care you need, or visit the Student Health Care Center website.

University Police Department: Visit UF Police Department website or call 352- 392-1111 (or 9-1-1 for emergencies).

UF Health Shands Emergency Room / Trauma Center: For immediate medical care call 352- 733-0111 or go to the emergency room at 1515 SW Archer Road, Gainesville, FL 32608;