

Computational Chemistry

Course Information

Course number: CHM 6586

Course title: Computational Chemistry

Credits: 3

Where: Room WEIL 0408D.

When: Mondays (period 3 and Wednesdays; Periods 2-3 (8:30 am –10:25am)

Classes start/end: 8/24/21 - 12/7/21

No class on Sep 5th and Nov 23th

List of Recommended Textbooks:

A.R. Leach, "Molecular Modeling: Principles and Applications", 2nd edition, Prentice-Hall, ISBN 0-582-38210-6 (2001)

Frenkel, D. and Smit, B., "Understanding Molecular Simulation", 2nd edition, Academic Press, San Diego (2002)

Course Description: We will cover different aspects of computational chemistry tools from quantum mechanical calculations to classical molecular dynamics simulations. The class will have lecture material and hands-on practical applications. By the end of the course students should be familiar with the best techniques to use for different types of molecules and how to set up and run relevant calculations on those systems.

Online material: Available through canvas (<https://elearning.ufl.edu/>)

It will contain the syllabus, homework and lecture notes. It will also serve as a mode of email communication (you can configure it to redirect the emails).

Instructor Information

Alberto Perez

Assistant Professor

Office: Room 240F Leigh Hall.

Office hours: By appointment.

Contact e-mail: perez@chem.ufl.edu

TA: Arup Mondal. – Leigh Hall 240.

Face to face learning

Attendance: Attendance to lectures is expected as this is a computational lab. We will combine a traditional lecture with application problems. In addition to the 3 hrs class a week, ~8-

10/week of reading, homework and general study are required. If possible, we will record lectures and post them on canvas for those that cannot make it to class.

Homework and Grading

Homework: Homework 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, although you are still responsible to finish it to be ready for the exams. Each homework problem has to show the full derivation, using SI units. No points will be given for a final result without justification.

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

Presentations: Students will prepare a presentation about chemical systems using sketchfab to present a guided 3D visualization of their systems along with their insights they have gained from their final projects.

Course Grading: The grade will be determined by homework (50%), final project (25%), presentations (15%) and in-class participation (10%).

There is NO FINAL in this class.

Course Evaluations: Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at <https://evaluations.ufl.edu>. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at <https://evaluations.ufl.edu/results/>.

HONOR CODE The student honor code can be found at <http://www.registrar.ufl.edu/catalog/policies/students.html>

The students, instructor and TAs are honor bound to comply with the Honors Pledge:

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.

Cheating on an exam will result in a grade of zero. Although homework is expected to be worked "in group", the submitted homework solution must be your individual work. If any homework or quiz assignment is suspect, a grade of zero will also be given for that assignment.

Information on current UF grading policies for assigning grade points is available at <https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>

Students with disabilities: Students requiring special accommodations need to register at the Dean of Student Offices and bring the documentation to the instructor.

Counseling services are available at <http://www.counsel.ufl.edu> or call (352)-392-1575 during regular service hours (8am-5pm). For other hours or weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352)-392-1171.

Campus Resources:

Health and Wellness

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; Visit the UF Health Emergency Room and Trauma Center website.

Academic Resources

E-learning technical support: Contact the UF Computing Help Desk at 352-392-4357 or via e-mail at helpdesk@ufl.edu.

Career Connections Center: Reitz Union Suite 1300, 352-392-1601. Career assistance and counseling services.

Library Support: Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center: Broward Hall, 352-392-2010 or to make an appointment 352- 392-6420. General study skills and tutoring.

Writing Studio: 2215 Turlington Hall, 352-846-1138. Help brainstorming, formatting, and writing papers.

Student Complaints On-Campus: Visit the Student Honor Code and Student Conduct Code webpage for more information.

On-Line Students Complaints: View the Distance Learning Student Complaint Process.

Course Objectives

By the end of this course students should be able to:

1. Understand when, which and how to use computational tools to gain insights into chemical systems.
2. Gain a basic understanding of how to run quantum mechanical calculations on small molecules.
 - a. Base superposition error
 - b. Counterpoise method
3. Gain a basic understanding of how to use classical mechanics tools for the simulating larger biomolecules.
4. An introduction to software packages for computational chemistry
5. Model building and molecular mechanics
6. Molecular orbitals and electronic structure
7. Solvation effects and molecular dynamics
8. Building large systems (polymers and solid surfaces)

Suggested Course itinerary:

Date	Topics
August 24 th	Introduction
August 29 th	Computational models
August 31 st	Molecular visualization, model building.
September 5 th	Holiday –no class
September 7 nd	Energy landscape. Exploration/exploitation, relation to observables.
September 12 th	Geometry optimization
September 14 th	Ab-initio methods, basis sets
September 19 th	Semi-empirical theories
September 21 st	DFT
September 26 rd	Solvation
September 28 th	Applications: Spectroscopy
October 3 th	Applications: Spectroscopy
October 5 th	Molecular Dynamics and Monte Carlo
October 10 th	Molecular Dynamics and Monte Carlo II
October 12 th	Molecular Dynamics and Monte Carlo III
October 17 th	Ensembles, periodic boundary conditions
October 19 th	“Equilibration” and “production” MD
October 24 st	Force Fields
October 26 th	Proteins and Nucleic acids
October 31 st	Proteins and Nucleic acids
November 2 nd	Implicit vs explicit solvation
November 7 th	Journal Club: “best practices in MD”

November 9 th	Advanced sampling techniques: umbrella sampling
November 14 th	Replica exchange
November 16 th	Markov State Models / Weighted ensemble
November 21 th	Applications: folding, binding
November 23 rd	Thanksgiving -- No class
November 28 th	Student Presentations
November 30 th	Student Presentations
Dec 5 th	Student Presentations
Dec 7 th	Student Presentations

Grading scale:

- A > 90
- A- 87.5 to 89.99
- B+ 82.5 to 87.49
- B 77.5 to 82.49
- B- 75 to 77.49
- C+ 72.5 to 74.99
- C 67.5 to 72.49
- C- 65 to 67.49
- D+ 62.5 to 64.99
- D 57.5 to 62.49
- D- 55 to 57.49
- E <60

Grade Values for Conversion

Grades	Grade Points		
A	4.0	D+	1.33
A-	3.67	D	1.0
B+	3.33	D-	.67
B	3.0	E	0
B-	2.67	WF	0
C+	2.33	I	0
C	2.0	NG	0
C-	1.67	S/U	0