Computational Chemistry
CHM6586 **(Fall 2020)**

Instructor: Coray Colina

Office Hours:
via Zoom: check zoom link via e-Learning, colina@chem.ufl.edu, 352-294-3488.

T period 4 (10:40-11:30) , or by appointment (please email the instructor for appointment).

Lectures (F2F: Room: CSE E231 , **Zoom:** check zoom link via e-Learning):
T Period 3 (9:35 AM – 10:25 AM),
Th Periods 3-4 (9:35 AM – 11:30 AM)

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

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

Course Website: This course has a Canvas page (e-learning) for notes and announcements.

F2F learning: We will have face-to-face (F2F) instructional sessions to accomplish the student learning objectives of this course. In response to COVID-19, the following policies and requirements are in place to maintain your learning environment and to enhance the safety of our in-classroom interactions.

- You are required to wear approved face coverings at all times during class and within buildings. Following and enforcing these policies and requirements are all of our responsibility. *Failure to do so will lead to a report to the Office of Student Conduct and Conflict Resolution*.
- This course has been assigned a physical classroom with enough capacity to maintain physical distancing (6 feet between individuals) requirements. Please utilize designated seats and maintain appropriate spacing between students. Please do not move desks or stations.
- Sanitizing supplies are available in the classroom if you wish to wipe down your desks prior to sitting down and at the end of the class.
- Follow your instructor's guidance on how to enter and exit the classroom. Practice physical distancing to the extent possible when entering and exiting the classroom.
- If you are experiencing COVID-19 symptoms (Click here for guidance from the CDC on symptoms of coronavirus), please use the UF Health screening system and follow the instructions on whether you are able to attend class. Click here for UF Health guidance on what to do if you have been exposed to or are experiencing Covid-19 symptoms**.**
- Course materials will be provided to you with an excused absence, and you will be given a reasonable amount of time to make up work. Find more information in the university attendance policies.

Online sessions: Our class sessions *may be* audio visually recorded for students in the class to refer back and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate orally are agreeing to have their voices recorded. If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

Course Description:
This course is an introduction to the field of computational chemistry and polymer science, providing an overview of current methods for modeling soft matter (polymers, surfactant solutions, etc.), nano-structured materials (nano-porous materials, etc.), and biomolecular systems (proteins, etc.) at the atomistic, meso and continuum scale levels.

Course Topics:
1. General overview of current methods for modeling soft matter (from quantum to the continuum). *2 weeks*.
2. Force fields. Contributions to intermolecular forces. Composite force fields. Parameterization of force fields. *2 weeks*.
3. Atomistic (molecular) simulation. General features. *3 weeks*.
4. Monte Carlo methods. Metropolis method. Isobaric, Grand, Gibbs ensembles. Reactive MC, free energies. *2 weeks*.
5. Molecular Dynamics methods. Constraint dynamics. Applications (e.g. proteins dynamics). 3 *weeks*.
6. Meso-scale simulation methods. Lattice MC. Brownian & Dissipative Particle Dynamics. Langevin Dynamics. Examples. *1 week*.
7. Continuum approach. Balance, phenomenological equations. Statistical Associating Fluid Theory. Overview, general features. Examples. *1 week*.

Course Objectives:
1. To provide students with an elementary understanding of the commonly used theoretical and simulation methods at the atomistic, meso and continuum scales.
2. To provide students with a basic knowledge to appreciate and understand the use of theory and simulation in research on fluids, soft matter, and nano-structured materials.
3. To provide students with the background and skills needed to read the simulation literature and evaluate it critically.
4. To teach students basic aspects in material chemistry modeling amenable to simulation, and to be able to identify on appropriate theory/simulation strategies to study them.
5. To teach students how the above material is related, so that they can make predictions for applications to fluids, interfaces, polymers, surfactants, colloids, nanostructured materials, biological systems.

Assessment Tools
1. Problem sets and homework that allow student collaboration and team-work.
2. Individual Projects.

Grading: Current UF grading policies for assigning grade points will be followed.

Software Use: All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Attendance: Lecture attendance is essential for your success in this class. However, we will not take roll. Repeated absence in class will make it very difficult to earn full participation points.

Disabilities: Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter, which must be presented to the instructor when requesting accommodations. Students with disabilities should follow this procedure as early as possible in the semester.

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; Visit the UF Health Emergency Room and Trauma Center website

Cell Phones: Please put all cell phones and other digital devices on "silent mode" during all class periods. During exams, your cell phone must be placed on the table in front of you, face down, for the entire test period.

Course evaluation: Students are expected to provide professional and respectful feedback on the

quality of instruction in this course by completing course evaluations online via GatorEvals. Click here for guidance on how to give feedback in a professional and respectful manner. 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 ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students here.

Honor Code: UF students are bound by The Honor Pledge which states,

"**We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code.**"

On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "***On my honor, I have neither given nor received unauthorized aid in doing this assignment.***"

The Honor Code specifies a number of behaviors that are in violation of this code and the possible sanctions. Click here to read the Honor Code. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.