Computational Chemistry
CHM6586 **(Fall 2017)**

Instructor: Coray Colina

Office Hours:
Room: WEIL 0408A, colina@chem.ufl.edu, 352-294-3488

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

Lectures (Room: WEIL 0408A):
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 for notes and announcements.

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. Force fields. Contributions to intermolecular forces. Composite force fields. Parameterization of force fields.
3. Atomistic (molecular) simulation. General features.
4. Monte Carlo methods. Metropolis method. Isobaric, Grand, Gibbs ensembles. Reactive MC, free energies.
5. Molecular Dynamics methods. Constraint dynamics. Applications (e.g. proteins dynamics).
6. Meso-scale simulation methods. Lattice MC. Brownian & Dissipative Particle Dynamics. Langevin Dynamics. Examples.
7. Continuum approach. Balance, phenomenological equations. Statistical Associating Fluid Theory. Overview, general features. Examples.

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.

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

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.

Honor Code: This class will operate under the policies of the student honor code, which can be found at: https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/

http://www.registrar.ufl.edu/catalog0809/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 by abiding by the Honor Code.***