Introduction to Computational Chemistry
CHM6586 (Fall 2019)

Course Description:
This course is an introduction to the field of computational chemistry, designed for graduate students and advanced undergraduate students. It will the cover theory and use of computational methods to study from small molecules (organic and inorganic chemistry), to soft matter (polymers, surfactant solutions, etc.), nano-structured materials (nano-porous materials, etc.), and biomolecular systems (proteins, etc.). We will introduce tools spanning atomistic, meso, and continuum scale levels. We will be using methods from quantum mechanics to classical mechanics.

Canvas e-learning site:
All communications must be done through the e-learning site, including homework, deadlines, grades and announcements. It is your responsibility to check this site for updates. Please do not email the instructors (or the TAs) personal email accounts.

Schedule:
Tuesdays: Period 3 (9:35 AM - 10:25 AM), Room WEIL 0408D
Thursdays: Period 3 - 4 (9:35 AM - 11:30 AM), Room WEIL 0408D

Professors:
Dr. Coray M. Colina. Leigh Hall, Room 354
Dr. Adrian E. Roitberg. Leigh Hall, Room 440

Office Hours: TBA

Textbooks (recommended):
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 Website: This course has a Canvas page for notes and announcements.

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. Introduction to software packages such as Gaussian.
7. Model building and molecular mechanics
8. Geometry optimization and potential energy surfaces
9. Semi-empirical molecular orbitals: Huckel, differential overlap approximations
10. Atomic orbital basis sets and electron integrals
11. Hartee-Fock and density functional calculations of bonding and properties
12. Optical, infrared and magnetic resonance spectra
13. Survey of electron correlation methods and sample results
14. Potential energy surfaces and reaction paths.
14. Solvation effects.

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 small molecules, 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 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 small molecule conformations, reactions, fluids, interfaces, polymers, surfactants, colloids, nanostructured materials, biological systems.

Assessment Tools
1. Problem sets and homework that allow student collaboration and team-work.
2. Group Projects (2or 3 students per group).

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.

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.***

GatorEvals:
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.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/.