

Computational Chemistry
CHM6586
Spring 16

Textbooks: 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)

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Office hours: Wednesday 10 am to noon, or upon request (send email to the instructor and/or TA).

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.

“Requirements for class attendance and make-up exams, assignments, and other work in this course are consistent with university policies that can be found at: <https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx>.”

Information on current UF grading policies for assigning grade points

This may be achieved by including a link to the web page: <https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>.

Academic Integrity

All University policies regarding academic integrity/academic dishonesty apply to this course and the students enrolled in this course. Team-work is encouraged for the laboratories provided that each team is comprised by 3 (max) people and the instructor is notified by email before each laboratory is started; otherwise, each student in this course is expected to work entirely on her/his own while taking any laboratory, to complete assignments on her/his own effort without the assistance of others, and to abide by University policies about academic integrity and academic dishonesty. Academic dishonesty can result in assignment of "F" by the course instructors or "XF" by Judicial Affairs as the final grade for the student.

Academic dishonesty is not limited to simply cheating on an exam or assignment.

Academic dishonesty includes, but is not limited to, cheating, plagiarizing, fabricating of information or citations, facilitating acts of academic dishonesty by others, having unauthorized possession of examinations, submitting work of another person or work previously used without informing the instructor, or tampering with the academic work of other students." Refer to the following URL for further details on the academic integrity policies:

In addition, any attempt to hack the homework server, any incidents of copying, saving, and/or transmitting materials from the on-line laboratories, and any attempts to tamper with the grades on CANVAS or the homework-server will be prosecuted through the academic integrity channels.

In addition, any attempt to hack the quiz server, any incidents of copying, saving, and/or transmitting materials from the on-line quizzes and homeworks, and any attempts to tamper with the grades on CANVAS or the quiz-server will be prosecuted through the academic integrity channels. The University and College guidelines can be found at the College Academic Integrity web site:

“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 (<http://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. 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.”

Accommodations for students with disabilities

The Office of Disability Services (www.dso.ufl.edu/dcr) requests and maintains disability-related documents; certifies eligibility for services; determines academic adjustments, auxiliary aids, and/or services; and develops plans for the provision of academic adjustments, auxiliary aids, and/or services.

“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 accommodation. Students with disabilities should follow this procedure as early as possible in the semester.”

Online course evaluation process

“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/>.”

Additional Information

Contact information for the Counseling and Wellness Center:

<http://www.counseling.ufl.edu/cwc/Default.aspx>, 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.