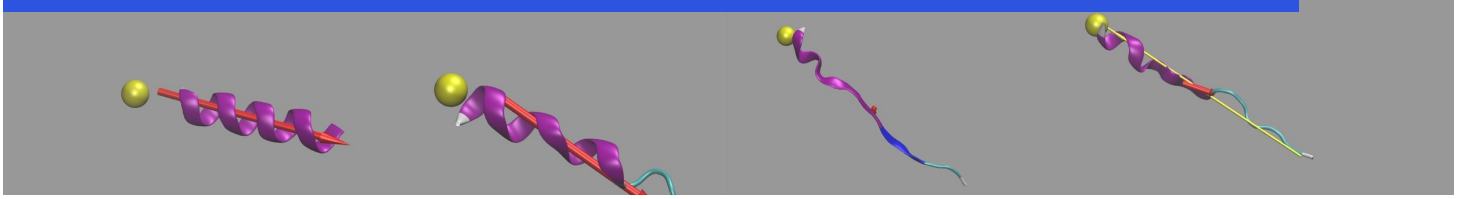
Introduction to Molecular Simulation CHEM 181



Course Description

This course enables chemistry and other science students to utilize computational tools for molecular simulation. Students who complete this class are able to understand the theory behind molecular dynamics and force-fields. In addition, students construct and execute molecular simulations using standard tools such as CHARMM, NAMD and VMD. Students then demonstrate an ability to analyze and present the data obtained from such simulations. Prerequisites: CHEM 025 and CHEM 027 with a grade of "C-" or better and permission of instructor.

This course is four (4) units. Students should expect to spend approximately seven hours a day, five days a week (or five hours a day, seven days a week), on coursework and assignments, and consulting with the instructor.

Although students may be physically present on campus, because this is an on-line course, Prof. McCallum will generally only interact with students via electronic means. This is to provide all students the same opportunity and quality of Prof. McCallum's attention.

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Canonical Text: Understanding Molecular Simulation by Frankel and Smit DOI: 10.1063/1.881812

This should be the first place you look for more detailed, specific information on simulation techniques. It is NOT required, as the lecture notes will be sufficient for the course. If you need one book on simulation, this is the one, however.

Course Goals

After successfully completing this course, students will understand the fundamentals of computer simulation: structure and coordinate files, basic theory of force fields, Newtonian molecular dynamics, equilibration and heating versus equilibrated systems, different solvation models, measurement, calculation, and display of dynamical information, visualization methods of both molecular systems and data, and an introduction to non-equilibrium molecular dynamics with a selection of advanced topics.

Student Responsibilities

Students are responsible for reading all the on-line text, viewing and comprehending the video lectures (two per week), completing all on-line tutorials (3-5 per week) and assignments (generally two formal assignments per week), any quizzes or other short assessment assignments (multiple times per week), and completing final project. By the first Tuesday of the first week, all required programs and files must be installed on the student's personal OS X

computer. Students are also required to attend any on-line chats or discussions that Dr. McCallum schedules for the course.

Student Learning Outcomes

- Understand fundamental concepts of thermodynamic and statistical mechanics necessary to competently prepare and perform modern molecular simulations.
- Understand the different file types required to describe molecules (proteins, peptides, etc) in a simulation
- Acquire, construct, and manipulate structural files using shell- and GUI-based (for example, VMD) tools
- Use VMD to manipulate and visualize molecular structure files (static and dynamic)
- Understand fundamental features of force-fields used in molecular dynamics
- Understand how to interpret and visualize molecular dynamics data
- Understand different solvation models and when they are useful
- Use actual molecular dynamics package NAMD to run simulations and acquire data
- Understand fundamental features of thermostats in simulations
- Understand simulation timing requirement

Course Schedule

Assignment Schedule

Week 1	Assignment 1	Due Thursday July 22 12:00 AM (Wednesday at midnight)
	Assignment 2	Due Sunday July 24 12:00 AM (Saturday at midnight)
	Quizzes 1,2	(On Canvas)
Week 2	Assignment 3	Due Thursday July 29 12:00 AM
	Assignment 4	Due Sunday July 31 12:00 AM
	Quizzes 3,4	(On Canvas)
Week 3	Assignment 5 (Double points)	Due Saturday Aug. 7 12:00 AM
	Quizzes 5,6	(On Canvas)
Week 4	Assignment 6	Due Thursday Aug. 12 12:00 AM
	Assignment 7	Due Sunday Aug. 14 12:00 AM
	Quizzes 7,8	(On Canvas)
Week 5	Quiz 9	
	Assignment 8 (Final Project)	Due Friday Aug. 20 12:00 NOON

Grading Breakdown	Weekly Assignments	20, 40 points	55% weight
	Quizzes	10 points	20%
	Final Project	@100	25%

Grading Scale: 93% A; 90% A–; 86% B+; 83% B; 80% B–; 76% C+; 73% C; 70% C–; 65% D.