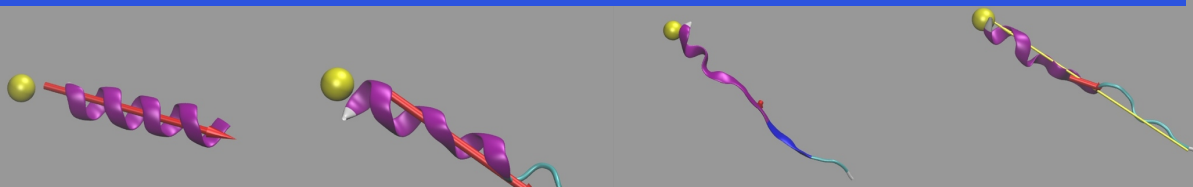


# Introduction to Molecular Simulation CHEM 181



## Course Description

This course enables Chemistry and other science students to utilize computational tools for molecular simulation. Students completing this class will be able to understand the theory behind molecular dynamics and force-fields. In addition, students will be able to construct and execute molecular simulations using standard tools such as NAMD, VMD and others. Students will demonstrate an ability to analyze and present the data obtained from such simulations. This course is four (4) units. Students should expect to spend three to four hours a day on coursework and assignments, and another five or so hours a week consulting with the instructor.

Professor C. Michael McCallum  
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Website: <http://www1.pacific.edu/~mmccallu/181>

## 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.

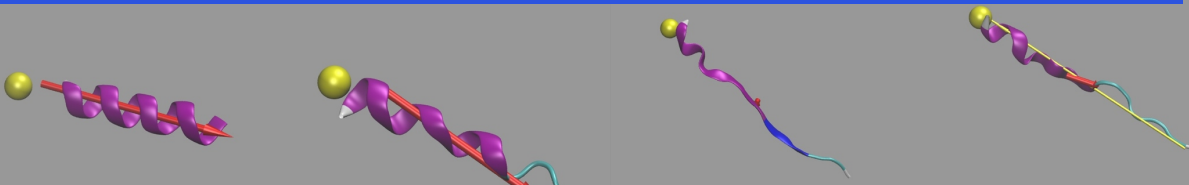
## Student Responsibilities

Students are responsible for completing all on-line tutorials and assignments (generally two formal assignments per week), any quizzes or other short assessment assignments, and the final project. Before the end of the first week, all required programs and files must be installed on the student's personal computer. Students are also required to attend any on-line chats or discussions that Dr. McCallum schedules for the course.

## Student Learning Outcomes

- 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)

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- 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 packages NAMD (and CHARMM) to run simulations and acquire data
- Understand basics of MMTSB toolset programming
- Understand simulation timing requirement

## Course Schedule

### Assignment Schedule

|               |                                 |                                                       |
|---------------|---------------------------------|-------------------------------------------------------|
| <b>Week 1</b> | Assignment 1                    | Due Thursday June 18 12:00 AM (Wednesday at midnight) |
|               | Assignment 2                    | Due Sunday June 21 12:00 AM (Saturday at midnight)    |
|               | Quiz 1                          | Sunday, June 21 (Sakai)                               |
| <b>Week 2</b> | Assignment 3                    | Due Thursday June 25 12:00 AM                         |
|               | Assignment 4                    | Due Sunday June 28 12:00 AM                           |
|               | Quiz 2                          | Sunday, June 28 (Sakai)                               |
| <b>Week 3</b> | Assignment 5<br>(Double points) | Due Saturday July 4 12:00 AM                          |
|               | Quiz 3                          | Sunday, July 5 (Sakai)                                |
| <b>Week 4</b> | Assignment 6                    | Due Thursday July 9 12:00 AM                          |
|               | Assignment 7                    | Due Sunday July 12 12:00 AM                           |
|               | Quiz 4                          | Sunday, July 12 (Sakai)                               |
| <b>Week 5</b> | Quiz 5                          | Wednesday, July 15 (Sakai)                            |
|               | Assignment 8<br>(Final Project) | Due Friday July 17 5:00 PM                            |

|                          |                    |            |     |
|--------------------------|--------------------|------------|-----|
| <b>Grading Breakdown</b> | Weekly Assignments | @20 points | 47% |
|                          | Quizzes            | @20        | 29% |
|                          | Final Project      | @80        | 24% |

### Grading Scale

|           |            |
|-----------|------------|
| <b>A</b>  | <b>93%</b> |
| <b>A-</b> | <b>90%</b> |
| <b>B+</b> | <b>86%</b> |
| <b>B</b>  | <b>83%</b> |
| <b>B-</b> | <b>80%</b> |
| <b>C+</b> | <b>76%</b> |
| <b>C</b>  | <b>73%</b> |

|    |     |
|----|-----|
| C- | 70% |
| D  | 65% |