

## **CME 327 Molecular Modeling for Chemical Engineers (Required)**

**Course Instructor:** *Dr. Dilip Gersappe*

**Website:** none

### **Course Goals:**

Introduction to molecular modeling techniques and simulation of complex chemical processes. Use of Monte Carlo methods and Molecular Dynamics methods. Special emphasis will be given to the simulation and modeling of biopolymeric systems.. [3 credits]

**Pre- or Corequisite(s):** ESG 111, AMS 261; AMS 361; PHY 132; CME 304; minimum of B- in CME 304

**Text(s):** *Computer simulation of liquids. A. Tiddlesey and B. Hall, Oxford University Press*

### **Class/ Laboratory Schedule:**

Spring: Lecture, Tuesday/Thursday 5:20-6:40 pm

### **Topics Covered:**

Week 1: Introduction to modeling in chemical systems

Week 2: Statistical mechanics – concept of ensembles

Week 3: Force fields and potentials

Week 4: Monte Carlo methods

Week 5: Constant pressure and Constant volume Monte Carlo

Week 6: Error analysis for Monte Carlo simulations

Week 7: Review and Mid-term

Week 8: Molecular Dynamics simulations

Week 9: Constant pressure and constant volume Molecular Dynamics

Week 10: Error analysis

Week 11: New advances in computer modeling

Week 12: New advances in computer modeling

Week 13: New advances in computer modeling

Week 14: New advances in computer modeling

Week 15: Review, final exam

**Contribution of course to meet professional component:**

**Relationship of course to program outcomes:**

<b>CTPC "3a-k" Outcomes</b>	<b>% contribution</b>
A. Ability to apply knowledge of math, engineering, and science	22%
B. Ability to design and conduct experiments, analyze data	22%
C. Ability to design system, component or process to meet needs	8%
D. Ability to function on multi-disciplinary teams	
E. Ability to identify, formulate, and solve engineering problems	22%
F. Understanding of professional and ethical responsibility	5%
G. Ability to communicate effectively	
H. Broad education	2%
I. Recognition of need and ability to engage in life-long learning	2%
J. Knowledge of contemporary issues	2%
K. Ability to use techniques, skills, and tools in engineering practice	15%
Any other outcomes and assessments?	
	100%

**Prepared by** \_\_\_\_\_

**Date Prepared:** \_\_\_\_\_