THE OHIO STATE UNIVERSITY
COLLEGE OF ENGINEERING

Molecular Dynamics Simulations

CBE 5780

Credit Hours:
3.00 - 3.00

Course Levels:
Undergraduate (1000-5000 level)
Graduate (5000-8000 level)

Course Components:
Lecture

Course Description:
Molecular dynamics simulations, especially as used in chemical engineering and soft materials science, from a practical perspective. Prior undergraduate courses in thermodynamics or statistical mechanics are recommended.

Prerequisites and Co-requisites:
Prereq: Jr standing or above in Engineering, Chemistry, or Physics; or Grad standing; or permission of instructor.

Course Goals / Objectives:
- After successful completion of the course students will: ? understand key statistical mechanical concepts relevant to molecular dynamics simulations
- ?be able to log in and submit jobs to a supercomputer
- ?be able to set up, run, and analyze molecular dynamics simulations
- ?have a foundation of knowledge of molecular simulations for use in your research or for further study

Course Topics:

- Statistical mechanics overview
- Molecular dynamics overview
- Data, inputs and outputs
- Software: LAMMPS and VMD
- Analysis methods, scripting
- Energy, temperature, and pressure
- Equilibration, mean squared displacement
- Coarse graining and mapping to real units
- Structural properties and calculations: g(r), S(k)
- Long-ranged interactions
- Dynamic properties and calculations
- Statistics, block averaging
- Dissipative particle dynamics

Designation:

Elective