Molecular M /W 5:30pm – 7pm or by appointment

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	316-978-6022 http://www.wichita.edu/gshwang M/W 7:00-8:35 pm, EB102 MATH 555 (Diff. Eqs. I), and ME 360C or AE 373 (Dynamics) or by instructor permission Basic knowledge of Matlab, Fortran, or C/C++ programming is preferred

Textbook: *Understanding Molecular Simulation: From Algorithms to Applications*, Academic Press, San Diego, by D. Frenkel and B. Smit, 1996

Course Description:

The aim of this course is to introduce the molecular simulation methods (classical molecular dynamics simulations and Monte-Carlo simulation) aiming at understanding fundamentals of the nanoscale mechanical, thermal, materials, energy, and bio systems and their engineering for desired functionalities. This course also includes the basics of the statistical thermodynamics (mechanics) and various key computer programing/simulation techniques.

Objectives:

a) To understand the fundamental knowledge of atomic-scale mechanical, material, and energy systems;

b) To make sound judgments on the quality of molecular simulation studies in the literature;

c) To decide whether molecular simulation is suited for application to the student research;

d) To know how to begin developing a simulation program applicable to the student research;

e) To understand the workings and limitations of commercial molecular simulation software.

Grading:

Homework	50%
Project Proposal Presentation	10%
Project Proposal Writing	10%
Final Oral Presentation	10%
Final Project Report	20%

Reading assignments & homework:

Project:

Tentative Class Schedule (subject to changes)

Week	Date	Subject	Remark
1	8/17	Introductions and Overview	
	8/19	Review: thermodynamics	
2	8/24	Statistical thermodynamics: equilibrium and thermodynamic properties	
	8/26	Statistical thermodynamics: ensemble average	
3	8/31	Statistical thermodynamics: ideal gas and equation of state	
	9/2	Statistical thermodynamics: applications	Project
4	9/7	No class (labor day)	
	9/9	Basics of molecular dynamics algorithm and programming methods	
5	9/14	Introduction to molecular dynamics simulation (commercial) codes	
	9/16	Interatomic potentials: hard sphere, LJ, SW potentials	
6	9/21	Intraatomic potentials: harmonic potential, bond, angle, and torsion	
	9/23		