Chemical & Biomolecular Engineering 631

Statistical Mechanics

Fall 2010

Tuesday 5:00 – 8:00 p.m.

DO 314

Lecturer: Dr. Stephen J. Paddison

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Office Hours: By appointment.

Textbook: Donald A. McQuarrie, Statistical Mechanics

Other Reference Books: (1) Mark E. Tuckerman, Statistical Mechanics: Theory and Molecular Simulation; (2) J.-P. Hansen and I. R. McDonald, Theory of Simple Liquids;

Lectures: Typically Tuesdays at 5:00 PM; Dougherty 314. Other lecture times arranged at mutual convenience with students and lecturer. There will be at least 2 guest lectures during the semester.

Examinations: There will be no examinations in this course.

Homework Problems: There will be no assignments in this course.

Grading:

Oral Presentation	50 %
Report	25 %
Participation	25 %

Final letter grades will be assigned according to the following scale: 85-100% = A, 70-84% = B, 55-69% = C, 40-54% = D, below 40% = F.

Course Objectives: Statistical mechanics is the study of macroscopic systems from a micro or molecular point of view. Statistical mechanics is the theory with which one may analyze the behavior of natural or spontaneous fluctuations. This theory allows one to understand the magnitudes and time scales of these fluctuations and the concomitant stability or instability of structures that spontaneous fluctuations inevitably destroy. The goals of statistical mechanics are the understanding and prediction of macroscopic phenomena and properties from individual molecules, atoms, or particles that make up the system.

Topics: This is an advanced graduate course and builds on the material covered in CBE 532, Statistical Thermodynamics. As such the students will be expected to demonstrate independent learning of topics and the presentation (oral & written) of a selected topic. There will be material presented on 2 or 3 advanced topics (see below) by the lecturer, but there will be choice of topics for which the student will be expected to select one topic for an in depth learning.

Covered in Lectures

(1) Classical Monoatomic Liquids: distribution functions
(2) Kinetic Theory of Gases: Boltzmann equation and beyond
(3) Transport Processes: Brownian Motion, Langevin equations
(4) Time Correlation Functions: Formalism and Applications

Independent Topics

(5) Theory of Liquids
(6) Statistical Mechanics of Polymers
(7) Statistical Mechanics for Molecular Simulation
(8) Other Topics (to be discussed and agreed upon with lecturer)

Oral Presentation: Each student will give a 90 minute presentation on their selected topic. There will be a 10-15 minute question and question period following the presentation where fellow students and the lecturer will participate. The presentations will be scheduled during the last 3 weeks of the course.

Report: A report must be handed in at the conclusion of the course (exact date to be announced) that covers the topic the student studied and also summary of the guest lectures.

Guest Lectures: We will have at least 2 guest lectures from prominent individuals in the field of statistical mechanics. Oct. 5th: Prof. Mark E. Tuckerman: use of statistical mechanics in molecular simulation; Nov. 23rd: Prof. Lawrence R. Pratt: theory of liquids and quasi-chemical theory.