Introduction to Statistical Thermodynamics (Ch/ChE 164) Winter 2007

Instructor:

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TAs:

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Course Designation:

Required for Ph. D. students in chemical engineering; elective for students seeking a master degree.

Catalog Description:

An introduction to the fundamentals and simple applications of statistical thermodynamics. Foundation of statistical mechanics; partition functions for various ensembles and their connection to thermodynamics; fluctuations; noninteracting quantum and classical gases; heat capacity of solids; adsorption; phase transitions and order parameters; linear response theory; structure of classical fluids; computer simulation methods.

Prerequisite:

Ch21abc or equivalent.

Text and References:

Principal textbooks: T. L. Hill, *Introduction to Statistical Mechanics* (Addison-Wesley, 1960) (A Dover edition is also available) and D. Chandler, *Introduction to Statistical Mechanics* (Oxford Univ. Press, 1987). Other references: D. A. McQuarrie, *Statistical Mechanics*; L. E. Reichl, *A Modern Course in Statistical Physics*; M. Plischke and B. Bergersen, *Equilibrium Statistical Mechanics*; L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Part I); K. A. Dill and S. Bromberg, *Molecular Driving Forces – Statistical Thermodynamics in Chemistry and Biology*.

Course Objectives:

To provide the microscopic (molecular) understanding of the thermodynamic behavior and properties. Specifically to connect the various thermodynamic functions (entropy, pressure, Helmholtz free energy, etc.) to the underlying statistical description (i.e., partition functions).

Relationship to Program Goals:

Modern chemical engineering has been shifting steadily toward a molecularly based discipline, where molecular design is an essential component both in the industrial base of our profession (pharmaceuticals, fine chemicals, advanced materials, etc.) and in the academic chemical engineering research. This molecular focus demands an understanding of the relationship between properties of matter and their microscopic (molecular) characteristics. Statistical thermodynamics provides the connection between the macroscopic, thermodynamic behavior to the molecular constitution and interactions.

This course is primarily aimed at Ph. D. students in chemical engineering, but also serves as an advanced science/engineering elective for master students. In addition, usually there are 1 or 2 senior undergraduate students taking this course.

Topics Covered:

1. Preliminaries: fundamentals of classical and quantum mechanics, fundamentals of thermodynamics, elementary probability theory;
2. Formulation of statistical mechanics: postulates of statistical mechanics; derivation of various ensembles; connection to thermodynamics; statistical fluctuations; equivalence of ensembles;
3. Simple applications: Bose-Einstein gas, Fermi-Dirac gas, Maxwell-Boltzmann gas, heat capacity of solids;
4. Classical statistical mechanics: Phase space, Maxwell velocity distribution, equipartition theorem;
5. Non-interacting systems: diatomic gases, chemical reaction equilibrium, Langmuir adsorption isotherm;
6. Interacting systems: lattice models, mean-field (self-consistent) theory, statistical thermodynamic variational principle, exact solution for 1-dimentional models;
7. Correlation and response functions: linear response theory;
8. Classical fluids: distribution functions, structure factor S(k) (or pair correlation function g(r)), measuring S(k), approximate schemes for calculating g(r);
9. Computer simulation: molecular dynamics, Monte Carlo method and importance sampling.

Class Schedule:

Lectures: T Th 10:00-11:30; TA sessions MW 4-6.

Grading:

Credit of the course will consist of three parts: the homework, the final exam, and the projects.