# Advanced Thermodynamics CHM 541/ /MSE524

Syllabus Fall, 2009

**Class Meetings:** MWF 11:50 am - 12:40 pm; ECG 227

**Instructors:** Jeff Yarger (jyarger@gmail.com) & William T. Petuskey (wpetuskey@asu.edu)
Office: ISTB1 470 & PS-D202 or D101
Office hours: Mon 4:45-6:00 pm
Wed 12:40-1:30 pm

**Teaching Assistant:** Grace(Hee-joung) Joun (hjoun@asu.edu)
Office: PSC 34 (basement)
Office hours: TuTh 11:00-12:00pm, or by arrangement

**Textbook:** *Physical Chemistry, 2nd Edition* (or *Matter in Equilibrium: Statistical Mechanics and Thermodynamics, 2nd Edition*)
by R. Berry, S. Rice and J. Ross
ISBN: 0195105893 (or 0195147499)

Other recommended or alternative textbooks include:
(1) Introduction to the Thermodynamics of Materials, by D. Gaskell
(2) Thermodynamics and an Introduction to Thermostatistics, by H. Callen
(3) Introduction to Modern Statistical Mechanics, by D. Chandler

**Course Description:**

This course emphasizes the application of thermodynamics to chemical systems. Although attention will be given to the intrinsic thermodynamic state of solids, liquids and glasses, most of the course will concentrate on the interactions between matter in relation to chemical reactions, phase transformations and phase stability. There will also be examples of biological systems. The course seeks to teach students to apply thermodynamics to real problems, to teach them how to estimate where basic information is scarce and how to interpret thermodynamic information in the context of case studies. Students are expected to learn and use one of the ASU site-licensed computational packages (e.g., Matlab, Maple or Mathematica) for application to specific thermodynamic problems. The course will discuss data resource gathering and the use of computer codes for multicomponent-multiphase systems.

**Mathematical Analysis Software**

Most scientific and engineering problems in the real world cannot be solved analytically, but require a numerical estimate of the answer. Some of the problems you will be faced with in this course, especially in the later two thirds, will require you to use a mathematics program (i.e., Mathematica™, MatLab™, Maple™). We strongly encourage you to learn how to use at least one of these packages.

The University has licenses for online versions of all three programs. These can be accessed through the "Mathematics and Statistics" link of the University Technology Office software web site, http://software.asu.edu/. A license for downloading Mathematica™ directly to your computer can also be purchased. Student versions can also be purchased at significantly discounted prices at the store located in the computer commons. Finally, the Department of Chemistry and Biochemistry's graduate student computer facilty has copies installed.

**Basis for Grades:**

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|---|---|---|
| | Midterm Exam #1 (in class & takehome) | 20% |
| | Midterm Exam #2 (in class & takehome) | 20% |
| | Homework | 30% |
| | Project | 30% |

**Tentative Exam Schedule:**

1st Midterm: Wednesday, October 7th
2nd Midterm: Monday, December 7rd.
Projects Due: Monday, December. 14th

**Study Groups and Class Interaction:**

Thermodynamics, like many areas of physical chemistry, is a demanding course that is best learned by working lots and lots of problems. You are strongly urged to form study groups of two or three people and work on homework together. In addition, problems will be presented in class for you and your study group to solve and discuss before the end of the period. There will be a series of case studies that will require you to conduct extensive mathematical calculations.

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**Topical Outline for Fall, 2009**

***Prof. Yarger***

**I. Thermodynamic Laws and Relationships (Chapters 12-19)**

- A. Definitions of systems, state functions and variables
- B. First, Second and Third Laws of Thermodynamics
- C. Relationships of Thermodynamic Properties: Maxwell's relations, Gruneisen's and compressibility relations, magneto- and electro-caloric effects
- D. Thermochemistry and its Applications.
- E. Nature of Equilibrium

**II. Aspects and Applications of Statistical Thermodynamics (Chapters 15-17)**

- A. The Partition Function
- B. Calculation of Thermodynamic Functions and Properties: Einstein and Debye Approximations of simple crystals, regular and subregular solutions, point defects, solid solutions with multiple sublattices, order-disorder transformations
- C. Electronic Contributions

***Prof. Petuskey***

**III. Thermodynamic Properties of Solids, Liquids and Gases: Data, Trends and Methods of Estimation (Chapters 20-23)**

- A. Rules of standard states and reference states (common uses and methods of conversion)
- B. Tabulation of thermodynamic data
- C. Trends in bonding enthalpy and entropy in solids, liquids and gases
    - a. Empirical and theoretical treatments
    - b. *Ab initio* methods
- D. Solution Thermodynamics
    - a. Regular and subregular solutions models
    - b. Molecular solutions: Margules, van Laar, and Wilson treatments
    - c. Aqueous electrolyte solutions: Debye and Pitzer treatments
    - d. Ternary and higher order solutions: polynomial and sublattice models, Kohler/Toop and Muggianu interpolations; Wagner Interaction Formulism

**IV. Phase Equilibria: Multicomponent and Multiphasic Systems (Chapters 19, 24)**

- A. Generalized phase rules,
- B. Phase diagrams, stability diagrams and other diagram types
- C. Computational methods: energy minimization versus mass action techniques; SOLGASMIX and FactSage® codes

**V. Special Topics (Chapters 25-26)**

- A Electrochemistry in solids and liquids (electrolyte and nonelectrolyte systems)
- B. Defect chemistry: thermodynamics of point defects and electronic defects in dilute and large concentrations (Boltzmann and Fermi-Dirac statistical systems)
- C. Surfaces and Interfaces
- D. Applications of computational thermodynamics to kinetics (CVD and diffusion)