CHM 6461: Introduction to Statistical Thermodynamics, Spring 2016

Instructor: Prof. Russ Bowers
Office: NPB 2360
Email: bowers@chem.ufl.edu
Office Hours: MW, 2:00-3:00pm or by appointment
Meeting Place and Time: TUR 2334, TR periods 2-3

Required Text: Terrell L. Hill, An Introduction to Statistical Thermodynamics (Paperback), Dover Publications (January 1, 1987) ISBN-10: 0486652424, ISBN-13: 978-0486652429

Important: Not all material presented during the lectures will follow this book! The lecture notes and exercises will also draw on the following auxilliary texts

Donald A. McQuarrie, Statistical Mechanics (Hardcover), Publisher: University Science Books; 2nd edition (May 2000), ISBN-10: 1891389157, ISBN-13: 978-1891389153.

Roger Bowley and Mariana Sanchez, Introductory statistical mechanics, Oxford Science Publications, Clarendon Press, Oxford, 2001,ISBN-13: 978-0198505761.

H. B. Callen, Thermodynamics and an introduction to thermostatistics, 2nd edition, John Wiley & Sons (1995).

Michel Le Bellac, Fabrice Mortessagne and G. George Batrouni, Equilibrium and Non-Equilibrium Statistical Thermodynamics, Cambridge University Press (available as ebook), eISBN: 9780511193705

Course Description

This course deals with the fundamentals of statistical thermodynamics with emphasis on molecular and chemical systems. We will introduce the probability and statistical laws, and derive thermodynamic relations from the statistical principles. Statistical mechanics connects the properties of the macroscopic material world to the basic constituents of matter at the deepest level. In this course we will study the interactions that govern the behavior of ensembles of atomic or molecular systems. These laws are statistical in nature, and the notion of probability will play an essential role. As a matter of fact, we will see that the laws of statistical physics are a statement about our incomplete knowledge of all the dynamical information about a many particle system. The interdisciplinary nature of statistical thermodynamics will be demonstrated throughout the course by studying problems that arise in material science, chemistry and biology.

Math Background

Although the course does not require any difficult math, you are expected to be familiar with:

- Differentiation and integration of elementary functions
- Taylor series
- Partial derivatives
- Infinite sums and products

Mathematica Software

Solutions to many of the homework problems are facilitated by Wolfram's Mathematica software package. Many examples and problems will be worked using this software, and students are encouraged to become proficient in this software. Access to Mathematica is available free of charge to all UF students through the UFApps platform: http://info.apps.ufl.edu/ or the student version may be purchased at https://www.wolfram.com/mathematica/pricing/students.php.

Grading

Homework assignments: 20%; Exams: 70%; class participation: 10%.
There will be a final exam, scheduled for April 25th. The final exam will constitute 35% of the total grade. There will also be two in-class exams. The higher score of the two in-class exams will constitute 35% of the total grade.

From the net numerical grade, a letter grade is computed. The grade limits will not be stricter than the following: 60% for a C minus, 70% for a B minus, and 80% for an A minus.

MAKE-UP EXAMS: Must be arranged in advance of the scheduled date. No make-up exams are allowed otherwise except for emergency situations.

Homework

Assignments will be distributed on Tuesday or Wednesday and will be normally due Tuesday of the following week, prior to the lecture. Solutions to the homework will be distributed after the problems have been collected. No late homework will be accepted!

Homework problems are a very important part of the course. The only way to learn the subject is to practice it as much as possible. Working problems is the only way to obtain a detailed understanding of the topic.

Attendance

Attendance of lectures and office hours is expected. In many instances (and as time allows), the 2-period class will combine a traditional lecture with discussion of problems. Reading the material BEFORE lecture time is paramount to keep up with the fast pace of the course. In addition to the 3 hrs class/week, ~8 hrs/week of reading, homework and general study are required.

Academic Integrity

You are encouraged to discuss the homework problems with your classmates. However, the final work you turn in must be your own. There is a distinction between discussing the work, and merely copying someone else's work. The idea here is that you should help each other to understand the problems and the concepts involved; you will learn more if you work on the assignments in groups and explain the methods to each other. You must engage in your own effort on solving the problems.

The student honor code can be found at
http://www.registrar.ufl.edu/catalog/policies/students.html

The students and instructor are honor bound to comply with the Honors Pledge: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

Students with disabilities

Students requiring special accommodations need to register at the Dean of Student Offices and bring the documentation to the instructor.

Course Evaluation

Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at https://evaluations.ufl.edu. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open.

Tentative Schedule:

WEEK	TOPIC	READING
1/4	Ensembles and Postulates	Hill 1.1-1.2
1/11	Canonical Ensemble and Thermodynamics	Hill 1.3-1.4
1/18	(MLK Day, No lecture on Jan 18) Grand Canonical Ensemble Microcanonical Ensemble	Hill 1.5-1.7
1/25	Fluctuations Second and Third Laws of Thermodynamics	Hill 2.1-2.4
2/1	Boltzmann Statistics, distribution function and Entropy	Hill 3.1-3.4
2/8	Ideal Monatomic Gas Internal Degrees of Freedom	Hill 4.1-4.4
2/11	**Exam 1**	
2/15	Molecular Partition Functions Ideal Diatomic Gas Vibrational, Rotational	Hill 8.1-8.4
2/22	Homonuclear Diatomics Ideal Polyatomic Gas	Hill 9.1-9.4 Hill 22.8
2/29	**Spring Break, no classes**	
3/7	Quantum Statistics Fermi-Dirac gas, electrons in metals, Ideal Bose-Einstein gas: helium	Hill 22.1-22.4
3/14	Monatomic Crystals (Einstein)	Hill 5.1-5.2
3/15	**Exam 2**	
3/21	Vibrations in Monatomic Crystals (Debye)	Hill 5.3-5.4
3/28	Chemical Equilibrium	Hill 10.1-10.4
4/4	Rates of Chemical Reactions	Hill 11.1-11.3
4/11	Absolute Rate Theory	Berry, Rice & Ross 30.6-30.7 (p 911-919)
4/18	Absolute Rate Theory Examples	
4/25	**Exam 3**	