004:231:001 Statistical Thermodynamics I

INSTRUCTOR: Prof. Claudio J. Margulis

Office: 118 IATL

Phone: office, 335-0615

Office Hours: T-Th 10:45-12:15 AM in 118 IATL. All other meetings by appointment only.

E-mail: claudio-margulis@uiowa.edu

LECTURES: 9:30A - 10:45A T-Th in 140 BHC. Attendance is required.

COURSE DESCRIPTION: This course will cover the subject of quantum and classical statistical thermodynamics. The course will mainly focus on systems in equilibrium but some limited non-equilibrium topics such as time correlation functions will be introduced.

1) To prepare and be successful for the close book tests, you must become proficient in solving problems and understanding the underlying theory behind them.

2) Sometimes a particular topic is more clearly explained in one book than in some other. Several textbooks on this topic are available. We will not follow one particular book in this course; however, a list of textbooks that I have used to prepare lectures appears later on this syllabus with their corresponding ISBN #.

3) This course is demanding; we will cover a large amount of material this semester. You must spend enough time to keep up with the lectures. If you fall behind it will be very hard to catch up because topics are interconnected. You will not be able to study for this class the night before an exam and expect to do well.

TEXTBOOKS: (recommended but not required)

Thermodynamics and an Introduction to Thermostatistics, 2nd Edition by Herbert B. Callen
Publisher: Wiley; 2 edition (August 29, 1985)
ISBN: 0471862568
(This book is used only during the first couple of weeks as a refresher on classical thermodynamics)

Introduction to Modern Statistical Mechanics by David Chandler
Publisher: Oxford University Press (September 1, 1987)
ISBN: 0195042778
(Much of the first part of this course is based on this book, however not all topics that will be discussed in class are covered)

Statistical Mechanics by Donald A. McQuarrie
Publisher: University Science Books; 2nd Ed edition (February 1, 2000)
ISBN: 1891389157
(This book covers nearly all the topics in this course and will be used extensively throughout the semester)

Statistical Mechanics: Principles and Selected Applications by Terrell L. Hill
Publisher: Dover Publications (August 1, 1987)
ISBN: 0486653900
(A classic, and still an excellent source for the equilibrium topics covered in this course)

Dynamic Light Scattering: With Applications to Chemistry, Biology, and Physics by Bruce J. Berne, Robert Pecora
Publisher: Dover Publications; Unabridged edition (August 1, 2000)
ISBN: 0486411559
(This is an advanced text book, difficult to read for the beginner. Only a few concepts from this book will be introduced in course)

If you wish to purchase a book I suggest either McQuarrie’s or Chandler’s book. I own a copy of all of the above books. These books will be available for checkout from my office for a maximum period of 2 hours at a time.

GRADING: The final course grade will be based on the following components:

Problem sets 20 %

2 Exams 20 % each (total 40%)

Final Project 40%

EXAMINATIONS: There will be 2 in-class exams and a final project. Exams are closed-book. Exams will be held on March 11 and April 29. The final project is due on Thursday, May 13, 2010 at 10:45 AM but can be submitted any time before this deadline. For each exam, emphasis will be placed on material covered since the preceding exam, however it is very important to understand that the material covered later in the course requires the application of concepts learned earlier. Announcements will be made in class regarding the material to be covered on each exam. All exams must be written in ink, but not red or erasable ink. Exams on which white-out was used or exams written in pencil, red or erasable ink will not be regraded. Exams will be returned in class as soon as possible.

Make-up exams must be arranged with the instructor and are only available in the event of a university recognized excuse (e.g. a documented medical emergency). Under no
circumstances will a make-up exam be given to take the place of a regular exam taken earlier. Scheduling of exams or classes in other courses is not an acceptable reason for taking a make-up, since the exam periods are already reserved in your schedule.

If you feel that an error was made in the grading of an exam, you may request a re-grade by notifying the instructor within one week of receiving the graded material. The request should be in writing and indicate the section of the exam that is in question. Please note that the entire examination will be subject to a regrade. No regrades after one week. No regrades for 1 point.

FINAL PROJECT: As part of this course you need to complete a final project. The final project which will most likely be relevant to your research must be agreed upon you and the instructor (me). By February 25 you must come up with one or more ideas that are related to theoretical chemistry and can be done computationally or analytically (i.e. with pencil and paper). During office hours we will outline a plan of action so that these can be completed by the project deadline. Hopefully this will provide you with skills that you can continue using for your research in the future.

HOMEWORK: Unless otherwise announced in class, a problem set will be due exactly one week after it was assigned (for example if the homework is assigned on Tuesday it will be due the following Tuesday at the beginning of class). The problem sets should represent the students own work. (Please see the section in the Student Academic Handbook on Rights and Responsibilities for University policy on academic misconduct). Late assignments and assignments submitted by email will not be accepted. Exceptions to the late assignment rule will only be made in the case of a valid excuse as described in the examinations section above. The homework assignments must be securely fastened with a staple. The problem sets are subject to the same regrade policy as for examinations, as described above.

*Administrative Home*

The College of Liberal Arts and Sciences is the administrative home of this course and governs matters such as the add/drop deadlines, the second-grade-only option, and other related issues. Different colleges may have different policies. Questions may be addressed to 120 Schaeffer Hall, or see the CLAS Student Academic Handbook.

*Electronic Communication*

University policy specifies that students are responsible for all official correspondences sent to their University of Iowa e-mail address (@uiowa.edu). Faculty and students should use this account for correspondences. (Operations Manual, III.15.2. Scroll down to k.11.)

*Accommodations for Disabilities*

A student seeking academic accommodations should first register with Student Disability Services and then meet privately with the course instructor to make particular arrangements. See www.uiowa.edu/~sds/ for more information.
*Academic Fraud*
Plagiarism and any other activities when students present work that is not their own are academic fraud. Academic fraud is a serious matter and is reported to the departmental DEO and to the Associate Dean for Undergraduate Programs and Curriculum. Instructors and DEOs decide on appropriate consequences at the departmental level while the Associate Dean enforces additional consequences at the collegiate level. See the CLAS Academic Fraud section of the *Student Academic Handbook*.

*CLAS Final Examination Policies*
Final exams may be offered only during finals week. No exams of any kind are allowed during the last week of classes. Students should not ask their instructor to reschedule a final exam since the College does not permit rescheduling of a final exam once the semester has begun. Questions should be addressed to the Associate Dean for Undergraduate Programs and Curriculum.

*Making a Suggestion or a Complaint*
Students with a suggestion or complaint should first visit the instructor, then the course supervisor, and then the departmental DEO. Complaints must be made within six months of the incident. See the CLAS *Student Academic Handbook*. Our departmental DEO is Prof. Wiemer (E331 Chemistry Building, 319-335-1350)

*Understanding Sexual Harassment*
Sexual harassment subverts the mission of the University and threatens the well-being of students, faculty, and staff. All members of the UI community have a responsibility to uphold this mission and to contribute to a safe environment that enhances learning. Incidents of sexual harassment should be reported immediately. See the UI *Comprehensive Guide on Sexual Harassment* for assistance, definitions, and the full University policy.

*Reacting Safely to Severe Weather*
In severe weather, class members should seek appropriate shelter immediately, leaving the classroom if necessary. The class will continue if possible when the event is over. For more information on Hawk Alert and the siren warning system, visit the Public Safety web site.

*These CLAS policy and procedural statements have been summarized from the web pages of the* College of Liberal Arts and Sciences *and The University of Iowa* Operations Manual.*
TENTATIVE OUTLINE OF THE COURSE

1) Review of macroscopic thermodynamics. Fundamental laws, maximum and minimum principles for the entropy and different free energies, the Gibbs-Duhem equation, Legendre transformations.

2) Introduction to equilibrium statistical mechanics. Ensembles, partition functions and the connection with thermodynamics.

3) Bose-Einstein, Fermi-Dirac and Boltzmann statistics.

4) Classical statistical mechanics. Reduced distribution functions. Thermodynamics from g(r).

5) Perturbation theory and the Van der Waals equation.

6) Time correlation functions.

7) Some other more advanced selected topics that will be cover if we have time. (Monte Carlo sampling, path integral formulations, etc.)