CHEM:5431-- Statistical Thermodynamics I  
LECTURES: 11:00A - 12:15P TTh 30 SH. Attendance is mandatory.  
Department of Chemistry: chem.uiowa.edu  

Course ICON site: To access the course site, log into Iowa Courses Online (ICON) https://icon.uiowa.edu/index.shtml using your Hawk ID and password.  

Course Home  
For Undergraduate Courses: The College of Liberal Arts and Sciences (CLAS) is the home of this course, and CLAS governs the add and drop deadlines, the “second-grade only” option (SGO), academic misconduct policies, and other undergraduate policies and procedures. Other UI colleges may have different policies.  
For Graduate Courses: The College of Liberal Arts and Sciences (CLAS) is the home of this course, and CLAS governs the policies and procedures for its courses. Graduate students, however, must adhere to the academic deadlines set by the Graduate College.  

INSTRUCTOR: Claudio J. Margulis  
OFFICE: 244 IATL  
PHONE: 5-0615  
Office Hours: W 1:00 pm- 4:00pm in 244 IATL. All other meetings by appointment only. E-mail: claudio-margulis@uiowa.edu  

DEO: MacGillivray, Leonard R; len-macgillivray@uiowa.edu  

COURSE DESCRIPTION/LEARNING OBJECTIVES: 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. See below tentative course outline.  

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, an abbreviated list of text books 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 and practice problems.
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 few weeks as a refresher on classical thermodynamics)

Introduction to Modern Statistical Mechanics by David Chandler Publisher: Oxford University Press (September 1, 1987)
ISBN: 0195042778
(This book covers most of the material and I may choose homework problems from it as well as other sources.)

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 is also an excellent source to study from.)

I have a copy of all of the above books. If you plan on purchasing a book it may be advantageous to borrow these from me first to see which one you like best. These books will be available for checkout from my office for a maximum period of 2 hours at a time.

Academic Honesty and Misconduct
All students in CLAS courses are expected to abide by the CLAS Code of Academic Honesty. Undergraduate academic misconduct must be reported by instructors to CLAS according to these procedures. Graduate academic misconduct must be reported to the Graduate College according to Section F of the Graduate College Manual.

A NOTE ON COLLABORATION

Collaboration in this course is encouraged except, of course, during exams.

Student Complaints
Students with a complaint about a grade or a related matter should first discuss the situation with the instructor and/or the course supervisor (if applicable), and finally with the Director or Chair of the school, department, or program offering the course.

Undergraduate students should contact CLAS Undergraduate Programs for support when the matter is not resolved at the previous level. Graduate students should contact the CLAS Associate Dean for Graduate Education and Outreach and Engagement when additional support is needed.
Drop Deadline for this Course
You may drop an individual course before the deadline; after this deadline you will need collegiate approval. You can look up the drop deadline for this course here. When you drop a course, a “W” will appear on your transcript. The mark of “W” is a neutral mark that does not affect your GPA. Directions for adding or dropping a course and other registration changes can be found on the Registrar’s website. Undergraduate students can find policies on dropping and withdrawing here. Graduate students should adhere to the academic deadlines and policies set by the Graduate College.

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

2 Exams 30% each (total 60%)
Final Computational/Stat. Thermo. Project 40% (described below)

EXAMINATIONS: There will be 2 in-class exams and a final project. Exams are closed-book. Exams will be held on October 20 and November 17. The final project write-up is due on November 15 but can be submitted any time before this deadline. The four lectures starting on November 29 are reserved for students to present their projects to the rest of the class. The time allotted for each presentation will be discussed in class. The combination of your project write-up and presentation is what will be considered for grading as “Final Project”. 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 if you want them to be regraded. Exams will be returned in class as soon as possible.

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.

FINAL PROJECT: As part of this course you need to complete a final project. The final project which you make choose to make relevant to your own future research must be agreed upon you and the instructor (me) by September 27. Notice that you cannot choose your own current research work as the project. It is important that we meet more than once before September 27 because it is possible that your idea of what is doable computationally as part of course work may be erroneous. The project should be challenging but not overly tolling, in other words it must be compatible with the workload of a graduate course. Your project must, to some extent, make contact with ideas related to the material presented in this course. Before I can approve your topic, you must demonstrate that you have acquired or at least thoroughly researched the tools and instruments that will enable the project to be completed successfully. By this I mean anything from input files, force field parameters,
hardware access or other things needed to see your project through. **I expect a write-up by September 27** describing what will be done and how it will be done. Feel free to discuss possible topics of interest with your research advisor if you so wish. The intention is that this project will provide skills that you can continue using for your research in the future. Please start work on the project early. I will not police this, but I guarantee that you will not be able to learn how to run simulations or write code in one or two weeks. Do not expect me to provide a project topic, set up your simulations or provide input files, this is your job. You must read scientific literature, software manuals, discussion forums or whatever else is needed to complete your project including learning how to program if this is needed. Unless you plan to install software and run simulations in your own computer or those in your research group, I suggest that during the **first week of class** you contact the high-performance computing administrators (for example Dr. Sai Ramadugu) with our course # and indicate you need an account on the chemistry queue. Please, be mindful of the fact that even the simplest task of using such machines will require learning the basics of Unix and protocols for job submission in queues; in other words, just getting started implies a time commitment.

HOMEWORK: Ungraded suggested problems will be posted on ICON through the semester. I will also post solutions to the problems assigned. Whereas your homework is not graded, it is important that you practice for the exams, these will provide the best way to achieve this. Do not skip working on these problems.

**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.
College of Liberal Arts and Sciences (CLAS) Course Policies

Attendance and Absences
University regulations require that students be allowed to make up examinations which have been missed due to illness or other unavoidable circumstances. Students with mandatory religious obligations or UI authorized activities must discuss their absences with me as soon as possible. Religious obligations must be communicated within the first three weeks of classes.

Exam Policies

Communication: UI Email
Students are responsible for all official correspondences sent to their UI email address (uiowa.edu) and must use this address for any communication with instructors or staff in the UI community.

University Policies
Accommodations for Students with Disabilities
Basic Needs and Support for Students
Classroom Expectations
Exam Make-up Owing to Absence
Free Speech and Expression
Mental Health
Military Service Obligations
Non-discrimination
Religious Holy Days
Sexual Harassment/Misconduct and Supportive Measures
Sharing of Class Recordings