CHEM:5431-- Statistical Thermodynamics I

LECTURES: 11:00A - 12:15P TTh BHC. Attendance is mandatory.
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Office Hours: W 1:00 pm- 4:00pm in 244 IATL. All other meetings by appointment only.
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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, 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. If you fall behind it will be very hard to catch up because topics are interconnected.

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 books 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
(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)

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.

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

Problem sets 20%
2 Exams 20% each (total 40%)
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 March 12 and April 16. The final project write-up is due on April 16 but can be submitted any time before this deadline. The four lectures after April 16 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 will most likely be relevant to your own research must be agreed upon you and the instructor (me) by February 25. It is important that we meet more than once before February 25 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 February 25 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 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: 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. 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 (such as a medical emergency). 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.

A NOTE ON COLLABORATION

Homework in this course is assigned to better prepare you for the closed-book exams. In this spirit, brainstorming sessions are encouraged, however, I expect you to do the homework on your own.

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)
Absences and Attendance
Students are responsible for attending class and for contributing to the learning environment of a course. Students are also responsible for knowing their course absence policies, which will vary by instructor. All absence policies, however, must uphold the UI policy related to student illness, mandatory religious obligations, including Holy Day obligations, unavoidable circumstances, or University authorized activities ([https://clas.uiowa.edu/students/handbook/attendance-absences](https://clas.uiowa.edu/students/handbook/attendance-absences)). Students may use this absence form to aid communication; the instructor will decide if the absence is excused or unexcused ([https://clas.uiowa.edu/sites/default/files/ABSENCE%20EXPLANATION%20FORM2019.pdf](https://clas.uiowa.edu/sites/default/files/ABSENCE%20EXPLANATION%20FORM2019.pdf)).

Academic Integrity
All undergraduates enrolled in courses offered by CLAS have, in essence, agreed to the College's Code of Academic Honesty. Misconduct is reported to the College, resulting in suspension or other sanctions, with sanctions communicated with the student through the UI email address ([https://clas.uiowa.edu/students/handbook/academic-fraud-honor-code](https://clas.uiowa.edu/students/handbook/academic-fraud-honor-code)).

Accommodations for Disabilities
UI is committed to an educational experience that is accessible to all students. A student may request academic accommodations for a disability (such as mental health, attention, learning, vision, and physical or health-related condition) by registering with Student Disability Services (SDS). The student is then responsible for discussing specific accommodations with the instructor. More information is at [https://sds.studentlife.uiowa.edu/](https://sds.studentlife.uiowa.edu/).

Administrative Home of the Course
The College of Liberal Arts and Sciences (CLAS) is the administrative home of this course and governs its add/drop deadlines, the second-grade-only option, and related policies. Other colleges may have different policies. CLAS policies may be found here: [https://clas.uiowa.edu/students/handbook](https://clas.uiowa.edu/students/handbook).

Communication and the Required Use of UI Email
Students are responsible for official correspondences sent to the UI email address (uiowa.edu) and must use this address for all communication within UI ([Operations Manual, III.15.2](https://clas.uiowa.edu/students/handbook/)).

Complaints
Students with a complaint about a course should first visit with the instructor or course supervisor and then with the Chair of the department or program offering the course; students may next bring the issue to CLAS in 120 Schaeffer Hall. For more information, see [https://clas.uiowa.edu/students/handbook/student-rights-responsibilities](https://clas.uiowa.edu/students/handbook/student-rights-responsibilities).

Final Examination Policies
The final exam schedule is announced around the fifth week of classes; students are responsible for knowing the date, time, and place of a final exam. Students should not make travel plans until knowing this information. No exams of any kind are allowed the week before finals. Visit [https://registrar.uiowa.edu/final-examination-scheduling-policies](https://registrar.uiowa.edu/final-examination-scheduling-policies).

Nondiscrimination in the Classroom
UI is committed to making the classroom a respectful and inclusive space for all people irrespective of their gender, sexual, racial, religious or other identities. Toward this goal, students are invited to optionally share their preferred names and pronouns with their instructors and classmates. The University of Iowa prohibits discrimination and harassment against individuals on the basis of race, class, gender, sexual orientation, national origin, and other identity categories set forth in the University’s Human Rights policy. For more information, contact the Office of Equal Opportunity and Diversity ([diversity.uiowa.edu](https://diversity.uiowa.edu)).

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 must uphold the UI mission and contribute to a safe environment that enhances learning. Incidents of sexual harassment must be reported immediately. For assistance, please see [https://osmrc.uiowa.edu/](https://osmrc.uiowa.edu/).