CHM 6461: Statistical Thermodynamics

Term: Spring 2021

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Class schedule: M,W,F | Period 2 (8:30 AM - 9:20 AM)

Books:

Required book: Terrell L. Hill, "An introduction to statistical thermodynamics", Dover Publications (January 1, 1987).

The course will follow closely Hill's book, but the lecture notes, presentations, exercises and for some particular topics we will also cover topics from the following auxiliary texts:

- Donald A. McQuarrie, "Statistical mechanics", University Science Books, 2nd Ed. (May 2000)
- Roger Bowley and Mariana Sanchez, "Introductory statistical mechanics", Oxford Science Publications, 2nd Ed. (2011)
- Leslie E. Ballentine, "Quantum mechanics: a modern development", World Scientific Publishing Co. Pte. Ltd., (1998)
- "Chemical reactivity theory: a density functional view", Ed: Pratim K. Chattaraj, CRC Press, (2009)
- Robert G. Parr and Weitao Yang, "Density-functional theory of atoms and molecules", Oxford University Press, (1989)

Course objective and goals:

This course will give a self-contained exposition of different topics on (equilibrium) statistical thermodynamics. We will discuss both the foundations of statistical thermodynamics, and some applications to different areas of chemical physics and chemical reactivity.

Course Outline:

- Ensembles and postulates.
- Canonical ensemble and thermodynamics.
- Grand canonical ensemble.
- Microcanonical ensemble.
- Fluctuations.
- Second and third laws of thermodynamics.
- Boltzmann statistics, distribution function and entropy.
- Ideal monoatomic gas.
- Internal degrees of freedom.
- Molecular partition functions (ideal diatomic gas, vibrational and rotational degrees of freedom).
- Homonuclear diatomics, ideal polyatomic gas.
- Quantum statistics (fermions and bosons).
- Statistical description of quantum states (closed and open states).
- Thermodynamic functions for quantum states, applications in chemical reactivity.
- Monoatomic crystals.
- Chemical equilibrium, rates of chemical reactions.

*NOTE: The course is designed to be flexible and adaptive. As we progress, we can discuss about touching on some particular topics depending on your particular interests.

Grading:

Exams (3 partial take-home exams)-----40%

Homework----40%

Class participation will also be taken into account (20%).

Letter grade	From	To
A	90	100
A-	84	89.99
B+	81	83.99

B	78	80.99
B-	75	77.99
C+	72	74.99
C	69	71.99
C-	66	68.99
D+	63	65.99
D	60	62.99
D-	50	59.99
E	0	49.99

More information on current UF grading policies for assigning grade points can be found at: link to the university grades and grading policies.

Accommodations for students with disabilities: Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center. Click here to get started with the Disability Resource Center. It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.

Privacy related issues: Our class sessions may be audio visually recorded for students in the class to refer back and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate orally are agreeing to have their voices recorded. If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

Homework:

Homework due date will be announced in class. Late homework will not be accepted. Each problem will have to show the full derivation. It is expected that the students will collaborate on some of the problems but, unless otherwise indicated, the homework must be delivered individually.

Exams and quizzes:

There will be 2 exams (midterm and final exam). Cheating will not be tolerated in any form and will automatically result in a zero mark for the given exam, homework, etc. If cheating is suspected it will be reported to the university as such.

Prerequisites:

Since the course is self-contained, we will cover many of the mathematical tools required to understand the foundations and applications of statistical thermodynamics (for instance, we will introduce and discuss topics on combinatorics that are profusely used in this field). Nonetheless, the students are expected to be familiar with:

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

Familiarity with standard concepts and tools from thermodynamics is also highly recommended (for instance, the notion of state functions and some common thermodynamic relations). We will also use different tools and concepts from quantum mechanics, most of which will be discussed in the course at the level necessary to our current needs. However, it is expected that the student is familiar with basic undergraduate-level quantum mechanics and the associated mathematical structure (i.e., state superposition, eigenvalues and eigenvectors).

Honor code:

The student honor code can be found at: www.dso.ufl.edu/sccr/honorcodes/honorcode.php.

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.

CampusResources:

Health and wellness:

U Matter, We Care: If you or someone you know is in distress, please contact umatter@ufl.edu, 352-392-1575, or visit U Matter, We Care website to refer or report a concern and a team member will reach out to the student in distress.

Counseling and Wellness Center: Visit the Counseling and Wellness Center website or call 352-392-1575 for information on crisis services as well as non-crisis services.

Student Health Care Center: Call 352-392-1161 for 24/7 information to help you find the care you need, or visit the Student Health Care Center website.

University Police Department: Visit UF Police Department website or call 352-392-1111 (or 9-1-1 for emergencies).

UF Health Shands Emergency Room / Trauma Center: For immediate medical care call 352-733-0111 or go to the emergency room at 1515 SW Archer Road,
Gainesville, FL 32608; Visit the UF Health Emergency Room and Trauma Center website.

Academic Resources:

E-learning technical support: Contact the UF Computing Help Desk at 352-392-4357 or via e-mail at helpdesk@ufl.edu.

Career Connections Center: Reitz Union Suite 1300, 352-392-1601. Career assistance and counseling services.

Library Support: Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center: Broward Hall, 352-392-2010 or to make an appointment 352- 392-6420. General study skills and tutoring.

Writing Studio: 2215 Turlington Hall, 352-846-1138. Help brainstorming, formatting, and writing papers.

Student Complaints On-Campus: Visit the Student Honor Code and Student Conduct Code webpage for more information.

On-Line Students Complaints: View the Distance Learning Student Complaint Process.