

# CHM 6461

## Statistical Thermodynamics

### Spring 2022

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Everything in this document is subject to change during the semester.

**Masks.** UF and The College of Liberal Arts and Sciences emphasizes that, considering CDC recommendations, **face coverings, are expected in all UF facilities.** Regardless of vaccination status, mask usage is a responsible and vital way of preventing transmission of COVID-19. Mask usage is mandatory in offices during one-on-one meetings (students can request a zoom alternative).

**Vaccination.** If you have not been vaccinated, please consider starting the process immediately. If you are currently at home, you can obtain a first dose where you are and receive a second dose here in Gainesville. If you are already in Gainesville, **you can schedule a vaccination appointment at ONE.UF.** Please keep in mind that being vaccinated for COVID-19 is the best way to protect yourself and others from the potentially life-threatening effects of the virus. Your action in this regard may help ensure the health and safety of yourself, your fellow UF/CLAS students, and the faculty and staff with whom you interact.

#### **Canvas e-learning site**

<https://ufl.instructure.com/courses/450117>

All communications must be done through the e-learning site, including homework, deadlines, grades, and announcements. It is your responsibility to check this site for updates. Please do not email the instructor personal email accounts.

#### **Schedule**

Room: TBA

Wednesday. Period 2-3 (8:30 AM - 10:25 AM)

Friday. Period 3 (9:35 AM - 10:25 AM)

#### **Books**

We will not use a particular book, but I will be discussing sections from the following texts:

“Statistical Mechanics: Theory and Practice through Molecular Simulation”, Oxford University press M. E. Tuckerman.

D.A. McQuarrie, Statistical Thermodynamics

D. Chandler, Introduction to Modern Statistical Mechanics

Often, material will be drawn from current literature in statistical mechanics.

I strongly recommend you being familiar with the level of basic statistical thermodynamics shown in the McQuarrie book.

### **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 (tentative)**

- 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:**

The course will have homeworks and computational projects, including a final project.

The Homework due date will be posted on the class calendar. Late homework (if it is turned in on the same day, but after deadline) will have a 20% deduction on the grade. No more homework will be accepted for grading after that. Each homework problem must show the full derivation. The homework answers should be present in a professional manner, with all steps explained. No points will be given for a result without justification.

### **Honor Code:**

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

**Attendance:** Lecture attendance is essential for your success in this class. However, we will not take roll. Repeated absence in class will make it very difficult to earn full participation points.

**Course Evaluations:** 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. Summary results of these assessments are available to students at <https://evaluations.ufl.edu/results/>.

### **Honor Code:**

The student honor code can be found at:

<http://www.registrar.ufl.edu/catalog/policies/students.html>

The students, instructor and TAs 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.*

*On all work submitted for credit by students at the university, the following pledge is either required or implied: On my honor, I have neither given nor received unauthorized aid in doing this assignment.*

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

Counseling services are available at <http://www.counsel.ufl.edu> . or call (352)-392-1575 during regular service hours (8am-5pm). For other hours or weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352)-392-1171

### **Class Recordings**

Students are allowed to record video or audio of class lectures. However, the purposes for which these recordings may be used are strictly controlled. The only allowable purposes are (1) for personal educational use, (2) in connection with a complaint to the university, or (3) as evidence in, or in preparation for, a criminal or civil proceeding. All other purposes are prohibited. Specifically, students may not publish recorded lectures without the written consent of the instructor.

A “class lecture” is an educational presentation intended to inform or teach enrolled students about a particular subject, including any instructor-led discussions that form part of the presentation, and delivered by any instructor hired or appointed by the University, or by a guest instructor, as part of a University of Florida course. A class lecture does not include lab sessions, student presentations, clinical presentations such as patient history, academic exercises involving solely student participation,

assessments (quizzes, tests, exams), field trips, private conversations between students in the class or between a student and the faculty or lecturer during a class session.

Publication without permission of the instructor is prohibited. To “publish” means to share, transmit, circulate, distribute, or provide access to a recording, regardless of format or medium, to another person (or persons), including but not limited to another student within the same class section. Additionally, a recording, or transcript of a recording, is considered published if it is posted on or uploaded to, in whole or in part, any media platform, including but not limited to social media, book, magazine, newspaper, leaflet, or third-party note/tutoring services. A student who publishes a recording without written consent may be subject to a civil cause of action instituted by a person injured by the publication and/or discipline under UF Regulation 4.040 Student