CHM 6461: Statistical Thermodynamics

Spring 2020

Professor: Ramón Alain Miranda Quintana

Office: Leigh Hall, 240H

Phone: 352 294 3489

Email: ramirandaq@gmail.com, quintana@chem.ufl.edu

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.

Grading:

Midterm-----35%

Final exam----35%

Homework----20%

Quizzes----10%

Class participation will also be taken into account.

Homework:

Homework due date will be announced in class and posted on the class calendar. 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.

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.