

CHM 4411, Physical Chemistry: Thermodynamics and Kinetics Spring 2016

"In this house, we obey the laws of thermodynamics!"

-Homer J Simpson

Instructor: Dr. Benjamin J Killian, LEI 202A, 392-0528, killian@chem.ufl.edu
Office Hours: M, W, F 3rd Pd.

Teaching Assistants: Martha Hermosilla-Palacios, her11193@ufl.edu
Wenxiao Guo, grandpacomp@ufl.edu

Objectives: In this course you will learn the physical and mathematical bases of macroscopic and statistical thermodynamics and kinetics with applications to chemical systems.

Texts: There is no required textbook for this course. You are, however, expected to have a PChem textbook for reference and extra problems. There are many textbooks that you may choose from. I have provided chapter information from two common textbooks,

- Atkins and De Paula, *Physical Chemistry* 9th Ed. W. H. Freeman and Co., New York (2010)
- McQuarrie and Simon, *Physical Chemistry: A Molecular Approach*. University Science Books (1997)

Grade Distribution:

Exams:	4 @ 200 pts.	800 pts.
Homework:	~10 weighted to 200 pts. total	200 pts.
Quizzes	~10 weighted to 200 pts. total	200 pts.
Total		1200 pts.

Grading Scale:

<u>Letter Grade</u>	<u>Total Points</u>	<u>Letter Grade</u>	<u>Total Points</u>	<u>Letter Grade</u>	<u>Total Points</u>
A	≥1080	B-	≥888	D+	≥696
A-	≥1032	C+	≥840	D	≥648
B+	≥984	C	≥792	D-	≥600
B	≥936	C-	≥744	E	<600

Tips for Success: This course is not easy. It may very well be one of the hardest courses you take while an undergrad. However, with attention you can pass this course and <gasp> actually learn something! Firstly, please be on time to lectures. Material will come primarily from the lectures. If you must miss a lecture, be sure to acquire the notes from a classmate. Remember, 2 periods is a lot of material to miss. If you must show up late, please be courteous to your instructor and fellow students by not being disruptive.

My lectures will only go so far toward teaching you this material. On a daily basis you should read the material and work problems. Work all assigned problems more than once. Practice on other problems. When you get graded material back, rework the problems. Try to find different ways to get the correct answer. Practice is crucial to mastering this material.

This subject matter is very mathematical. You will have to call upon the Calculus that you probably haven't had to use for several years. Dust off your old Calculus text and make friends with it again. Don't get bogged down in the math. Understand the concepts and fill in the blanks later.

Finally, be sure to maintain a positive attitude. Thermodynamics can be a little dry. I will do everything I can to make it interesting for you. No matter how boring and tedious you find the material, remember that the universe runs on thermodynamics.

Course Mechanics: Homework will be assigned weekly, and will generally comprise 5 problems. Be sure to show your work on homework assignments *with correct units throughout*. Homework must be submitted on paper. No e-mailed assignments will be accepted. I, as well as TAs, will be available to answer questions during office hours. If you need to speak with me outside of office hours, please make an appointment. The final homework grade will be based on a scale of 200 points. Each assignment will be equally weighted.

There will be quizzes throughout the semester. These are intended to indicate problem areas before they are encountered on exams. Be sure to understand the quiz questions completely. *No make-up quizzes will be given.* You will be allowed to drop two (2) quiz scores. The final quiz grade will be based on a scale of 200 points. Each quiz will be equally weighted.

There will be four (4) exams through the course of the semester, each worth 200 points. The exams dates are Jan 28, Feb 25, March 31, and Apr 19.

During quizzes and exams, you are expected to do your own work. I do not require that you use a non-programmable calculator; however, I reserve the right to require you to reset it if warranted. Students may not share calculators. Cell phones, mp3 players, personal computers, and all other electronic/wireless devices are prohibited during quizzes and exams. *Violations will result in a grade of zero on the assignment.*

Schedule of Lecture Topics: The following broad topics will be covered through the semester, as time permits.

	Atkins	McQuarrie
1. Fundamentals and Gas Laws:		
a. Energy Levels and Partition Functions	15	17,18
b. Ideal and Real Gases	1	16,18
c. Indicator Diagrams	2	19
d. Kinetic Theory of Gases	20	27
2. The First Law:		
a. Energy, Heat, and Work	2,16	19
b. Legendre Transforms (an introduction)	N/A	N/A
c. Enthalpy and Thermochemistry	2,16	19
d. A first look at Differential Forms	2	N/A
3. The Second and Third Laws:		
a. Carnot Cycle and efficiency	3	20
b. Entropy and Spontaneity	3,16	20
c. Absolute Entropy and Third Law		21
4. Mathematical Tools and Techniques:		
a. Legendre Transforms and Free Energies	3,4	22
b. Differential forms and Maxwell Relations	3	22
5. Equilibrium and Transitions:		
a. Chemical potential	3,4	23
b. Phases and Phase Changes	4,5	23
c. Chemical equilibrium	6	23-26
d. Pure Liquid Mixtures	5	24,25
e. Colligative Properties	5	25
6. Equilibrium and Solutions:		
a. Activities	5	24
b. Acid/Base Reactions	N/A	N/A
c. Electrochemistry	6	N/A
d. Solubility	N/A	N/A
7. Kinetics and Reaction Dynamics:		
a. Introduction to Kinetics	21	28
b. Integrated Rate Laws	21	28
c. Elementary Reaction, Complex Mechanisms, Simplifications	21	28,29
d. Temperature Dependence and Equilibrium	21	28
e. Unimolecular Reaction and Transition State Theories	22	28,29
f. Catalysis	23	29

Class Attendance: Requirements for class attendance and make-up assignments are consistent with university policies that can be found at <https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx>.

Students with Disabilities: Students with disabilities requesting accommodations should first register with the Disability Resource Center (352.392.8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter, which must be presented to the instructor when requesting accommodations. Students with disabilities should follow this procedure as early as possible in the semester.

Grading Policies: Information about the most current UF grading policies for the assigning of grade points can be found at <https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>.

Course Evaluations: Students are expected to provide feedback on the quality of instruction in this course by completing on-line 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/>.

Academic Honesty: UF students are bound by The Honor Pledge, which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code." On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment."

Additional information may be found at <https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/>. If you have specific questions, please consult with the instructor or your TA.

Student Wellness: We hold student success very highly, and we hope that any concerns of both an academic and a personal nature can be addressed in a timely and helpful manner. The Counseling and Wellness Center is an important service provided by the university to help with a variety of personal issues and concerns. The center can be contacted at 352.392.1575. More information is available at <http://www.counseling.ufl.edu/cwc/Default.aspx>.