Chem 4501 **Introduction to Thermodynamics, Kinetics, and Statistical Mechanics** 3 Credits

Syllabus: Fall Semester 2017
(last updated: August 17, 2017)

Prerequisites: One prior year chemistry, one prior year physics, one prior year calculus.

Time and Location: MWF 11:15 – 12:05, 312A/B Bruininks Hall.

Instructor: Chris Cramer (cramer@umn.edu, @ChemProfCramer)

TA: Katelyn (Katie) Youmans (youm0013@umn.edu)

Office Hours: CC: By appointment, see contact details above
KY: During classtime if an active learning session is *not* scheduled (312 Bruininks), or by appointment, see contact details above

Required textbook: *Molecular Thermodynamics*, D. A. McQuarrie and J. D. Simon, University Science Books: Sausalito, CA, 1999. Note that this book is essentially 40% of a larger text by the same authors, entitled *Physical Chemistry: A Molecular Approach*, where the other 60% of the latter text covers quantum mechanics and kinetic theories. So, if you already have *Physical Chemistry: A Molecular Approach*, you do *not* need to acquire a copy of *Molecular Thermodynamics*. Similarly, if you anticipate that you are going to take a quantum mechanics course that will use *Physical Chemistry: A Molecular Approach*, you may want to purchase the larger book instead of the smaller *Molecular Thermodynamics*. [To be specific, Chapters 2–12 of *Molecular Thermodynamics* are almost verbatim Chapters 16-26 of *Physical Chemistry: A Molecular Approach*. We *will* cover Chapter 1 of *Molecular Thermodynamics*, which is essentially a primer of key quantum mechanical principles that we will be using "without proof" and may be thought of as an ultra-condensed version of Chapters 1–6 of *Physical Chemistry: A Molecular Approach*. We will also be covering Chapter 13 of *Molecular Thermodynamics*, which *is* unique to that text; however, I will (with permission having been secured from the publisher) distribute that chapter to everyone.] *You will want to have access to at least one of these texts.*

Class Website: The *administrative* website for the course is pollux.chem.umn.edu/4501 — this site includes various useful materials. The *curricular* website for the materials covered in Modules 1–8 of the course is hosted on the Coursera platform at coursera.org/learn/statistical-thermodynamics-2/. This material is *also* available, along with the material for Modules 9–13, in playlists on the YouTube website youtube.com/channel/UCQWne9DleuGu0q9TmA70jWQ/playlists. (Note that pdf versions of all slides are available on the admin and Coursera sites, and you are welcome to use the upper division microcomputer lab in 101D Smith Hall if you want to print these free of charge.)

Coursework: The class will proceed with the lecture content to be accessed entirely online; active-learning (problem-solving) sessions will be scheduled for many course meeting times, but there will be no presentation of additional conceptual material that is not available online. All of the topics to be covered are outlined in greater detail below. Students are expected to keep up with online and textbook content and to work on assigned homework problems (see below). Classroom attendance will not be taken, but you are likely to have a *much* more difficult time if you fail to attend classes, as that is where we will work with the material. You should *complete* the assigned content *before* the corresponding active-learning session.

Homework: Homework sets for the first portion of the course (8) will consist of 10 multiple choice problems, each of which will be graded (correct or not). Homework sets for the second portion of the course (4) will be taken from McQuarrie and Simon and will be more derivational in nature, with one problem from each of these latter sets being chosen for complete grading and the others examined more cursorily. All homework assignments are worth 10 points towards your final grade. Homework may be done individually, or in groups of up to 4 people (all members of a group will receive the same grade). *Homework is due at the beginning of the class period on the indicated date* (vide infra).

Exams: Three in-term exams will be taken during normal class periods; they will be cumulative on all class materials up to that point, with heavy emphasis on new material covered since any prior exam. The final exam will cover the entire semester, with some additional emphasis on topics covered in the last module of the course (which will follow the third in-term exam). The format of the exams will combine multiple choice with short problems chosen to have close correspondence to assigned homework. Arriving at the answer to either type of problem may well involve some mathematical calculations; space and relevant formulae required to perform such calculations will be provided as appropriate. The exams will emphasize *conceptual* details over detailed mathematical manipulations, but testing on a certain amount of the latter cannot be avoided. The final exam is 1:30 p.m. - 3:30 p.m., Wednesday, December 20, 2017. ***Under no conditions will it be possible to reschedule the final exam, nor can that exam somehow be dropped or otherwise substituted.***

Grading: Each of the 3 in-term exams during the semester will be worth 120 points, the cumulative homework will be worth 120 points, and the final exam will be worth 240 points, giving a total of 720 points in the course. If an in-term exam is missed for a proven and documented personal emergency or university-approved activity, then the comprehensive final exam will be weighted more heavily. You must notify me of any documented reason for missing an exam within one week following the date of that exam (and preferably well before, if you have advance warning). ***Under no conditions will it be possible to reschedule the final exam, nor can that exam somehow be dropped or substituted***. The class will be graded on an *absolute scale*: The total number of possible points in the course is 720, and you must earn at least 580 points for an A–, 450 points for a B–, 340 points for a C–, and 300 points for a D. Thus, earning approximately 80% of possible points enters the A range, 63% the B range, 47% the C range, 42% the D range, and earning less than 42% of possible points will result in a failing grade. As warranted, "+" and "–" grades will be awarded within each range (typically the top and bottom one or two percent in a range, at my discretion).

Calculators: No calculators, nor any other electronic devices, will be allowed during exams. You will generally be provided with all formulae required to solve problems and answers will be expressed in terms of constants that need not be reduced to decimal values.

Preparing for Exams: There is (as you may have heard) no free lunch. The most effective method to prepare for an exam is to study the lecture slides, the assigned homework, and the in-class active-learning problems. Look for common concepts or formula manipulations that arise in multiple exercises as these are likely to be of key importance and utility.

Academic Misconduct: I rigorously adhere to the CSE policy on scholastic conduct and academic integrity. This is a challenging course affording significant opportunity for individual initiative. Insofar as some of the graded requirements are to be completed outside of class, you will have the opportunity to discuss them with your peers, and also to work in groups. This does not become inappropriate *unless* it is designed to arrive at the required results without actually performing the antecedent work. I trust you to act within what should be common-sense limits (because I want to live in that kind of world; don't you?) Students who are judged to have engaged in academic misconduct will receive a failing grade for the course and the incident will be reported to the relevant collegiate student conduct board.

Anything unclear? If so, just ask me.

Appendix. There are a number of items intended for inclusion on every University of Minnesota syllabus. You can find them at:

policy.umn.edu/Policies/Education/Education/SYLLABUSREQUIREMENTS_APPA.html

and you should certainly read them there.

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COURSE OUTLINE

For the entire course—Modules 1-8 on the Coursera website and 9-13 on a YouTube playlist—you are free to proceed at your own pace; the day-by-day outline below will help you align your reading and prepare for in-class active learning exercises (you should have completed the relevant reading by classtime on the indicated date). Note that the homework deadlines are hard deadlines, i.e., you must submit the homework by the deadline or it will not be graded. Dates indicate whether we will be in the classroom at the normally scheduled time. The "AL N" notation indicates an active-learning/problem-solving session for module # N. The "AMA" notation means "Ask Me Anything" (i.e., these are effective office hours). There will also be occasional catch-up/review sessions, as indicated in the schedule. If no formal activities are planned, "(no class)" is entered, but Katie will be available in the normal classroom for an office hour (or to receive homework, when due).

Date	Topic/Reading
6-Sep	Discussion of Syllabus. Summary overview of thermodynamics and its continuing topicality.
8-Sep AL 1	Molecular energy levels from quantum mechanics. (Module 1)
11-Sep (no class)	**Homework 1 due** (may be submitted electronically). Ideal gases. Equations of state. PV diagrams. Gases and liquids. (Module 2)
13-Sep AL 2	Corresponding states. Dispersion. Intermolecular interactions. Real gases. (Module 2)
15-Sep AL 1, 2	Sample exam problems.
18-Sep (no class)	**Homework 2 due** (may be submitted electronically). Boltzmann probability and connection to energy. Ensemble properties. (Module 3)
20-Sep AMA	Heat capacity. Partition functions. (Module 3)
22-Sep AL 3	Atomic and molecular partition functions. Connection to quantum mechanics (statistical thermodynamics). (Module 3)
25-Sep (no class)	**Homework 3 due** (may be submitted electronically). Electronic and translational partition function for gases. (Module 4)
27-Sep AMA	Rovibrational partition functions. (Module 4)

29-Sep AL 4	Rovibrational partition functions continued. Heat capacities. (Module 4)
2-Oct AMA	**Homework 4 due** (may be submitted electronically). Problem solving. Review.
4-Oct	**EXAM I**
6-Oct (no class)	First law. Energy. PV Work. State functions. (Module 5)
9-Oct (no class)	Adiabaticity. Reversibility. Heat and work. Enthalpy. Heat capacity. (Module 5)
11-Oct AL 5	Heat of transition. Enthalpy of chemical reaction. Heat of formation. Standard enthalpy. (Module 5)
13-Oct AL 5	Sample exam problems.
16-Oct (no class)	**Homework 5 due** (may be submitted electronically). Spontaneity and entropy. (Module 6)
18-Oct AMA	Statistical thermodynamics and entropy. Reversibility. (Module 6)
20-Oct AL 6	Entropy and the interconversion of heat and work. Entropy and the partition function. (Module 6)
23-Oct (no class)	**Homework 6 due** (may be submitted electronically). Third law. Temperature limits. Perfect crystals. (Module 7)
25-Oct AL 7	Phase transitions. Experimental determination of third-law entropies. Standard entropy. (Module 7)
27-Oct AMA	Helmholtz and Gibbs free energies. Ensemble conditions. (Module 8)
30-Oct (no class)	**Homework 7 due** (may be submitted electronically). Maxwell relations. Ideal gas state functions. (Module 8)
1-Nov (no class)	Independent variables. Gaseous standard state. Gibbs-Helmholtz equation. Fugacity. (Module 8)
3-Nov AL 8	Overflow/catch-up
6-Nov AMA	**Homework 8 due** (may be submitted electronically). Problem solving. Review.
8-Nov	**EXAM II**
10-Nov (no class)	Phase equilibria. Phase diagrams. Free energy connections. (Module 9)
13-Nov AL 9	Chemical potentials. Clausius-Clapeyron equation. Partition functions and phase equilibria. (Module 9)
15-Nov AMA	**Homework 9 due** (may be submitted electronically). Solutions. Partial molar quantities. Gibbs-Duhem equation. (Module 10)

17-Nov (no class)	Raoult's law. Ideality and non-ideality. Vapor-liquid equilibria for solutions. Activity. (Module 10)
20-Nov AL 10	Standard states. Non-ideal solutions and molecular thermodynamics. (Module 10)
22-Nov (no class)	**Homework 10 due** (may be submitted electronically). Solutes in solutions. Solid/liquid solutions. Activity. (Module 11)
27-Nov AL 11	Colligative properties. Osmotic pressure. Electrolyte solutions. Debye-Hückel theory. (Module 11)
29-Nov AL 9-11	Sample exam problems.
1-Dec (no class)	Chemical equilibria. Equilibrium constants. Reaction quotients. Standard states. Spontaneity. van't Hoff equation. (Module 12)
4-Dec AL 12	Equilibrium constants and partition functions. Experimental data. Fugacities. Activities. (Module 12)
6-Dec AL 9-12	**Homework 11 due** (may be submitted electronically). Problem solving. Review.
8-Dec	**EXAM III**
11-Dec (no class)	Electrochemistry. Half cells and electrochemical cells. Electromotive force. (Module 13)
13-Dec AL 13	**Homework 12 due** (may be submitted electronically). Experimental utility of electrochemical measurements. Batteries. Fuel cells. Course evaluations. (Module 13)
20-Dec	**FINAL EXAM, 1:30–3:30 PM**