CHEM 631 SYLLABUS

Course title and number	Chem 631: Statistical Thermodynamics
Term	Fall 2020
Meeting times and location	Tuesday-Thursday 1:30-2:45 PM CHEM 2122

Instructor Information

Name	Daniel Tabor
Email address	daniel.tabor@chem.tamu.edu
Office hours	To be determined and also by appointment
Office location	Chemistry 2307C

For quick questions, sometimes the best time to ask those is either right before or right after class. For longer questions, office hours are recommended. I will try to respond to any emailed questions (during the week) within 24 hours. Please include CHEM 631 in the subject line.

Course Description

Fundamental chemical thermodynamics with applications to chemical and phase equilibria and the study of solutions; introduction to statistical mechanics and calculation of thermodynamic quantities from microscopic models; statistical theories of gases, solids, and liquids, applications to modern physical and chemical problems such as polymers, solutions, biophysics, and surfaces; stability and fluctuations.

Course Objectives

The objective of this course is to make the concepts and methods of statistical thermodynamics/mechanics clear and interesting to students who are pursuing careers in the physical sciences. A particular emphasis is placed on techniques for solving modern research problems, both from a mathematical and numerical perspective. By the end of the course, students will be able to be conversational in the fundamental concepts and methods of statistical mechanics (as applied to chemistry) with their peers, collaborators, and research advisors.

Textbook and/or Resource Material

Often a Stat. Mech. course in a chemistry department with be taught from three different sources: 1) McQuarrie 2) Chandler 3) Lecture Notes. We are taking a linear combination of the three, but primarily taking from 1) and 3).

The main text for this course is:

1. Statistical Mechanics, 1st edition by McQuarrie (rough basis for the lectures, chapter numbers for relevant topics in brackets below). I highly recommend buying a used version online. In general, we will follow the book a bit more closely for the beginning of the course and gradually move to approaching some concepts/problems with a slightly different point of view later in the course, particularly with phase transitions and more modern problems. Even in those cases, reading the text will give you a complementary perspective compared to the lectures and this might help clarify some of the challenging concepts.

Lecture material is also derived from some of the following books, which you may find interesting or more suited for your style. I have copies in my office you can borrow.

2. Introduction to Modern Statistical Mechanics, by David Chandler. This little green book arguably contains more information than McQuarrie. I would argue that for most cases, it is an ideal book to read *after* you think you have a concept down, as nearly everything is described as briefly and

elegantly as possible. Some think of it as the “stat mech book for people who already know stat mech.” A large fraction of physical chemists took a course that is driven by this book. This book also has a solutions manual for some of its exercises, but there is certainly more emphasis on “manual” than “solutions” in that companion text.

3. Molecular Driving Forces, by Dill and Bromberg. This book is on average, probably a bit too simple for an intro graduate course and too complicated for most undergraduate courses, but it contains a lot of mathematical review, and has some interesting perspectives (it is also where we take some of the helix-coil model notes from).

Finally, this course may involve some mathematics that you haven’t used in quite a while or never had a full course of instruction on. You may want to check out some low-cost texts with problems/solutions in the following topic areas:

1. Vector/Multivariable Calculus
2. Calculus-Based Probability and Statistics
3. Linear Algebra
4. Differential Equations (typically the simpler ones)

I’ll be sure to point out the mathematical technique we are using to solve certain problems and where you might have first seen it.

Grading Policies

There will be two midterm exams and one final exam. The final exam is cumulative. The final course grade will be based on the following weighted average:

1. Problem Sets: 35%
2. Midterm 1: 20%
3. Midterm 2: 20%
4. Final Exam: 30%

The midterms might be scheduled either in class time or be given as take-home exams (to be decided near the exam date). This term, all final exams are administered remotely, so the final will be a take-home exam to be submitted online.

Grading Scale

If it were up to me, we wouldn’t have grades, particularly in graduate school. In an ideal world, at the end of the semester, we would say farewell for having had a great semester learning new stuff and at some point in the near or distant future you would come across a situation where you needed something that you learned in this course and you’d either know it or you’d know where to go to relearn it.

Alas, we do not live in ideal world and this course is graded. But there is some good news. I grade with an absolute scale as opposed to a curve. This way you are not competing against your colleagues (an important lesson to learn and carry through your entire career!) and can help each other out throughout the semester for mutual gain.

You may have noticed that the maximum score for the course is 105. If you make at least an 80, you will earn an A. If you make at least a 65, you will earn a B. These cutoffs will not be raised, but may be lowered as sometimes, it is difficult for me to know how difficult a problem on a problem set or an exam is before I have seen how the class does on it (though I am getting better at this). So, I will carefully consider if the course was more difficult than anticipated. Cs are extremely rare and Fs are generally reserved for academic misconduct.

Problem Sets

This is by far the most important part of the class from a pedagogical perspective (and this is also why it is the single largest component of your weighted average) and I expect that a great deal of your learning will happen outside of class as you work on these problems.

Homework assignments will be given (approximately) weekly. Assignments will usually be due in class one week after assignment. You may discuss homework problems with other students in the class (and I

encourage this!), but must write up your own independent solutions and turn them in. Late homework will not be accepted so that solutions may be immediately posted on the due date. This way you can get instant feedback on your answers.

The problem sets may consist of both conceptual pencil-and-paper problems and practical computer-based calculations. The goal for the latter is to give you the tools you need to solve realistic problems you may encounter in your own research. There are several options here:

1. Mathematica (access provided by the University)
2. Other computer algebra systems (such as Maple, Matlab, MathCad)
3. Fortran, C/C++, Python, etc.

The problem sets are sometimes challenging because real life applications of statistical mechanics are challenging—not because I am trying to classify you into grading bins (see above on my disdain for converting your mastery of the course into a single letter). This may be one of the first instances in your educational career where you come across a problem and do not even know how to start, much less finish, a problem and this is completely okay!

Extra credit: Periodically, extra credit may be offered on the problem sets. With this, you can get over a 100 on the problem set part of your grade.

Exams

The exams will contain a mixture of techniques developed in the lecture and the problem sets (typically in less exhaustive scenarios) and conceptual questions that test the ability to synthesize multiple concepts in new contexts. There are also usually a few True/False questions.

Course Topics, Calendar of Activities, Major Assignment Dates

The following topics should be covered. Some changes may be made due to time constraints. In brackets are the relevant chapters from McQuarrie, where applicable. I will try to give advanced notice to the next topic we are covering so that you can read ahead; the lectures focus more on clarifying the more difficult concepts.

In class questions and discussion are *strongly encouraged* and almost always benefit the entire class, due to us all coming from a diverse set of academic backgrounds and experiences. *Please feel free to speak up at any time* as I will sometimes forget to ask, “Any questions?”

1. Thermodynamics “Boot Camp” [1]
2. Boltzmann Distribution and Partition Functions [2]
3. Connections Between Thermodynamic Properties and Partition Functions [2]
4. Fluctuations [3]
5. Generalized Ensembles [3]
6. Lattice Models for Gases
7. Non-Interacting Systems, Indistinguishable Particles, Boson and Fermion Gases [3-6, 8, 10]
8. Classical Partition Functions and Equipartition Theorem [7, 16]
9. Chemical Equilibrium/Activity [9]
10. Solids, Phonons, Einstein Model, Debye Model [11]
11. Phase Transitions, Ising Model, Mean Field Theory
12. Helix-Coil Models for Biomolecules
13. Gibbs Phase Rule, Surfaces
14. Virial Expansion [10, 12]
15. Classical Fluids [13-14]
16. Fluctuation-Dissipation Theorem, Flux, Stokes-Einstein, Fokker-Planck [20]

Americans with Disabilities Act (ADA)

Texas A&M University is committed to providing equitable access to learning opportunities for all students. If you experience barriers to your education due to a disability or think you may have a disability, please contact Disability Resources in the Student Services Building or at (979) 845-1637 or visit disability.tamu.edu. Disabilities may include, but are not limited to attentional, learning, mental

health, sensory, physical, or chronic health conditions. All students are encouraged to discuss their disability related needs with Disability Resources and their instructors as soon as possible.

Academic Integrity

For additional information please visit: http://aggiehonor.tamu.edu

"An Aggie does not lie, cheat or steal, or tolerate those who do."

"Texas A&M University students are responsible for authenticating all work submitted to an instructor. If asked, students must be able to produce proof that the item submitted is indeed the work of that student. Students must keep appropriate records at all times. The inability to authenticate one's work, should the instructor request it, may be sufficient grounds to initiate an academic misconduct case" (Section 20.1.2.3, Student Rule 20).

You can learn more about the Aggie Honor System Office Rules and Procedures, academic integrity, and your rights and responsibilities at aggiehonor.tamu.edu.

Attendance

The university views class attendance and participation as an individual student responsibility. Students are expected to attend class and to complete all assignments.

Students will be excused from attending class on the day of a graded activity or when attendance contributes to a student's grade, for the reasons stated in Student Rule 7, or other reason deemed appropriate by the instructor.

Please refer to Student Rule 7 in its entirety for information about makeup work, including definitions, and related documentation and timelines. As stated above, late work will not be accepted.

"The instructor is under no obligation to provide an opportunity for the student to make up work missed because of an unexcused absence" (Student Rule 7, Section 7.4.2).

Students who request an excused absence are expected to uphold the Aggie Honor Code and Student Conduct Code. (See Student Rule 24.)

Title IX and Statement on Limits to Confidentiality

Texas A&M University is committed to fostering a learning environment that is safe and productive for all. University policies and federal and state laws prohibit gender-based discrimination and sexual harassment, including sexual assault, sexual exploitation, domestic violence, dating violence, and stalking.

With the exception of some medical and mental health providers, all university employees (including full and part-time faculty, staff, paid graduate assistants, student workers, etc.) are Mandatory Reporters and must report to the Title IX Office if the employee experiences, observes, or becomes aware of an incident that meets the following conditions (see University Rule 08.01.01.M1):

- The incident is reasonably believed to be discrimination or harassment.
- The incident is alleged to have been committed by or against a person who, at the time of the incident, was (1) a student enrolled at the University or (2) an employee of the University.

Mandatory Reporters must file a report regardless of how the information comes to their attention – including but not limited to face-to-face conversations, a written class assignment or paper, class discussion, email, text, or social media post. Although Mandatory Reporters must file a report, in most instances, you will be able to control how the report is handled, including whether or not to pursue a formal investigation. The University's goal is to make sure you are aware of the range of options available to you and to ensure access to the resources you need.

Students wishing to discuss concerns in a confidential setting are encouraged to make an appointment with Counseling and Psychological Services (CAPS).

Students can learn more about filing a report, accessing supportive resources, and navigating the Title IX investigation and resolution process on the University's Title IX webpage.

Mental Health and Wellness

Texas A&M University recognizes that mental health and wellness are critical factors that influence a student's academic success and overall wellbeing. Students are encouraged to engage in proper self-care by utilizing the resources and services available from Counseling & Psychological Services (CAPS). Students who need someone to talk to can call the TAMU Helpline (979-845-2700) from 4:00 p.m. to 8:00 a.m. weekdays and 24 hours on weekends. 24-hour emergency help is also available through the National Suicide Prevention Hotline (800-273-8255) or at suicidepreventionlifeline.org.

Fall 2020 Campus Safety Measures

To promote public safety and protect students, faculty, and staff during the coronavirus pandemic, Texas A&M University has adopted policies and practices for the Fall 2020 academic term to limit virus transmission. Students must observe the following practices while participating in face-to-face courses and course-related activities (office hours, help sessions, transitioning to and between classes, study spaces, academic services, etc.):

- Self-monitoring—Students should follow CDC recommendations for self-monitoring. **Students who have a fever or exhibit symptoms of COVID-19 should participate in class remotely and should not participate in face-to-face instruction.**
- Face Coverings—Face coverings (cloth face covering, surgical mask, etc.) must be properly worn in all non-private spaces including classrooms, teaching laboratories, common spaces such as lobbies and hallways, public study spaces, libraries, academic resource and support offices, and outdoor spaces where 6 feet of physical distancing is difficult to reliably maintain. Description of face coverings and additional guidance are provided in the Face Covering policy and Frequently Asked Questions (FAQ) available on the Provost website.
- Physical Distancing—Physical distancing must be maintained between students, instructors, and others in course and course-related activities.
- Classroom Ingress/Egress—Students must follow marked pathways for entering and exiting classrooms and other teaching spaces. Leave classrooms promptly after course activities have concluded. Do not congregate in hallways and maintain 6-foot physical distancing when waiting to enter classrooms and other instructional spaces.
- To attend a face-to-face class, students must wear a face covering (or a face shield if they have an exemption letter). If a student refuses to wear a face covering, the instructor should ask the student to leave and join the class remotely. If the student does not leave the class, the faculty member should report that student to the Student Conduct office for sanctions. Additionally, the faculty member may choose to teach that day's class remotely for all students.

Personal Illness and Quarantine

Students required to quarantine must participate in courses and course-related activities remotely and **must not attend face-to-face course activities**. Students should notify their instructors of the quarantine requirement. Students under quarantine are expected to participate in courses and complete graded work unless they have symptoms that are too severe to participate in course activities.

Students experiencing personal injury or Illness that is too severe for the student to attend class qualify for an excused absence (See Student Rule 7, Section 7.2.2.) To receive an excused absence, students must comply with the documentation and notification guidelines outlined in Student Rule 7. While Student Rule 7, Section 7.3.2.1, indicates a medical confirmation note from the student's medical provider is preferred, **for Fall 2020 only, students may use the Explanatory Statement for Absence from Class form in lieu of a medical confirmation. Students must submit the Explanatory Statement for Absence from Class within two business days after the last date of absence.**

Copyright Notice

disseminated or sold.

Final Remarks

Above all I hope you have fun in this course. I'll give you interesting, sometimes challenging, problems in addition to the routine problems you must do to develop your technique. When you get frustrated please seek help—from classmates, from me, or from whomever you have around to help. If you never get frustrated, then please come see me; I'll arrange for something more challenging. (I'm serious.)