Syllabus for CHEM5579: Thermodynamics and Statistical Mechanics
Core Curriculum (Fall Semester, 2026)

Class schedule: August 31 – December 11; Monday, Wednesday, and Friday, 12:00 PM – 12:50 PM

Note: We have the last lecture scheduled on **December 11 (Friday)**.

Location: Merkert 130

Course website: *Canvas*

I may update the course syllabus and homework problem sets on the course website (*Canvas*, Chem5579, Files). Solutions to the homework and exams may be posted on *Canvas* as well.

Instructor: Prof. Lucas Bao (email: lucas.bao@bc.edu)

Office hours: Monday & Wednesday, 1:00 PM – 2:00 PM

Office: Merkert 224

Prerequisites. This course requires **active learning**. To take this course, we require the following undergraduate prerequisites: multivariable calculus, basic linear algebra, basic differential equations, thermodynamics, and basic quantum mechanics.

Description and scope of the course. This course provides a foundation connecting the microscopic behavior of particles to macroscopic observables in chemistry. Core topics include classical Hamiltonian mechanics, distribution functions, and both classical and quantum equilibrium statistical mechanics. These principles are applied to gases, materials, spectroscopy, and reactivity. Advanced topics, such as path integral formalism, statistical field theory in phase transitions, and nonequilibrium systems, are introduced as time permits.

Course style. In order to create a flexible and more interactive learning experience for this graduate-level course, we adopt a hybrid of ***active learning***, the ***traditional teacher-centered classroom***, and if time permits, the ***flipped classroom*** strategy.

How do we help you learn?

- **Automatically recorded lectures**: Real-time recorded videos of our lectures will be available on *Canvas* ("Panopto Recordings").
- **Office hours**: We provide help and hints, but **not** straightforward solutions (we do not do homework for you), to your homework problems.
- **Communication channel**: Office hours and email.
- **Dynamic feedback collection**: Email me about any topics that you struggled with the most, and we will go through them either during one-on-one meetings, during office hours, or in class.

How should you learn in graduate school?

A graduate-level course is fundamentally different from an undergraduate-level course, not only in terms of the expectation, course content, and the pace of the lectures, but, more importantly, we rely heavily on ***active learning***. This is why you attend graduate school, and this is what you need to perform well in scientific research. In research, you need to develop problem-solving skills on your own (with some advice from your advisor, of course), learn the background material, and be highly self-motivated. I highly recommend studying the material *ahead* of our schedule since it requires a substantial time investment to digest the course content.

Since this is a 3-credit course, I expect, on average, you will spend **~ 2–3 hours studying the course material** *and* **~ 5–7 hours on problem sets** *every week*. If you find yourself spending far more time than this expectation, it probably means that you may have missed a couple of pieces of the puzzle in undergraduate thermodynamics, quantum mechanics and/or mathematics (this is perhaps due to different curriculum focus implemented at various schools). Do not panic! You could first focus on grasping the big picture and key ideas rather than on the detailed mathematical derivations. Nevertheless, I do not believe it is possible to truly understand and apply statistical mechanics without going through the math. Different students come in with different backgrounds. Everybody will advance in understanding at a different rate. That is expected; that is graduate school.

Textbook (required):

(1) Donald McQuarrie, *Statistical Mechanics*, published by University Science Books

(2) Mark E. Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation*, 2nd edition, published by Oxford University Press

Note: Textbooks in PDF format may be available for download online (e.g., Library Genesis).[1]

Reference mathematics book:

If you have trouble understanding the course material due to a lack of related mathematical background, I highly recommend you use the following book (which is written by a physical chemist) as your reference:

D. A. McQuarrie, *Mathematical Methods for Scientists and Engineers*, University Science Books

Note: In this course, I will assume you have studied *multivariable calculus* and *linear algebra* and are familiar with *complex numbers* and basic *ordinary differential equations*. It is perfectly fine to study these topics or refresh your memory along with the lectures.

Reference textbook (optional):

(1) Mehran Kardar, *Statistical Physics of Particles*, published by Cambridge University Press

(2) David Chandler, *Introduction to Modern Statistical Mechanics*, published by Oxford University Press

[1] I do not support downloading any textbooks from unknown resources. I do not suggest you use the Library Genesis without checking the copyright.

Written exam, quiz, and grading:

Item	Full marks	Contribution
Midterm exam 1 (2-hour; closed-book, allow one-page handwritten note)	100	20%
Midterm exam 2 (2-hour; closed-book, allow one-page handwritten note)	100	20%
Homework (Graded based on completion, not correctness)	30	15%
In-class quizzes (5 min; closed-book, closed-note)	30	10%
Final exam (3-hour; closed-book, allow one-page handwritten note)	150	35%

The above weighted average determines the absolute course score. The final course grade is assigned as:

Z = (absolute course score – class average)/class standard deviation

A: $Z \geq 1.433$; **A–**: $1.433 > Z \geq 1.233$; **B+**: $1.233 > Z \geq 0.766$; **B**: $0.766 > Z \geq 0$;
B–: $0 > Z \geq -0.333$; **C+**: $-0.333 > Z \geq -0.766$; **C**: $-0.766 > Z \geq -1.000$;
C–: $-1.000 > Z \geq -1.333$; **D**: $Z < -1.333$.

Midterm 1 (four questions) will cover classes 1 through 15; midterm 2 (four questions) will cover classes 16 through 30; the final exam (six questions) will likely cover all lectures. ***Exam problems are either direct drawn from or adapted from, with some variations, homework problem sets, plus problems directly testing the lecture note content on critical topics***.

The in-class quizzes are designed to help you review the course material in real-time. They will primarily test your fundamental understanding of the topics just covered. Each quiz will typically consist of a single multiple-choice question. Please note that the use of notes or books is not permitted. **I highly encourage you to spend ~1 hour just before my class (starting at noon) for review, which could be highly effective.**

Homework. Homework/Problem sets will be announced in class, assigned, and posted on *Canvas* after completing a certain topic or chapter in the textbook. **Each problem set contains three parts: (1) Due date, (2) Learning goals, and (3) Reading assignment (lecture notes, chapters, or sections from textbooks, research papers).** To fulfill the learning goals defined, you need to finish the reading assignments and do active learning. In the lectures and the in-class discussion sessions, I sometimes skip some details in derivations. It is your responsibility to fill these gaps with the help of reading material and online recorded lectures. Homework is designed to be pedagogical (and perhaps, challenging to some students); in other words, you can learn a lot (including some important topics that I did not cover in the lectures) by working out the questions assigned. **Homework will be graded based on completion, not correctness**, and solutions will be posted on *Canvas***. Each** **Problem** (a Problem contains many questions and parts) **fully completed earns you 1 point; half completion or minimum attempt earns zero points. Note that you do not have to solve the questions marked as "optional" unless you are interested in the content. You only need to turn in 30 completely solved Problems in order to reach full marks (30) for the homework item.**

You are highly encouraged to work *independently* on homework. If you choose to work with others as a team (or with Gemini or GPT), you have to turn in your own solution and show your understanding. Academic dishonesty is strictly forbidden.

If you choose to submit a scanned version of your written HW solutions, please email your file as a *single* PDF to the course TA *before* the deadline. You usually have about one week to finish a problem set. **Start these well ahead of their due dates as they require a substantial time investment to complete** (on average, ~ 3–4 hours every week). I am certain that you will NOT be able to solve all problems within 24 hours. ***No homework will be accepted after the deadline.***

Academic Integrity Policies. Please refer to https://www.bc.edu/bc-web/academics/sites/university-catalog/policies-procedures.html.html#tab-academic_integrity_policies for a statement about the importance of academic integrity and a reference to the university's academic integrity policy.

Plagiarism refers to the act of taking the words, ideas, data, illustrations, or statements of another individual or source and presenting them as one's own. This also encompasses the use of artificial intelligence (AI) text generators to fulfill key requirements of an assignment, such as reading, synthesizing, interpreting, writing, coding, or programming, *without* providing proper attribution and citation for any AI-assisted components. While AI can be a valuable learning tool (similar to Google), it should not be relied upon as a source for direct answers to complete assignments. Popular AI tools, like ChatGPT, are known to sometimes produce inaccurate information regarding math, physics-related inquiries, and tasks that necessitate careful quantitative reasoning.

Course Outline:

- (~3 classes) Recap of thermodynamics laws and functions; Legendre transform
- (~6 classes) Classical Hamiltonian mechanics, phase space, Liouville's theorem
  Applications: Classical molecular vibration analysis
- (~2 classes) Recap of probability concepts and combinatorics; Stirling's Approximation; Shannon entropy.
- (~4 classes) Principles of statistical mechanics, classical phase-space density and ensemble in Gibbs' approach; classical equipartition principle
- (~14 classes) Classical equilibrium statistical mechanics: Gibbs entropy; microcanonical ensemble and principle of maximum entropy, Boltzmann entropy.
  Ensembles in Boltzmann's approach: canonical ensemble, grand canonical ensemble, isothermal-isobaric ensemble; equilibrium fluctuation; liquid structure and radial distribution function.
  Applications: Ideal gas; Flory–Huggins solution theory for polymers; Debye–Hückel theory for electrolyte solution; Manning condensation – DNA and counterions; Langmuir adsorption isotherm
- (~5 classes) Quantized energy levels in statistical mechanics for ideal gas & Molecular partition functions
  Applications: Nanoparticle aggregation and design; Chemical equilibrium; Transition-state theory for reaction rates
- (~4 classes) Principles of quantum statistics, thermal density matrix; Von Neumann entropy; Feynman path integral formulation of equilibrium quantum statistics
- (~4 classes) Bose-Einstein statistics of photons, and Fermi-Dirac statistics of non-interacting electron gas
  Applications: Phonons and heat capacity of solids; Electronic heat capacity of conductors; Blackbody radiation and laser cavity

Only if time permits:

- Deviation from equilibrium by external driven forces (Non-equilibrium): fluctuation–dissipation theorem; classical linear response; quantum linear response
- Advanced topics (selective coverage and introductory):
  (1) Interacting particles for real gas: Mayer cluster expansion and graph theory
  (2) Interacting neurons in neural network: Use statistical mechanics to build machine learning
  (3) Time correlation functions in molecular spectroscopy
  (4) Ising model and phase transition, Landau-Ginzburg theory

Course Schedule:

- First lecture date: August 31 (Monday)
- We will NOT have in-person lectures on the following dates: Sept. 16 (Wednesday), and Sept. 18 (Friday). **Nevertheless, we will do active learning (e.g., pre-recorded lecture videos and lecture notes) on these two days.**
- We will NOT have lectures or office hours on the following university holiday dates: September 7 (Monday; Labor Day), October 12 (Monday; Fall break), November 25 & 27 (Wednesday, Friday; Thanksgiving)
- The **last** lecture is on **December 11** (Friday).
- Final exam date (**3 hours**): **December 14**, 9:00 AM – 12:00 noon.