

CHEM 6481: Statistical Mechanics, Fall 2026

Instructor Information

Instructor: Jesse McDaniel

Email: mcdaniel@gatech.edu

Meeting Times: Tuesday/Thursday 12:30–1:45 PM

Location: TBD

Office Hours: Day/time TBD, Molecular Sciences (MoSE) 2100L

Prerequisites: Undergraduate physical chemistry and multivariable calculus (exceptions may be permitted with permission of instructor).

General Course Information

Description

This is a graduate-level course on statistical thermodynamics and statistical mechanics. Topics include: review of thermodynamics, theory of ensembles, chemical and statistical thermodynamics of ideal monatomic and diatomic gases, heat capacity of insulating and metallic crystals, statistical thermodynamics of imperfect gases, structure of liquids, phase transitions/critical phenomena, and Monte Carlo methods.

Course Learning Outcomes

By the end of this course, students will learn the formalism for predicting/deriving macroscopic thermodynamic properties from either microscopic molecular models or first-principles/quantum-mechanical Hamiltonians using the framework of equilibrium statistical mechanics. Students will develop fluency with the canonical, microcanonical, and grand canonical ensembles, and understand basic fluctuation theory as applied to the different ensembles. Students will learn how to explicitly evaluate partition functions for the classes of systems that permit standard analytic treatment, including ideal monatomic and diatomic gases, phonons in crystals, 1D Ising model, and simple model Hamiltonians. Students will learn how to compute thermodynamic quantities from these partition functions, including internal energy, heat capacity, entropy, free energy, and chemical potential. Students will develop skills in standard statistical mechanical manipulations involving ensemble averages and fluctuation formulas. Students will additionally develop practical computational skills by implementing a Monte Carlo simulation of the 2D Ising

model in Python, gaining hands-on experience connecting theoretical predictions to numerical results.

Required Course Materials

Required Text: D.A. McQuarrie, “Statistical Mechanics” (University Science Books, 2000).
Additional Text: D. Chandler, “Introduction to Modern Statistical Mechanics” (Oxford, 1987) — PDF will be provided on Canvas. Reference texts for PhD research available on course page.

Grading System:

- Problem Sets 30%
- Midterm Exam 30%
- Final Exam 30%
- Ising Model Project 10%.

Problem Sets (30%): Approximately 7 problem sets that extend and supplement lecture material. Important derivations and concept extensions are covered in the problem sets. Problem sets will be posted to Canvas, and students will typically have 1.5 weeks to complete each problem set.

Ising Model Project (10%): Students will develop a Monte Carlo code to simulate a 2D Ising model, analyze thermodynamics, and visualize phase transitions using Python (Jupyter notebook, numpy, matplotlib). A template code will be provided for students with limited programming experience

Midterm Exam (30%): will be held on Tuesday, October 13, during the usual class time. The midterm exam will be closed book and closed notes.

Final Exam (30%): TBD, 11:20 AM – 2:10 PM. The final exam will be cumulative, and will be closed book and closed notes.

Final Grade Metric:

Your final grade will be assigned as a letter grade according to the following scale:

- A 85 – 100%
- B 70 – 85%
- C 55 – 70%
- D 40 – 55%
- F Less than 40.0%

Course Policies

Attendance and/or Participation

In-person attendance is mandatory. If a student has any concerns with in-person attendance, this should be discussed with Dr. McDaniel as soon as possible. There will be no class on Tuesday, October 6, due to the Institute-mandated fall break.

Academic Integrity

Students are expected to maintain the highest standards of academic integrity. All work submitted must be original and properly cited. Plagiarism, cheating, or any form of academic dishonesty will result in immediate consequences as outlined in the university's academic honor code: <https://policylibrary.gatech.edu/student-life/academic-honor-code>

Accommodations for Students with Disabilities

It is the responsibility of any student with a learning disability to request special accommodation if desired. Students must provide a letter of documentation from the Office of Disability Services for verification purposes. Such requests should be made well in advance of the time that the accommodation is required. [contact the Office of Disability Services](#) (404-894-2563) as soon as possible to make an appointment to discuss your special needs and to obtain an accommodations letter. Please also e-mail me as soon as possible in order to set up a time to discuss your learning needs.

Use of AI

AI can increasingly solve many homework problems at both the undergraduate and graduate level. AI is a powerful tool, but is not a substitute for your learning. Students are strongly encouraged to critically think through and work all problems on their own, without the use of AI. Students who solve problems themselves are the ones who learn the material effectively and do well on exams. The act of critically thinking through a problem is how you learn; copying down an answer found online (via AI or elsewhere) does not lead to learning and effective problem solving.

Student-Faculty Expectations Agreement

At Georgia Tech, we believe that it is important to strive for an atmosphere of mutual respect, acknowledgement, and responsibility between faculty members and the student body. [The Student-Faculty Expectations](#) articulate some basic expectations that you can have of me and that I have of you. In the end, simple respect for knowledge, hard work, and cordial interactions will help build the environment we seek. Therefore, I encourage you to remain committed to the ideals of Georgia Tech while in this class.

Campus Resources for Students

Course materials and announcements will be posted to Canvas. While general resources for graduate students at Georgia Tech are available through the Office of Graduate Education, good resources are typically found within your home department. For example, in the School of Chemistry and Biochemistry, Dr. Kenyetta Johnson is the Director of Graduate Studies, and serves as a central point of contact for first-year, chemistry PhD students.