

**CHE 720 Applied Statistical and Molecular Thermodynamics
Fall 2008 Syllabus and Schedule**

Instructor: Professor Brian Anderson
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Lecture Room: Rm 449 ESB

Lecture Time: Mon, Wed 3:00pm – 4:50pm

Text: Hill, Terrell L., *An Introduction to Statistical Thermodynamics*, Courier Dover Publications, 1986.

Course Philosophy: Statistical Thermodynamics is the study of the large-scale effects of fluctuations in physical systems. Since science and technology are operating at ever-smaller scales, understanding and controlling the role of fluctuations has become critical. Statistical mechanics has thus both provided the underpinning for the modern era of molecular-scale sciences, as well as undergone a revolution in its own conceptual and technical basis due to experimental and computational advances. The goal of this course is to equip you with the broad concepts and tools of Statistical Mechanics and Statistical Thermodynamics that are a cornerstone of contemporary science and engineering.

In addition, part of the time in this course will be allotted for you to work on special topics applying Statistical Mechanics in an area related to your research work or other interests.

Course Policies (exceptions at discretion of instructor):

1. There are no make-up exams.
2. All problem sets are due at the beginning of class or at the stated time.
3. A late assignment = no assignment.
4. Exam grading appeals must be submitted in writing on the day the exam is returned. If you miss that class, you lose the opportunity for regrading.
5. Any classes canceled due to inclement weather (or any other reason) will be rescheduled.
6. If the fire alarm goes off during an exam, the resolution of the situation is solely at the discretion of the instructor.
7. You may (and are encouraged to) work in groups on problem sets. However, what you submit must be your own work except for assignments that are designated as group assignments. Assignments that are obviously copied will receive no credit.
8. Problem sets and exams should be neat and easy to follow. Each problem should start on a new page. Your answer should be boxed, have units as appropriate, and have the correct number of significant figures. No credit will be given for answers without work. Credit will be deducted for missing or incorrect units, sloppy work that is hard to follow, and for the incorrect number of significant figures.
9. If you carry a cellular phone, it should be turned off during class. All cell phones are expected to be turned off or silenced during all class lectures and during exams. This type of interruption is disruptive to fellow classmates and will not be tolerated.

Grading:	Two Exams @ 20%	40%	The nominal grading scale is	$\geq 90\%$	A
	Journal Review	10%		$\geq 80\%$	B
	Homework	30%		$\geq 70\%$	C
	Project	20%		$\geq 60\%$	D
				$< 60\%$	F

At the instructor's discretion, this scale may be lowered, but not raised.

Journal Review: Each student will review a journal article from the contemporary literature that employs statistical mechanics. This can be theoretical or experimental, and preferably is in an area related to the student's research or other interests. Meetings will be set up with the professor to discuss the choice, understanding of the article, and presentation of the review. The review will be a two-page written report accompanied by a 10-minute presentation to the class.

Project or Literature Research: Each student will have the choice of either doing a project or literature research on a topic to be developed in consultation with the professor, again preferably in an area related to the student's interests or research. The project or literature research will be written up as a ten-page report, accompanied by a 20-minute presentation to the class. Project grading will reflect work put into the project, quality of work, and evaluations by the class.

Exams: There will be two exams in this class. Since the final week or two of the semester will be devoted to presentations by students on their projects or papers, there will be no final exam.

Some Ideas and Areas for Literature Research or Projects: Below are a few topical areas of Statistical Mechanics that are in active development today. These topics could be the subject of literature research (either a broad survey, or on a more specific topic), or a project (e.g., performing a Molecular Dynamic or Monte Carlo simulation on a system of your choice).

1. Nucleation and Growth
2. Rare Events
3. Transition Path Sampling
4. Glasses
5. Polymers
6. Non-Equilibrium Work Theorems and Single-Molecule Measurements
7. Microcanonical Statistical Mechanics and Density-of-States Monte Carlo
8. Brownian Ratchets, Maxwell's Daemons, and Biomolecular Motors
9. Chaos, Quantum Chaos, and Ergodicity

Other Recommended Texts: Chandler, David, *Introduction to Modern Statistical Mechanics*, Oxford University Press, 1987.

Hill, Terrell L., *Statistical Mechanics: Principles and Selected Applications*, Dover, 1987.

McQuarrie, Donald A., *Statistical Mechanics*, University Science Books, 2000.

Days of Special Concern:

WVU recognizes the diversity of its students and the needs of those who wish to be absent from class to participate in Days of Special Concern, which are listed in the Schedule of Courses. Students should

notify their instructors by the end of the second week of classes or prior to the first Day of Special Concern, whichever is earlier, regarding Day of Special Concern observances that will affect their attendance. Further, students must abide by the attendance policy of their instructors as stated on their syllabi. Faculty will make reasonable accommodation for tests or field trips that a student misses as a result of observing a Day of Special Concern.

Social Justice:

West Virginia University is committed to social justice. I concur with that commitment and expect to maintain a positive learning environment based upon open communication, mutual respect, and non-discrimination. Our University does not discriminate on the basis of race, sex, age, disability, veterans status, religion, sexual orientation, color or national origin. Any suggestions as to how to further such a positive and open environment in this class will be appreciated and given serious consideration.

If you are a person with a disability and anticipate needing any type of accommodation in order to participate in this class, please advise me and make appropriate arrangements with the Office of Disability Services (293-6700).

Course Syllabus and Tentative Schedule

Week	Topic	Notes
8/25	Introduction and Review of Thermodynamics	
9/1	Statistical-Mechanical Ensembles	Monday – Labor Day (no class)
9/8	2 nd and 3 rd Law	
9/15	No class	
9/22	Model Systems	
9/29	Ideal Gases (monatomic and diatomic)	
10/6	Monatomic Crystals	Exam I
10/13	Classical Statistical Mechanics	Meet to discuss journal article and project: 2-page journal review due
10/20	Journal Reviews	
10/27	Ising Model, Lattice gas	
11/3	Monte Carlo	
11/10	Chemical Equilibrium	Exam II Meet to discuss presentations
11/17	No Class – AIChE	Draft reports due Monday
11/24	No Class – Thanksgiving	
12/1	Student Presentations	Last Class – Wed 12/3