CHE 210A: Thermodynamics and Statistical Mechanics (F15)
UCSB Department of Chemical Engineering

schedule:	Monday, Wednesday, Friday 12:30-1:45pm (see schedule)
location:	Engineering II 3301
web page:	www.engr.ucsb.edu/~shell/che210a/

Course description

At their most basic level, thermodynamics and statistical mechanics are the sciences of equilibrium. Thermodynamics takes a macroscopic, bulk point of view, whereas statistical mechanics establishes the principles of equilibrium at the microscopic, molecular level. This course will integrate both perspectives to discuss the general features and properties of equilibrium, the relationships and constraints among thermodynamic variables, and simple models of gases, liquids, and solids. A strong emphasis will be placed on understanding the relationship between macroscopic, bulk behavior and molecular interactions.

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Main course text

Thermodynamics and Statistical Mechanics: An Integrated Approach, M. Scott Shell, Cambridge University Press, 2015

Other recommended texts

Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience, Ken Dill and Sarina Bromberg, Garland Science, 2010

An excellent modern introductory text to the subject particularly well-suited for self-study.

Statistical Mechanics, Donald A. McQuarrie, University Science Books, 2000 (2nd edition)

A classic statistical mechanics text, with clear, concise explanations of the subject material. It serves well as both an introduction to the subject and a reference. This book is also frequently used in ChE 210B.

An Introduction to Statistical Thermodynamics, Terrell Hill, Dover Books, 1987

This inexpensive paperback is a tour-de-force in laying out the foundations and early theoretical advancements of statistical mechanics. Hill discusses many of the subtleties that other texts glance over, and provides detailed derivations. It is an essential reference for anyone involved in research broadly related to molecular science.

Course policies

1. Final grades are computed from: 20% class interaction, 30% midterm, 50% final exam.
2. Students are expected to maintain the upmost ethics in all aspects of the course. This includes working problem sets independently and not seeking external solutions or answers online or otherwise.

How to succeed in this course

Thermodynamics and statistical mechanics can be difficult subjects to grasp. A number of healthy habits will make them clear and coherent:

1. **You, not me, are responsible for the learning.** At a graduate level, you must take full responsibility for deeply understanding the *subject*, regardless of the specific homework problems and lectures. Thoroughly read the course materials, work through problems in detail, and seek out other resources as necessary to aid your understanding. The point is to *know* thermodynamics and statistical mechanics, not to pass the course. These subjects are basics required of any research scientist.
2. **Take note of concepts and statements that you do not understand.** Write them down, jot things in the margins, constantly keep tabs on things that are a source of difficulty and confusion for you. Then, seek out answers. Work through problems a second time. Consult a different text book. Ask a peer. Visit office hours. If you don't understand it well enough to teach it to someone else, you're not there yet.
3. **Be an independent learner.** Work on problems by yourself first. Try to resolve blocks by taking different approaches, working on different examples, or reading other texts. *Then*, consult your peers for discussion of the best approach. Don't work with others on problem sets from the get-go because that will let things you don't understand slip by unnoticed.
4. **Pose yourself questions.** After working through a problem, ask yourself, "What would happen in that problem if X were changed to Y?" Challenge yourself to think of possible variations beyond the examples in the lectures and problem sets.
5. **Invest time.** Thermodynamics requires quality practice to become familiar with the concepts, calculus, and mathematical manipulations involved. Don't be afraid to work extra examples in the book, or find new books to consult. Your goal should not be to master the problem sets, but to master the subject.
6. **You are supposed to struggle.** This is a challenging course, and you will only understand the material by struggling with it through reading, thinking, and working problems. Don't expect to know the answer right away, and avoid feeling competitive with other students as you will find that everyone has different backgrounds. Your job is to learn and understand, not to beat the curve.

Assigned homework problems

2.6	7.6	12.11	17.11
3.5	7.16	12.21	18.7
3.6	7.24	12.28	18.11
3.9	8.7	12.29	18.14
3.11	8.8 (g)	14.1	18.20
3.16	8.21	14.13	18.24
4.3	9.13	15.8 (c,f,g,h only)	18.28
4.10	9.21	15.16	19.9
5.9	10.9	16.1	19.16
5.13	10.11	16.8	19.20
6.3	10.12	16.11	19.21
6.10	11.6	16.12	20.19
6.20	11.10	16.23	20.26
6.25	12.7	17.10	

Additional problems recommended for study

2.10	9.1	12.25	18.16
3.14 (a only)	9.10	14.4	18.29
4.14	9.18	14.8	18.30
5.3	10.17	14.14	18.32 (a only)
6.18	10.19	14.19	19.11
7.13	10.20	15.14	20.3 (a,b,c only)
7.19	10.22	16.9	21.7
7.27	11.1	16.17	
8.3	11.14	17.2	
8.11	12.22	17.13	

Tentative schedule

lecture	date		topic	HW (book)
1	9/25	F	Equilibrium and entropy Probability and how to count	
2	9/28	M	How the microscopic world works	2.6, 3.5
3	9/30	W	How the macroscopic world works	3.6, 3.9, 3.11
	10/2	F	***no class – Graduate Student Symposium***	
4	10/5	M	The fundamental equation	3.16, 4.3, 4.10
5	10/7	W	The first law and reversibility	5.9, 5.13, 6.10
6	10/9	F	Legendre transforms and other potentials	6.20, 6.25
7	10/12	M	Maxwell relations and measurable quantities	7.6, 7.16, 7.24
8	10/14	W	Gases	8.7, 8.8g, 8.21
9	10/16	F	Phase equilibrium	9.13, 9.21
10	10/19	M	Stability	10.9, 10.11, 10.12
11	10/21	W	Solutions	11.6, 11.10, 12.7
12	10/23	F	Solutions	12.11, 12.21
13	10/26	M	Solids	12.28, 12.29
14	10/28	W	***MIDTERM***	
15	10/30	F	The third law review midterms	14.1, 14.13
16	11/2	M	The canonical partition function	15.8cf, 15.16
17	11/4	W	The canonical partition function	16.1, 16.8, 16.11
18	11/6	F	Fluctuations	16.12, 16.23
	11/9	M	***no class – MSS travel***	
	11/11	W	***no class – holiday***	
19	11/13	F	Statistical mechanics of classical systems	17.10, 17.11, 18.7
20	11/16	M	Statistical mechanics of classical systems	18.11, 18.14, 18.20

21	11/18	W	Other ensembles	18.24, 18.28
	11/20	F	***no class – MSS travel***	
22	11/23	M	Chemical equilibrium	19.9, 19.16
23	11/25	W	Reaction coordinates and rates	19.20, 19.21
	11/27	F	***no class – holiday***	
24	11/30	M	Molecular simulation methods	20.19, 20.26
	12/2	W	***no class – MSS travel***	
	12/4	F	***no class – MSS travel***	