CHM 6461

Statistical Thermodynamics

Syllabus, Spring Semester 2015

Statistical thermodynamics provides the connection between the microscopic and macroscopic descriptions of systems. For chemistry, this means the connection between the atomic and molecular nature of materials and their thermodynamic properties. Traditionally, the three major areas of physical chemistry are thermodynamics, quantum mechanics, and statistical mechanics (reaction dynamics could be a fourth). There is often too little time to cover statistical thermodynamics in the undergraduate curriculum, but it is a necessity for physical chemistry (and other subfields) at the graduate level. [The term "statistical thermodynamics" refers to systems at equilibrium. When non-equilibrium as well as equilibrium processes are considered, one refers "statistical mechanics."]

Instructor

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Office Hours: Tuesday 3-5 pm

Time and location

TR 9:30-10:45, CP 115

Required text

Statistical Mechanics, Donald McQuarrie (University Science Books: Sausalita, CA, 2000), ISBN-13: 978-1891389153, ISBN-10: 1891389157.

Recommended texts:

Almost any undergraduate physical chemistry text

An Introduction to Statistical Thermodynamics, Terrell Hill (Dover: New York, 1986), ISBN-13: 978-0486652429, ISBN-10: 0486652424.

Introduction to Modern Statistical Mechanics, David Chandler (Oxford University Press: Oxford, 1987), ISBN-13: 978—105042771, ISBN-10: 0195042778.

The required text is very good, and it is the classic text on the subject and the most widely used text for graduate level introductory study in chemistry departments. However, it may be helpful to read alternative approaches. Most undergraduate texts will have a chapter on statistical mechanics, which may be a good source to consult if you become confused about the general "lay of the land." McQuarrie largely based his text on the book by Hill, but occasionally Hill's presentation is different from McQuarrie's, and it has the advantage of being a Dover edition and thus inexpensive ($10.21 according to my latest check at www.amazon.com). Both McQuarrie and Hill are two-semester texts. The text by Chandler is a slender volume, and in fact I used it as the required text the first time I taught the course. The presentation is often quite different from the other McQuarrie's and Hill's. I changed to McQuarrie because students found that Chandler was sometimes difficult to follow because of a high level of abstraction and because steps were omitted from derivations. Nevertheless, I highly recommend Chandler for an alternative perspective.

Prerequisite

CHM 3411 or permission of instructor. Essentially, one should have thermodynamics and quantum mechanics at the undergraduate level before taking statistical thermodynamics.

Grading

Grades will be based on homework (15%), one lecture presentation (10%), one mid-term exam (25%), and a final exam (50%).

Homework

Problem sets will be assigned at roughly two week intervals. Due dates will be firm. I may assign each student a topic to present to the class, for experience teaching and because one learns most by teaching. We will discuss this possibility after the mid-term exam.

Exam schedule

Mid-term exam: take-home, Fri-Sun Apr 27-29 (anticipated but could change)
Final exam: During week of Apr 27 – May 2, precise time and date TBA

Course Outline

Topic	*Chapter*
Introduction and Review	1
The Canonical Ensemble	2
Other Ensembles and Fluctuations	3
Boltzman Statistics, Fermi-Dirac Statistics, and Bose-Einstein Statistics	4
Ideal Monatomic Gas	5
Ideal Diatomic Gas	6
Classical Statistical Mechanics	7
Ideal Polyatomic Gas	8
Chemical Equilibrium	9
Quantum Statistics	10
Crystals	11
Imperfect Gases	12
~~Distribution Functions in Classical Monatomic Liquids~~	~~13~~
~~Phase Transitions~~	~~Handouts~~

We will spend approximately one week on each topic. Chapter 1 is a brief review of pertinent concepts from thermodynamics, quantum mechanics, mathematics and statistics. You will be largely responsible for this on your own. Chapters 2 and 3 lay the conceptual foundation for statistical mechanics. Be certain that you understand this material. Chapter 4 is also basic. Chapters 5, 6 and 8 apply the principles to the simplest of quantum mechanical systems, ideal gases. Chapter 7 extends the basic formalism to classical statistical mechanics. The difference is that, since quantum mechanical systems are generally discrete (in terms of energy levels, for example), a discrete formulation of statistical mechanics is generally needed for chemical systems. Classical statistical mechanics is based on continuum, rather than discrete, distributions. Chapters 12 and 13 apply the principles to more complicated systems of chemical interest (imperfect gases and monatomic liquids). The last topic, not covered in McQuarrie but very important to chemists, is phase transitions.