

# STATISTICAL THERMODYNAMICS & MECHANICS OF MATERIALS

MSE 500

Fall 2026

**Instructor:** Professor Ken Schweizer

206 MSEB

kschweiz@illinois.edu

**MWF 9-10:20 am** (often ends earlier)

**136 Loomis Lab of Physics**

## LOGISTICS

In the pre-covid era, the course was delivered on the blackboard with students taking notes. During fall 2020 the course was taught on Zoom, and I developed a full set of “lecture notes” and visual aids (called “vugraphs” in pre-covid days) organized in PDFs which mimic precisely how the blackboard lectures were given. This fall I will lecture using these PDFs with computer projection. ***So, you really do not need to take detailed notes, so please ask questions, they benefit everyone. However, I must emphasize that lectures do not simply read the PDFs, there is a lot explanations not on the slides.*** I will also use the blackboard to answer specific questions or further elaborate on a topic. *I will send you the PDF lecture slides by email in packets of roughly 3 as we go through the material. I will send you the full packet of vugraph slides for each of the 3 course parts in one document each. **So do check your email regularly.***

I urge everyone to regularly attend class. Unfortunately, attendance in this class, and many/most other MSE courses post-covid, has significantly dropped. Not good. MSE 500 is a demanding graduate course, and **falling behind generally has serious consequences**. Trying to learn the material solely by reading lecture slides is **not** a good idea. Not attending class also conflicts with the goal of building community in graduate school, and everyone learns when students ask questions.

***\*\*Lectures will NOT be recorded\*\****

If you have a question not asked during class, you can generally ask me right after the lecture, or email me. If more in depth questions arise, I am **always** happy to arrange a 1-on-1 meeting.

All homework sets and answers (and all other course materials per above) are sent to you directly by email. **I do not upload anything on a course website (none exists).**

**Office Hours:** The class is large, with students with many different schedules and from different departments. Not practical to set one time. Please email me and we can arrange a meeting. I reply quickly.

**Homework:** There is **no TA**, so homework is **not** collected/graded. I will give you answers. **It is your job to carefully study it** and see what you did not get correct. If you have any questions, please contact me.

Problem sets will be given every week and are a **key to learning**. I suggest you first work hard on it **alone**. If you have difficulties, then discuss the problems with each other. ***If you look at the answers before working hard on problems by yourself then you will learn nothing.*** Students who have trouble with the course almost always make this mistake of not first working hard by themselves on the problems and/or fall behind early in the course and do not promptly resolve things they do not understand.

**EXAMS:** Two midterms on parts I and II plus a final exam.

**First exam on Part I** (expect material covered ends by October 2)

**1<sup>st</sup> exam** in it likely October 16

**Second exam on Part II** (expect material covered ends by Nov. 4 or 6)

**2<sup>nd</sup> exam** likely Nov. 18 or 20

**Final Exam:** comprehensive, but **strongly emphasizes Part III**. The time and date are set by the University and not changeable: **8 am, Monday, December 14**. Last class is Wednesday, December 9.

Exams are in class. Mid-terms are 80 minutes. Final exam 3 hours. **All exams are closed book and notes.** You are allowed to create one sheet (1 side) of formulas/information in order to avoid having to memorize. Putting it together is a good experience to identify what is really important. But do **not** overemphasize its importance. Exams are meant to test your understanding and critical thinking ability, not deliver facts from a summary sheet.

### Course Grading:

Exams 1 and 2: 20 or 30% each      Final: 40 or 60 %

*I determine weighting factors to maximize your composite exam average and hence final course grade.*

### My Travel.

I will be out of town Monday-Thursday, October 26-29. As usual, one class will be canceled. For the other, a link to a recorded lecture will be sent. I will be in town to proctor both mid-term exams this year.

**\*REQUIRED TEXT: KD:** Ken A. Dill & Sarina Bromberg, *Molecular Driving Forces – Statistical Thermodynamics in Chemistry & Biology*, Garland Science, Taylor & Francis Group, NY and London, **2<sup>nd</sup> edition**.

For some topics I follow the Dill book. For **many** I do not. For a few topics there is **nothing** in the book. Even if I “follow” Dill to some extent, I almost always do things differently for further clarity and to give you an additional perspective not in any textbook which helps deepen understanding.

### SUPPLEMENTAL BOOKS *on reserve in Grainger Engineering Library*

**DC:** David Chandler, *Introduction to Modern Statistical Mechanics*, 1987.

**McQ:** Donald A. McQuarrie, *Statistical Mechanics*, 2000.

**TLH:** T.L.Hill, *Introduction to Statistical Thermodynamics*, 1960.

**NG:** N.Goldenfeld, *Lectures on Phase Transitions & Renormalization Group*.

**PM:** P.M. Morse, *Thermal Physics*, second edition, 1969.

*Book abbreviations employed in the suggested reading for each topic in the course outline given below.*

### **\*\*Friendly Advice\*\***

*I urge you to not fall behind, especially since this is a fundamental physics-based course that continuously builds on prior material, and integrates concepts and methods throughout the semester. It is not easy to recover from a “bad start”. For MSE PhD graduate students, this is especially important since you must receive a “B” or higher so that it counts towards passing the qualifying exam.* Typically a few students receive a course grade below “B” each year, and need to effectively re-take the course. But there is **NO** mandate nor quota this must happen, and it can be avoided by good study habits and effort.

Statistical thermodynamics and mechanics is a quantitative, physics-based, fundamental science that requires mathematics. *If your math skills are rusty, I urge you to brush up on basic calculus.* The Dill book has very nice review material on math tools. I will **not** cover these in class, but I suggest to read these chapters immediately if needed. *This includes the elementary probability and statistics of Dill chapter 1 which is briefly covered in mainly the first two lectures.*

## COURSE OUTLINE 2026

**NOTE #1:** The estimated number of lectures for each topic is indicated in parentheses. Relevant reference material available from the Dill textbook (**KD**) and other supplementary books is indicated using their abbreviations given above. **Reading this material is optional. By far the most important thing is to deeply understand what is presented in the class lectures/notes.** The references in *ITALICS* are best to read if you want extra information/explanations beyond what I present. You will need to decide if it is helpful.

**NOTE #2:** On the copies of the PDF lecture slides I distribute you will see a **Lecture #** is indicated for each class. I will often switch back and forth to the **“Vugraph” file** during class. It has extra information, illustrates specific points, show graphs, conceptual images, and experimental data. Each vugraph slide is numbered as **VG #**. They are referred to on the lecture notes slides.

**NOTE #3:** This course is **not** about classical macroscopic thermodynamics. That is an undergrad pre-requisite. I briefly review key aspects of thermodynamics as needed as we go through different topics.

### PART I: Fundamentals and Elementary Applications (16)

#### I. Brief Introduction to Probability and Statistics (1-1.5)

*\*\*Read ALL of KD Ch.1                      not all will be covered in class*

#### II. Thermodynamics, Entropy, First & Second Laws, and Boltzmann Law Concepts (7)

- A. Extremum Principles            *KD, Ch.2*
- B. Heat, Work, Energy and the First Law    *KD, Ch.3; DC, Ch. 1.1*
- C. Boltzmann Entropy and Introductory Statistical Thermodynamics    *K2, Ch.5*
- D. Free Energies, Temperature, Equilibrium and Ideal Gas  
*KD, Ch. 7, Ch.8 ; DC, Ch. 1.2,1-1.4 ; PM, Ch.17*

#### III. Statistical Mechanics and Elementary Applications (8)

- A. Boltzmann Distribution Law, Partition Function, Ensembles  
Ensembles, Heat Capacity, Energy Fluctuations  
*KD, Ch.10; Ch.12, p.230-232; DC, Ch.3.1-3.4; PM, Ch.18,19*
- B. Discrete Systems  
flexible molecules, paramagnetism via Boltzmann & “order parameter” approaches  
*KD, Ch.10, p.184-188*
- C. Continuum Systems  
Ideal atomic gas, Classical vs. Quantum, Particle-in-a-Box model  
Vibrations, Harmonic Oscillators, Einstein model of solids  
Molecules, degrees of freedom, and Partition function factorization  
*KD, Ch.11 and Ch. 12, p228-232 ; PM, Ch.18,21,22*

## PART II: Gases, Fluids, Liquids, Mixtures, Phase Behavior & Surfaces (12)

### IV. Phase Equilibria & Thermodynamics of 1-Component Fluids (5)

---

#### A. Interactions & Generic Phase Equilibria

*KD, Ch.24, p.471-479*

*KD, Ch. 14, 1<sup>st</sup> two sections; Ch.25*

#### B. Classic Van der Waals Model

Equation-of-State, Virial expansion, Liquid-Vapor phase transition, Isothermal compressibility, Law of corresponding states *KD, Ch.24, p.479-483* ; NG, Ch 4.1-4.4

#### C. Microscopic Lattice Fluid Model

Partition function, athermal limit, mean field approximation, attractions, connection to van der Waals model *DC, Ch.5.2* ; *KD, Ch.24, p.485-486*

### V. Continuum Fluids: Thermodynamics, Structure and Freezing (3)

*\* Dill book has virtually nothing on this section \**

#### A. Hard Sphere Fluids (relevant to atoms, molecules, colloids)

1-dimensional Tonks model, comparison to lattice fluid model

#### B. Correlation functions, Radial Distribution function $g(r)$

*DC, Ch. 7.2, 7.3, 7.5* ; *McQ, Ch. 13.1-13.3* *KD, Ch.24, p.483-485*

#### C. Thermodynamic Properties, Structure and Crystallization

3-dimensional packing effects, repulsive vs. attractive forces

*DC, Ch. 7.4* ; *McQ, Ch.2.1-12.3, 13.9, 14.3*

### VI. Two Component Liquid Solutions and Solid Alloys (3)

Phase Diagrams & mean field theory for Liquid-Liquid phase separation

*KD, Chapters 15 and 25*

*TLH, Ch.14.4, 20.1*

### VII. Surfaces (1)

Physical Adsorption, Monolayers & Langmuir Isotherm *KD, Ch.27, p.541-546*; *TLH, Ch 7.1+14.1*

## PART III: Crystals, Magnets, Biopolymers and Quantum Statistics (11)

*Last class is Wednesday December 9 and you are responsible for the lecture material that day.*

### VIII. Thermal Properties of Crystals (1)

Collective phonons, vibrational properties, heat capacity, Debye model, comparison of Debye and Einstein models, characteristic temperatures

*McQ Ch. 11.1-11.3 + 11.6 + Handout*      DC, Ch.4.3 ; PM, Ch.20

### IX. Cooperative Phenomena (7 or 8 ; likely will skip section E this year)

#### A. Order Parameters, Critical Phenomena, Broken Symmetry

General concepts, Landau approach      *KD, Ch 26*

#### B. Spatial Correlations and Susceptibility

Spin correlation functions, density fluctuations, correlation length

#### C. Ising Model, Spins, Magnets

1-d Ising model, Curie-Weiss Mean Field theory, Fluctuation effects and energy-entropy competition; Effect of spatial dimension; External fields

*DC, 5.1, 5.3,5.4 ; NG, Ch. 3.7, 4.5      KD, p.525-527*

#### D. Order-Disorder Phase Transitions in Solids

Description of ordered state (e.g. Cu-Zn alloy), Mean Field theory

*Handout*

#### E. Helix-Coil Conformational Transition in Biopolymers

Polypeptides, Conformation, Hydrogen-bonding, Entropy vs. Energy

*KD, Ch.26, p.527-535*

### X. Quantum Electronic Phenomena (3 or 2) *\*topics not covered in the Dill book\**

#### A. Quantum Statistics

Non-interacting systems, Fermi-Dirac statistics, Fermi level

*DC, Ch. 4.3, 4.4 ;    McQ, Ch.4.2 ;    PM, Ch 24*

#### B. Electron Gas and Metals

Ideal Fermi gas of electrons, Electronic heat capacity

*DC, Ch.4.5 ;    McQ , Ch. 10.1,10.2 ;    PM, Ch.26*