BioE 103: Engineering Molecules II

Department of Bioengineering, UC Berkeley

> “Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you anymore.”
>
> - Arnold Sommerfeld

Course Format: Three hours of lecture and one hour of discussion per week.

Instructor:

Terry Johnson (418 HMMB)

GSI:

Suraj Makhija

Office Hours:

- Terry - Mondays 4:30-6PM in 418 HMMB
- Suraj - Fridays 9-10:30AM in the b1 Stanley Atrium

Textbook: Molecular Driving Forces by Dill and Bromberg, 2nd edition

Recommended: a standard (52 card) playing card deck and a set of RPG dice (d4, d6, d8, d10, d12, d20, d100)

Important dates:

- Midterm review session - Friday 10/13 in class
- No class meeting - 10/18 3-4PM
- Midterm - Wednesday 10/18 8-10PM in 10 Evans
- Final exam - Wednesday 12/13 7-9PM in 160 Kroeber

Course Description

This course is designed to introduce undergraduates to the thermodynamics and kinetics in the context of design. Chemical manipulations of or by biological molecules are informed by an understanding of these subjects, and will prepare students to approach complex problems in synthetic and systems biology, cell and tissue engineering, and biomaterials.

While this syllabus is meant to be accurate description of the course and its content, it may be modified at the instructor's discretion.

Objectives

To introduce students chemical kinetics and thermodynamics, in the context of molecular design.

Grading Policy

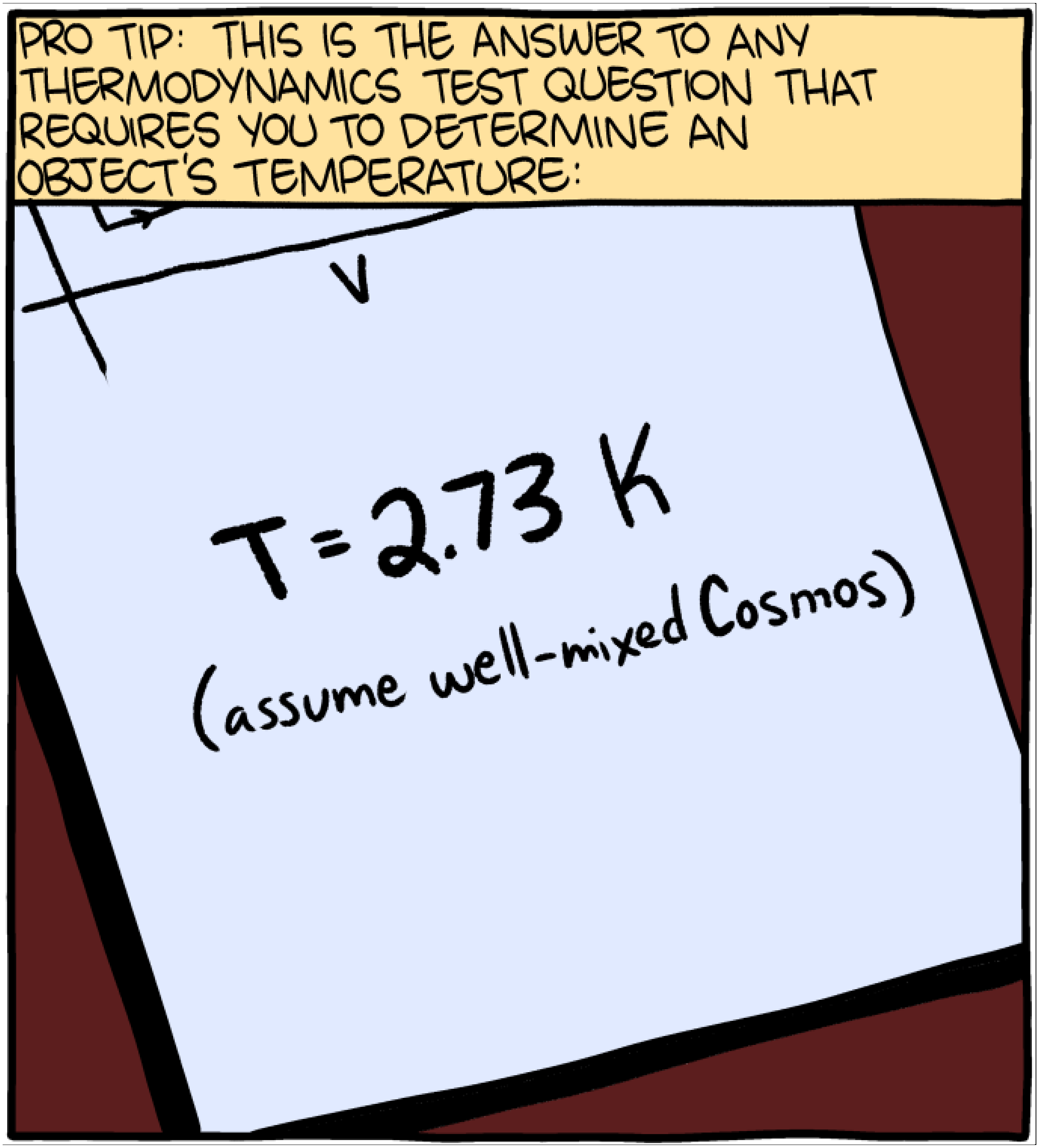

Image credit: smbc.com

34% Homeworks (1/2 credit for late homeworks turned in before solutions are posted, no credit afterwards)

33% Midterm

33% Final exam

Please note: we expect you to work with others in this class. While outright copying is not allowed, collaboration on assignments is very much encouraged. Find a study group and make them a regular part of your week!

If you would like to contest a homework grade, you must turn the homework or exam back in to one of the instructors with a note briefly describing the issue. The regrade will be considered during the next grading cycle. You should not expect that the instructor or the GSI will regrade anything while in conversation with you - that would not be fair to the other students in the class, whose homeworks were graded without them present.

Homeworks must be written in ink to be considered for regrades. Regrade requests should be based on an error on our part (e.g., adding up the points incorrectly) or what you suspect is a misunderstanding of your work (e.g., arriving at the correct answer using an unexpected technique). Regrade requests that argue with the rubric (e.g., “this is wrong, but you took too many points off”) will be returned without consideration.

Your homeworks should stand alone. If a homework is disorganized or ambiguous, and requires an extensive explanation to the grader, you will likely still lose points. The homeworks are not only evaluating your understanding of the material - they are also meant to evaluate your ability to communicate that understanding clearly and concisely. Also, be aware of UC Berkeley's Code of Student Conduct. Plagiarism or cheating will not be tolerated.

When deliverables are missed due to unavoidable circumstances, alternate arrangements can be made at the instructor's discretion. Don’t be shy! Dealing with unavoidable circumstances is part of my job. The sooner you contact me regarding issues such as these, the better. If something is preventing you from a satisfactory engagement with this course, let me know so I can take the appropriate steps to accommodate you.

Course Content

You will not be responsible for material in the chapters and sections in red below.

1 Principles of Probability

The Principles of Probability Are the Foundations of Entropy

What Is Probability?

The Rules of Probability Are Recipes for Drawing Consistent Inferences

Correlated Events Are Described by Conditional Probabilities

Combinatorics Describes How to Count Events

Collections of Probabilities Are Described by Distribution Functions

Distribution Functions Have Average Values and Standard Deviations

2 Extremum Principles Predict Equilibrium

What Are Extremum Principles?

What Is a State of Equilibrium?

An Extremum Principle: Maximizing Multiplicity Predicts the Most Probable Outcomes

Simple Models Show How Systems Tend Toward Disorder

3 Heat, Work, & Energy

Energy Is a Capacity to Store and Move Work and Heat

Energy Is Ubiquitous and Important

Some Physical Quantities Obey Conservation Laws

Heat Was Thought to Be a Fluid

The First Law of Thermodynamics: Heat Plus Work Is Conserved

Atoms and Molecules Have Energies

Why Does Heat Flow?

The Second Law of Thermodynamics Is an Extremum Principle

4 Math Tools: Multivariate Calculus (review on your own)

5 Entropy & the Boltzmann Law

What Is Entropy?

Maximum Entropy Predicts Flat Distributions When There Are No Constraints

Maximum Entropy Predicts Exponential Distributions When There Are Constraints

What Is the Reason for Maximizing the Entropy?

6 Thermodynamic Driving Forces

Thermodynamics is Two Laws and a Little Calculus

The Fundamental Thermodynamic Equations, $S = S(U,V,N)$ or $U = U(S,V,N)$, Predicts Equilibria

The Fundamental Equations Define the Thermodynamic Driving Forces

The Second Law Predicts Thermal, Mechanical, and Chemical Equilibria

7 The Logic of Thermodynamics (old school)

8 Laboratory Conditions & Free Energies

Switch from Maximum Entropy to Minimum Free Energy

Free Energy Defines Another Extremum Principle

Thermochemistry: The Enthalpy of a Molecule Is the Sum of the Enthalpies of Its Covalent Bonds

Theresa Head-Gordon’s notes on Standard States (posted on bcourses)

9 Maxwell’s Relations & Mixtures (a bit advanced for a first course in the subject)

10 The Boltzmann Distribution Law

Statistical Mechanics Gives Probability Distributions for Atoms and Molecules

The Boltzmann Distribution Law Describes the Equilibria Among Atoms and Molecules

What Does a Partition Function Tell You?

Thermodynamic Properties Can Be Predicted from Partition Functions

Theresa Head-Gordon’s notes on Molecular Energy (posted on bcourses)

End of Midterm Material

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11 The Statistical Mechanics of Simple Liquids and Gases (old school)

12 What Is Temperature? What Is Heat Capacity? (very interesting, but not essential)

13 Chemical Equilibria

Simple Chemical Equilibria Can Be Predicted from Atomic Structures

Le Chatelier's Principle Describes the Response to Perturbation from Equilibrium

The Temperature Dependence of Equilibrium Is Described by the Van't Hoff Equation

14 Equilibria Between Liquids, Solids, & Gases

Phase Equilibria Are Described by the Chemical Potential

The Clapeyron Equation Describes p(T) at Phase Equilibrium

How Do Refrigerators and Heat Pumps Work?

Surface Tension Describes the Equilibrium Between Molecules at the Surface and the Bulk

15 Solutions & Mixtures

A Lattice Model Describe Mixtures

Interfacial Tension Describes the Free Energy of Creating Surface Area

What Have We Left Out?

16 Solvation & the Transfer of Molecules Between Phases

The Chemical Potential Describes the Tendency of Molecules to Exchange and Partition

Solvation Is the Transfer of Molecules Between Vapor and Liquid Phases

A Thermodynamic Model Defines the Activity and Activity Coefficient

Adding Solute Can Raise the Boiling Temperature of the Solvent

Adding Solute Can Lower the Freezing Temperature of a Solvent

Adding Solute on One Side of a Semipermeable Membrane Causes an Osmotic Pressure

Solutes Can Transfer and Partition from One Medium to Another

Dimerization in Solution Involves Desolvation

17 Physical Kinetics, Diffusion, Permeation, and Flow (will be covered in BioE 104)

18 Microscopic Dynamics (will be covered in BioE 104)

19 Chemical Kinetics & Transition States

Chemical Reaction Rates Depend on Temperature

The Mass Action Laws Describe Mechanisms in Chemical Kinetics

At Equilibrium, Rates Obey Detailed Balance

Chemical Reactions Depend Strongly on Temperature

Activated Processes Can Be Modeled by Transition-State Theory

Catalysts Speed Up Chemical Reactions

The Brønsted Law of Acid and Base Catalysis: The Stronger the Acid, the Faster the Reaction it Catalyzes

A First Approximation: The Evans–Polanyi Model of the Brønsted Law and Other Linear Free Energy Relationships

Funnel Landscapes Describe Diffusion and Polymer Folding Processes

20 Coulomb's Law of Electrostatic Forces

21 The Electrostatic Potential

22 Electrochemical Equilibria

23 Salt Ions Shield Charged Objects in Solution

24 Intermolecular Interactions

25 Phase Transitions

26 Cooperativity: the Helix–Coil, Ising, & Landau Models

29 Bio & Nano Machines

Biochemical Machines Are Powered by Coupled Binding Processes

Oxygen Binding to Hemoglobin Is a Cooperative Process

Binding Polynomials Can Treat Multiple Types of Ligand

Rates Can Often Be Treated by Using Binding Polynomials

The Molecular Logic of Biology Is Encoded in Coupled-Binding

Biochemical Engines Harness Downhill Processes to Drive Uphill Processes

Theresa Head-Gordon’s notes (posted on bcourses) on:

- Binding
- Enzyme Catalysis

30 Water

31 Water as a Solvent

Oil and Water Don't Mix: the Hydrophobic Effect

The Signature of Hydrophobicity Is Its Temperature Dependence Alcohols Constrict the Volumes in Mixtures with Water

Ions Can Make or Break Water Structure

Ion Pairing Preferences in Water Depend on Charge Densities

32 Polymer Solutions

Polymer Properties Are Governed by Distribution Functions

Polymers Have Distributions Conformations

Polymer Solutions Differ from Small-Molecule Solutions

The Flory–Huggins Model Describes Polymer Solution Thermodynamics

Flory–Huggins Theory Predicts Nonideal Colligative Properties for Polymer Solutions

The Phase Behavior of Polymers Differs from that of Small Molecules

The Flory Theorem Says that the Intrinsic Conformations of a Chain Molecule Are Not Perturbed by Surrounding Chains

Everything below this line is if we have time for it!