Class I

Thermodynamic ~ motion of heat

Energy, entropy, free energy

1800's — empirical

behavior of molecules on average

↔ bulk thermodynamics

Chemistry:

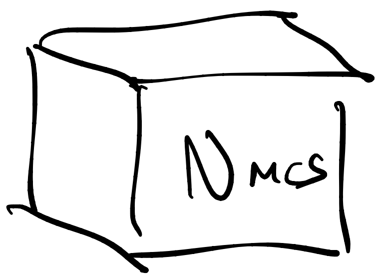
Chemical reaction

Equilibrium

Kinetics – motion of atoms

– how long rxn occur

Statistical thermodynamics



3N degrees of freedom (6N)

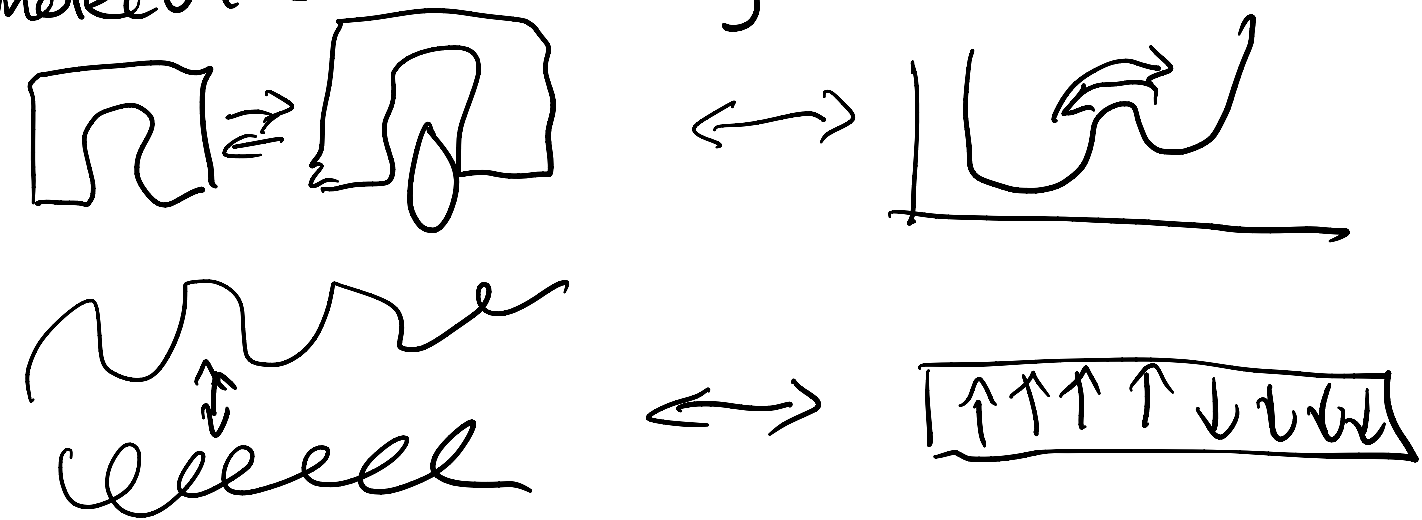
$x_1, y_1, z_1, \; v_x^1, v_y^1, v_z^1$ } few quantities

$\vdots \qquad \vdots$

3N → state variables

(N, V/P, T)

Biomolecular Thermodynamics



Mathematics – language

probabilities

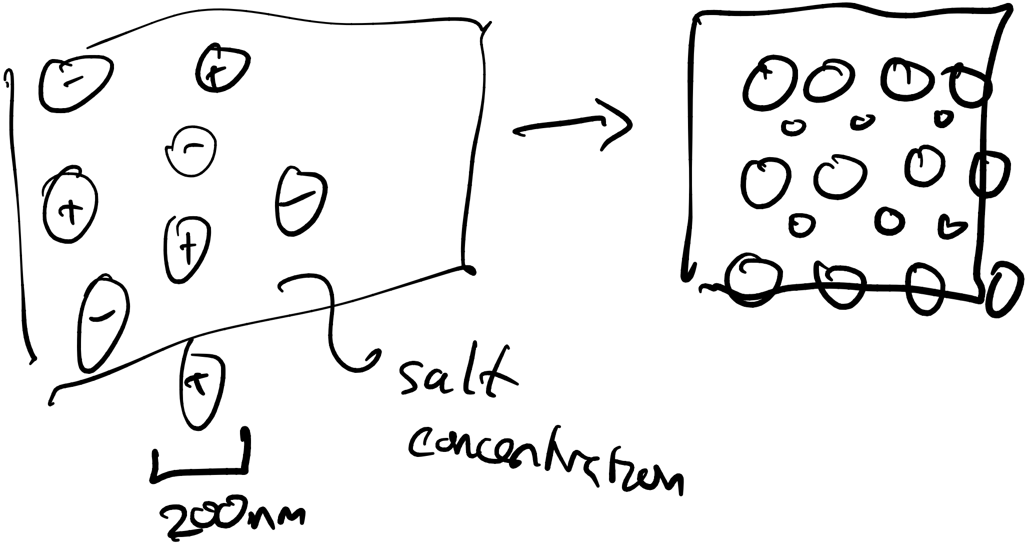
calculus ← maximum minimum

Data & programming

Empirical

self assembly

Sacanna Lab



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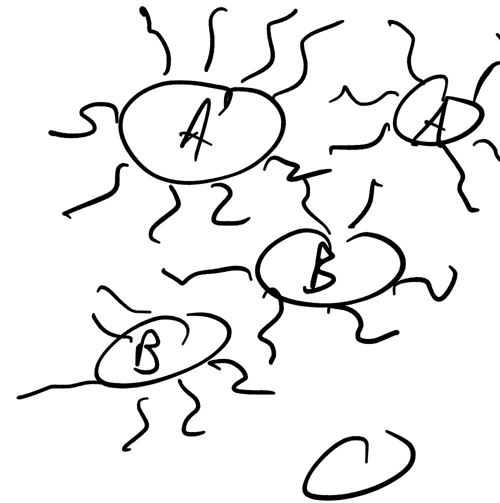

Biophysics

Free energy landscape
how do protein complexes activate

Molecular dynamics simulation

CHEM UA 652 - PHYSICAL CHEMISTRY: THERMODYNAMICS AND KINETICS
SPRING 2024

Class Time/Room: Tuesday, Thursday, 2PM-3:15 PM. Silver 101A
Instructor: Glen Hocky hockyg@nyu.edu

Teaching Asst.: Nicodemo Mazzaferro

Office Hours: Glen Hocky TBD, Location TBD
Nicodemo Mazzaferro TBD, Location TBD

survey

Office hours start the second week of classes.

Course Overview:
This class covers the topics of thermodynamics and kinetics, which are *fundamental* to understanding all chemical reactions.

This semester, the course will use as its example problems drawn from biology. This is so that we have concrete modern examples for each topic. Don't worry, all of the traditional topics will still be covered. Moreover, as you will see, there are deep connections between the examples from biology and from other areas of chemistry and materials science. For example, at the end of the class you will see how the temperature dependence of a peptide folding is deeply connected to the magnetization transition in materials.

Overarching goals for the class:
By the end of the course, every student should have improved their understanding and skills in the following areas.

1. Learn about the fundamental laws and quantities in thermodynamics. That means answering the questions, what are energy, heat, work, entropy, and how are they connected? What is free energy and how does it relate to equilibrium constants. How and why do phase transitions occur? What are the molecular underpinnings of potential and kinetic energy, and how do these relate to reaction rates? Can we derive the fundamental macroscopic ideas of thermodynamics from microscopic principles ("statistical mechanics")?
2. Improve and refresh abilities in certain key areas of calculus including partial differential equations.
3. Improve abilities in the area of probability and statistics, and how these connect to entropy and free energy via statistical mechanics.
4. Have a working knowledge python programming and its application to physical chemical problems, including mathematical and statistical simulations and data analysis.

Course websites*:*
Course material and assignments will be available on ***NYU Brightspace***. Also, I will be sending email communications via *Brightspace.*

There may be an interactive programming assignment for the course, in which case the assignments will be completed at a website such as:
https://chemua-652-spring.rcnyu.org/ ← check

Required reading:
The main text will be "***Biomolecular thermodynamics: from theory to application***," by Doug Barrick (Johns Hopkins University).

1) Digital access is available for free via the NYU Library:
https://doi-org.proxy.library.nyu.edu/10.1201/9781315380193

2) A copy of the book is on 2-hour reserve at Bobst library
3) The book is available from the NYU bookstore, and also can be purchased from Amazon and from CRC Press
https://www.crcpress.com/Biomolecular-Thermodynamics-From-Theory-to-Application/Barrick/p/book/9781439800195

Additional resources
There are many textbooks on thermodynamics that approach the topic from different perspectives. Some ones you may want to take a look at to supplement your knowledge, and which I may draw from for the topic of Chemical Kinetics include the following. They are all on course reserve at Bobst.
1) *Physical Chemistry: A Molecular Approach* by Donald A. McQuarrie
2) *Physical Chemistry: Principles and Applications in Biological Sciences.* Ignacio Tinoco, Jr. et al
3) *Molecular Driving Forces*. Ken Dill, Sarina Bromberg

Recitations:
Recitations will be used to review key concepts, as well as to go over exams and past homework in more detail. They may also be used to introduce extra material, such as in the first recitation. You need to be registered for one of the recitation sections.

Office hours:
There will be regularly scheduled office hours held by the Professor and the TA. If you cannot attend either and would like to meet, please **message through brightspace**.

Purpose of office hours. What is the point of office hours? Many people never attend office hours, or they do so only right before or right after an exam. But office hours can be so much more than for emergencies! This is a great chance for us to get to know each-other better. It is also a good time to clear up confusions you (or we) have about the material. We never want people to feel like they are behind. It's also a great time to discuss how the course material relates to your other interests, or to discuss more advance topics. So please consider attending as many office hours as you can from the beginning!

Class Attendance:
We know that you will sometimes have to miss class or recitation. However, attendance is *strongly* encouraged. Although it is possible to learn this material from a book, I am going to spend many hours per week trying to digest complex ideas and produce the best 1.25 hour presentation of those ideas that I can. To do that, I need feedback from you! Making this a great class requires input from all of you. This goes for recitation as well.

Online contingencies — The intention is to have this course fully in person. However, for various extenuating purposes it may be necessary to offer the class through Zoom, in which case the link will be made available through brightspace.

There will sometimes be worksheets (see next section) contributing to a participation grade in lecture. Although it is not currently the intention to give quizzes, if attendance drops off in recitation then we may start giving quizzes that also go in the participation part of your grade.

Participation
Research has shown that taking an active role in learning is much more effective than passively listening in lecture. Hence, we will incorporate some activity and discussion into our course. One way this may be done is with some in class worksheets that you will work on with a neighbor and turn in together. Another way in which this is done will be Just-In-Time (JIT) learning. JIT is a technique that will help us gauge your understanding of the material as well as spark discussion. Occasionally, you'll receive a few simple problems that will be due 9pm the evening before lecture. Then during lecture, we will discuss the results

and that will help us know what material needs further review. These will not be graded for correctness, but for completion, and will contribute to a participation grade.

Respect and inclusion
Another goal of this course is to create a learning environment that is inclusive and fosters contributions from all students. No one in the course should be made to feel uncomfortable because of the identity or background. If you feel like your performance in the class is being impacted by your experiences outside of class, please don't hesitate to come and talk with me.

Problem sets:
Problem sets will be given every 1-1.5 weeks and will be due approximately 1 week later. Problem sets will be turned in by scanning and uploading them to Brightspace. Problem sets turned in during the next 24 hours will receive ¾ credit, and ½ credit during the next 24 hours. After that, answers will be posted and problem sets will no longer be accepted. Partial credit will be given for partial solutions, so please turn in whatever you have done on time.

Some problem sets will have a computational/programming component. The reason for this is that some programming and data analysis is an essential skill for future work in science, and it will also look great on your resumé. These will be done in Python3 through a dedicated course website, on which some problems may be automatically graded. These should be completed by their assigned due date with the same policy as above. Please contact us if you believe there is a technical problem with the course site or in one of the problems.

To make sure everyone is on the same page with regards to introductory python programming, a python crash course assignment will be given first, and more concepts will be introduced as needed.

In both cases, you are encouraged to work with your peers on problems, but *please then go and write your own solutions/programs*. You can list up to two people that you worked with on the homework, and it's okay for those solutions to be the same.

Exams:
There will be four exams, three midterms and a final. These exams will be closed book, but you can bring a 1-page (double sided) equation/study sheet of your own making. You can also bring a standard calculator (*non-graphing, no-calculus)*. This is so that everyone has equal resources and opportunity.

Questions will generally be in the same style as the problem sets. The final will be on the scheduled exam date. The final will likely cover both the last bit of material as well as some questions covering key topics from earlier parts of the course.

For fairness, anyone missing an exam without an excused absence from NYU Student Health (or similar) will be given a zero on the exam.

Grading:
Grading will be weighted with the following breakdown:

(drop one)

Participation:	10%
Homework:	20%
Midterms:	15% each (45% total)
Final:	25%

Regrade policy
Mistakes happen, so you may need to have an exam regraded. If so, you must adhere to the following policy:

- Do not make any marks on the exam.

- On a separate, hand-signed cover sheet stapled to the exam, list your email address, state the problems that were mis-graded, and affirm that no changes to the exam were made after grading
- Submit the regrade request within two days of receiving the graded exam.
- Arithmetic errors in adding up points will be corrected immediately. Any other regrade request will cause the entire exam to be regraded; therefore, your overall score may increase or decrease.
- Oral or late requests for regrading will not be accepted.

Academic Integrity and Plagiarism:
As you know, we take academic honesty very seriously at NYU. The instructors for this course have no tolerance for plagiarism or cheating. The NYU policy on plagiarism will be enforced. Students who fail to conform to NYU's standards on academic integrity will be subject to stringent disciplinary action. Inform yourself in advance of proper academic conduct. In brief (and quoting from the College of Arts & Science policy), "Academic honesty means that the work you submit – in whatever form – is original." When in doubt, ask. Please consult: http://cas.nyu.edu/page/academicintegrity

Note, as stated above for problem sets, you are encouraged to work together and list other people that you actually wrote out the solutions with. Actually copying someone else's work outside of this policy will be considered plagiarism and given a zero. Cheating on an exam or attempted cheating on a regrade will result in a zero, as well as possible further disciplinary consequences. Also, uploading coarse material to or use of web resources that solve problems for you (e.g. Chegg) constitutes cheating as well.

Disability Disclosure Statement
Academic accommodations are available for students with disabilities. Please contact the Moses Center for Students with Disabilities (212-998-4980 or mosescsd@nyu.edu) for further information. Students who are requesting academic accommodations are advised to reach out to the Moses Center as early as possible in the semester for assistance.

Approximate Lectures Overview

Date	Subject	Reading
Section Week 1	~~*No Recitation the first week*~~	
Jan 23, Jan 25	**Intro**, Calc, Probabilities and elementary events	Ch 1, Ch 2 up to page 46
	probabilities of combinations, probability distributions	
Section Week 2	Python, data analysis, plotting, curve fitting	Ch 2, pp 47-60
Jan 30, Feb 1	Classical thermo: thermodynamic framework, first law	Ch 3, pp 87-101
	Classical thermo: work	Ch 3, pp 101-126
	Classical thermo: heat	Ch 4, pp 131-137
Section Week 3	TBD	
Feb 6,8	Classical thermo: 2^{nd} law, spontaneous processes	Ch 4, pp 137-142
	2^{nd} law, heat engines and Carnot cycles	Ch 4, pp 142-147
	2^{nd} law: general cycles and the entropy.	Ch 4, pp 147-151, 157-168
Section Week 4	TBD	
Feb 13,15	2^{nd} law: irreversible processes, S potential, statistics	Ch 5, pp 173-187
	Classical thermo: potentials (G, A)	Ch 5, pp 187-201
	Classical thermo: mixtures, molar quantities	Ch 6, pp 209-223
Section Week 5	Review and Exam prep	
Feb 20	**EXAM 1**	
Feb 22	Classical thermo: phase transitions	Ch 7, pp 233-241
Section Week 6	TBD	
Feb 27 Feb 29	Classical thermo: phase transitions	Ch 7, pp 241-254
	Classical thermo: chemical potentials, standard states	Ch 7, pp 254-261
	Classical thermo: mixtures and mixing	Ch 7, pp 258-268

Section Week 7	TBD	
March 5 March 7	Conformational equilibrium and transitions	Ch 8, pp 273-286
	Denaturation of proteins	Ch 8, pp 286-291
	Protein stability curves and calorimetry	Ch 8, pp 291-295, 301-302
Section Week 8	TBD	
March 12,14	Chemical kinetics	Supplemental materials
		E.g. Dill Ch 17-19
		McQuarrie Ch 27-29
March 19 March 21	**Spring break**	
Section Week 9	TBD	
March 26, 28	Chemical kinetics	Supplemental materials
Section Week 10	Review and Exam prep	
April 2	**EXAM II**	
April 4	Stat thermo: ensemble concepts, Lagrange multipliers	Ch 9, pp 303-316
	Stat thermo: partition functions, heat exchange model	Ch 9, pp 316-324
Section Week 11	TBD	
Apr 9, Apr 11	Stat thermo: the Boltzmann distribution and *Q*	Ch 10, pp 327-338
	Stat thermo: kT and thermodynamic functions	Ch 10, pp 338-343
	Stat thermo: examples, isothermal isobaric ensemble	Ch 10, pp 343-355
Section Week 12	TBD	
Apr 16, 18	Molecular and reaction partition functions	Ch 11, pp 359-370
	Helix-coil theory—framework and independent sites	Ch 12, pp 373-384
	Exam review, Helix-coil theory—zipper model	Ch 12, pp 384-389
Section Week 13	TBD	
Apr 23, 25	Helix-coil theory—matrix approach	Ch 12, pp 389-394
	Binding equilibria (BE): single sites	Ch 13, pp 403-413
	BE: multiple sites, macro treatment, binding polynomial	Ch 13, pp 413-420
Section Week 14	Midterm review	
April 30	**EXAM III**	
May 2	Course review	
Section Week 15	Course review	
Finals, May 8-14, TBD	**Final Exam**	

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Chem UA 631

Glen M. Hocky

Worksheet 1 – Thermodynamics in the wild

Person 1: ______________ Person 4: ______________

Person 2: ______________ Person 5: ______________

Person 3: ______________

Some thermodynamics keywords

Energy | Entropy | Temperature | Pressure | Volume | Free-Energy

Phases | Gas Solid | Liquid | Crystal | Glass

Viscosity | Diffusion | Emulsion | Mixture | Equilibrium

Binding | Folding | Enzymes | Catalyst | Battery

You will be assigned one topic from below (circle it)

Car | Plane | Light bulb | Refrigerator | Washing machine

Water | DNA | Mammal | Tree | Pizza | Computer | Cell Phone

Write some thoughts on how "thermodynamics and kinetics" apply

Glen M. Hocky

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<u>Write some thoughts on how "thermodynamics and kinetics" apply</u>

Computer — T

— energy usage/transfer

Pizza specific heat of pizza?

phase change

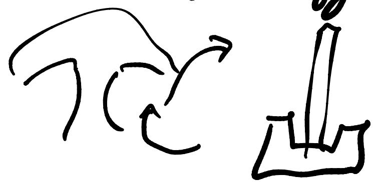
| Yeast →

gas → energy

Tree Photosynthesis

Energy absorption

Crystal?



Fridge cycling.

coolant.

Washing machine detergents