CHEM UA 652 - PHYSICAL CHEMISTRY: THERMODYNAMICS AND KINETICS
SPRING 2020

Class Time/Room: Tuesday, Thursday, 2PM-3:15 PM. Bobst LL1-50

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Office Hours: Glen Hocky   Wed 10:30am-noon, Silver 1018
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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. Why? Many people who take this class are interested in pursuing careers in more biological areas and in biochemistry.

What about the people who don't care about biology? 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 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 Classes*. Also, I will be sending email communications via *Classes*.

Interactive programming assignments will be completed at a special website (more info later):
https://chemua-652.rcnyu.org/

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:
   http://bobcat.library.nyu.edu/permalink/f/ci13eu/nyu_aleph005530026
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 **email us**.

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.

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, at the beginning of class. 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.

In order to make sure everyone is on the same page with regards to introductory python programming, a python crash course assignment will be given the first week, 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 three exams, two 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 last regularly scheduled class day (May 7). 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:

Participation:	10%
Homework:	25%
Midterms:	20% each (40% 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.

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 28, Jan 30	**Intro**, Calc, Probabilities and elementary events probabilities of combinations, probability distributions	Ch 1, Ch 2 up to page 46
Section Week 2	Python, data analysis, plotting, curve fitting	Ch 2, pp 47-60
Feb 4, Feb 6	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 11, 13	Classical thermo: 2nd law, spontaneous processes	Ch 4, pp 137-142
	2nd law, heat engines and Carnot cycles	Ch 4, pp 142-147
	2nd law: general cycles and the entropy.	Ch 4, pp 147-151, 157-168
Section Week 4	TBD	
Feb 18, 20	2nd 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	TBD	
Feb 25, 27	Classical thermo: phase transitions	Ch 7, pp 233-241
	Classical thermo: phase transitions	Ch 7, pp 241-254
	Classical thermo: chemical potentials, standard states	Ch 7, pp 254-261

Section Week 6	Review and Exam prep	
March 3	**EXAM I**	
March 5	Discuss exam, Classical thermo: mixtures and mixing	Ch 7, pp 258-268
	Intro to conformational equilibrium	Ch 8, pp 273-282
Section Week 6	TBD	
March 10	Conformational equilibrium and transitions	Ch 8, pp 282-286
March 12	Denaturation of proteins	Ch 8, pp 286-291
	Protein stability curves and calorimetry	Ch 8, pp 291-295, 301-302
Section Week 7	TBD	
March 17, 19	**No Class, Spring Recess**	
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March 17	Chemical kinetics	Supplemental materials
March 19		E.g. Dill Ch 17-19
		McQuarrie Ch 27-29
Section Week 8	TBD	
March ==24==, 26	Chemical kinetics	Supplemental materials
Section Week 9	TBD	
March 31, Apr 2	Stat thermo: ensemble concepts, Lagrange multipliers	Ch 9, pp 303-316
	Stat thermo: partition functions, heat exchange model	Ch 9, pp 316-324
	Stat thermo: the Boltzmann distribution and Q	Ch 10, pp 327-338
Section Week 10	TBD	
Apr 7, Apr 9	Stat thermo: kT and thermodynamic functions	Ch 10, pp 338-343
(Passover)	Stat thermo: examples, isothermal isobaric ensemble	Ch 10, pp 343-355
	Molecular and reaction partition functions	Ch 11, pp 359-370
Section Week 11	Review and Exam prep	
Apr 14	**EXAM II**	
Apr 16	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 12	TBD	
Apr 21, 23	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 13	TBD	
Apr 28, 30	BE: macroscopic treatment, interacting sites	Ch 13, pp 420-430
	BE: microscopic treatment and stepwise constants	Ch 14, pp 441-450
	BE: micro overall constants, interacting sites	Ch 14, pp 450-462
Section Week 14	TBD	
May 5	**Final Exam Review**	
May 7	**Final Exam**	