

## Chemistry 422/522: Statistical Mechanics: Modern Aspects

David Case, instructor. Office: 208b Proteomics, skype: dacase; cell: 609-751-8668

email: [david.case@rutgers.edu](mailto:david.case@rutgers.edu)

Spring 2021, Mondays and Wednesdays, 9:15 to 10:35am Eastern + asynchronous lectures

This is a one-semester physical chemistry course with an emphasis on applications of thermodynamics and statistical mechanics to chemical and biochemical systems. It is an advanced course, and will build on the introduction to chemical thermodynamics you may have received in physical chemistry courses like CCB 327, or 525.

The course text is *Molecular Driving Forces, 2nd ed*, by Ken Dill and Sarina Bromberg. We will skip around some in this book, and there will be additional handouts for most topics. The table below gives an approximate time schedule; detailed reading assignments will be made as the class proceeds.

**Note:** Although there will be some overlap with material that Prof. Khare used for Chemistry 525 in the Fall, I will try to keep that to a minimum. Chem 525 is *not* a pre-requisite for this course. Even where there is necessarily some overlap with Chem 525, you will be getting a different perspective here.

Week starting	Subject	Chapter
Jan 20, 25	Quick review of classical of thermodynamics	3,5,6,8
Feb 1	Fundamentals of statistical thermodynamics	10,11
Feb 8, 15	Microscopic dynamics	18,24
Feb 22, Mar 1	Microscopic electrostatics	20,21,23
Mar 8	Mixtures: salt-water in biophysics	30,31
Mar 22, 29	Chemical reaction rates	19, (27)
Apr 5	Cooperativity and allostery	26,28,29
Apr 12, 19	Simulations of liquids; connections to experiment	
Apr 26, May 3	Student project presentations	

The course website is <http://casegroup.rutgers.edu/lnotes.html>. Reading and homework assignments and additional course materials will be posted there. Final grades in the class will be based on assigned homework/problem sets (30%), projects/presentations (40%) and exams (30%). Midway through the semester, each student will choose a project, which can be related to research you are carrying out, or to some facet of thermodynamics, statistical mechanics, or kinetics that interests you. Students will be expected to make a short oral presentation to the rest of the class, as well as to attend and provide feedback to other student presentations. A written summary of the project will also be required. Two take-home exams will be given during the course of the semester and announced as least one week beforehand; there will not be an exam during the Final Exam period.

**Please note:** Students are expected to adhere the university policies on academic integrity and student conduct in all assignments, assessments and other matters regarding this course. These policies can be found online: <https://nbprovost.rutgers.edu/academic-integrity-students>. You may consult with fellow students on homework and on class projects, but you must personally prepare and understand any written material you hand in. You may *not* consult with fellow students on the exams.

## Notes on course administration

1. The course website is here: <https://casegroup.rutgers.edu/lnotes.html>
2. I will post two recorded lectures per week on the course website; there will also be a PDF version of the slides for each lecture.
3. Since we have a small enrollment, I am going to try a “tutorial” approach, meeting individually with each of you about once every other week. These might be short meetings if there is not much to discuss, but I will spend as much time as is needed. (We can have group meetings you want, but let’s start this way.)
4. This means that there will generally *not* be any presentation at the scheduled class times, although individual meetings might take place then. The exception to this will be on *April 26, April 28 and May 3*, when you will each make a presentation, and listen to your fellow students. (Details about this will be announced later.)
5. Homework assignments will generally be posted weekly on the course website. Please submit homework via email in a PDF or similar format.
6. Please send an email to [david.case@rutgers.edu](mailto:david.case@rutgers.edu) with the following information
  - Name, email address, and the time zone where you live.
  - Are there good or bad times for you to meet with me?
  - Did you take CCB 525 from Prof. Khare last semester? Have you completed an undergraduate course in Physical Chemistry?
  - Do you have questions or suggestions?
7. Please let me know if you are having problems or questions! Generally, I find that email usually works best – I should always be able to answer promptly. But you are welcome to use Skype (my Skype id is “dacase”) or text (to +1-609-751-8668) as well.