CHEM 430/530A – FALL 2015

INSTRUCTOR: Ziad Ganim
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REFERENCE BOOKS: *Statistical Mechanics*; D.A. McQuarrie

(recommended) Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience; K.A. Dill, S. Bromberg

(recommended) An Introduction to Statistical Thermodynamics; Terrill L. Hill

COURSE WEBSITE: http://canvas.yale.edu, then add this course

TIME/LOCATION: *MW 9.25-10.15 in Sterling Chemistry Lab 19*

F(optional) 9.25-10.15 in Rosenkranz Hall, Room 01
Off-hours computer lab: Kline Biology Tower, CSSSI

General Description:

The fundamentals of statistical mechanics developed and used to elucidate gas phase and condensed phase behavior, as well as to establish a microscopic derivation of the postulates of thermodynamics. Topics include ensembles; Fermi, Bose, and Boltzmann statistics; density matrices; mean field theories; phase transitions; chemical reaction dynamics; time correlation functions; Monte Carlo and molecular dynamics simulations.

Grading: Homework, Examinations, and Final:

Problem sets will be assigned and due approximately weekly. The problem sets and final emphasize the skills necessary to use statistical mechanics in research. As such, many Friday class meetings are dedicated to working through practical issues relevant to the problem sets and course material in a discussion format, and those sessions are *optional*. Midterm examinations will be scheduled by majority opinion of the class and will take place in the late afternoon.

Problem Sets	50%	Six assignments
Midterm I	15%	Between Sep 25 – Oct 2
Midterm II	15%	Between Nov 2 – Nov 9
Final Project	20%	Final Report: Dec 18, Oral Presentations: Dec 21, 9am-2pm

In lieu of a final examination, you will have an opportunity to demonstrate your understanding of the course material with a final project that will consist of a written report and oral presentation. The topic and scope of work should be approved by the instructor by Nov 20. The final project topic may be drawn from your research interests, a topic outside your thesis, or by extending any problem set from the course. The written component should be in *J. Phys. Chem. Lett.* format (template http://pubs.acs.org/page/jpclcd/submission/authors.html). The oral component will be a 20 min presentation of your work followed by a question/answer period with the class.

Course Schedule:

2-Sep	**Lec 01**	*Assemblies, Ensembles, and The Ergodic Hypothesis*	*PS1 Assigned*
4-Sep	Lab 01	*Optional: Discussion/PS1*	
9-Sep	**Lec 02**	*Macroscopic Properties from Microscopic Probabilities, Canonical Distribution*	*PS1 Due / PS2 Assigned*
11-Sep	**Lec 03**	*Information Theory and Statistical Mechanics*	
14-Sep	**Lec 04**	*Macroscopic Properties from the Canonical Partition Function*	
16-Sep	**Lec 05**	*Microcanonical Ensemble and Fluctuations*	
18-Sep	Lab 02	*Optional: Discussion/PS2*	
21-Sep	**Lec 06**	*Separable Hamiltonians, Distinguishable vs. Indistinguisable Particles*	
23-Sep	**Lec 07**	*Boltzmann, Fermi-Dirac, and Bose-Einstein Statistics*	*PS2 Due*
		Midterm I Covers Lec01-07, PS1-2	
25-Sep	**Lec 08**	*Molecular Partition Function, Translational Part of Boltzmann Partition Function*	
28-Sep	**Lec 09**	*Quantum vs. Classical Qtrans . Equipartition. Internal Degrees of Freedom*	*PS3 Assigned*
30-Sep	**Lec 10**	*Internal Degrees of Freedom for Atoms and Diatomic Molecules*	
2-Oct	Lab 03	*Optional: Discussion/PS3*	
		Midterm I Deadline	
5-Oct	**Lec 11**	*Rotational Partition Function. Equipartition*	
7-Oct	**Lec 12**	*Polyatomic Molecules*	
9-Oct	Lab 04	*Optional: Discussion/PS3*	
12-Oct	**Lec 13**	*Polyatomic Molecules*	*PS3 Due / PS4 Assigned*
14-Oct	**Lec 14**	*Nuclear Spin Statistics: Symmetry Number, Sigma*	
16-Oct	Lab 05	*Optional: Discussion/PS4*	
19-Oct	**Lec 15**	*Catch up*	
26-Oct	**Lec 16**	*Introduction to Density Matrices*	*PS4 Due / PS5 Assigned*
28-Oct	**Lec 17**	*Density Matrices and Application to Spin Systems*	
30-Oct	Lab 06	*Optional: Discussion/PS5*	
		Midterm II Covers Lec08-17, PS3-5	
2-Nov	**Lec 18**	*Model Intermolecular Potentials, Virial Equation of State*	*PS5 Due / PS6 Assigned*
4-Nov	**Lec 19**	*Simple Liquids*	
6-Nov	Lab 07	*Optional: Discussion/PS6*	
9-Nov	**Lec 20**	*Einstein and Debye Solids*	
		Midterm II Deadline (Covers Lec08-16, PS3-6)	
11-Nov	**Lec 21**	*Free Electron Theory of a Metal*	
13-Nov	Lab 08	*Optional: Discussion/PS6*	
16-Nov	**Lec 22**	*Chemical Equilibrium and Phase Transitions*	
18-Nov	**Lec 23**	*Chemical Reaction Rate Theory*	
20-Nov	Lab 09	*Optional: Discussion/PS6*	*PS6 Due*
		Final Project Topic Approval Deadline	
30-Nov	**Lec 24**	*Special Topics 1 (i.e., Non-equilibrium Statistical Mechanics, Onsager relations)*	
2-Dec	**Lec 25**	*Special Topics 2 (i.e., Macromolecules, Statistical Mechanics of Water)*	
4-Dec	Lab 10	Final Project Work	
7-Dec	**Lec 26**	*Thermodynamics I*	
9-Dec	**Lec 27**	*Thermodynamics II*	
11-Dec	Lab 11	Final Project Work	
18-Dec	**Final**	Written Final Due	
21-Dec	**Final**	9am-2pm, Final Presentations	

Computer Lab / Matlab Programming:

Friday computer lab meetings will take place in Rosenkranz Hall (Prospect 115), Room 01. Hours and further information: http://schedule.yale.edu/csssi_rkz

A closer option to the chemistry buildings is the CSSSI Classroom in the Kline Biology Tower, C27, subject to availability when other classes are not in session: http://schedule.yale.edu/csssi_kbt

You are also encouraged to download and run Matlab on your personal machine, which is available free of charge to all Yale students. Begin by navigating to: http://software.yale.edu/Library/chooseOS and following your OS-specific instructions.