Course Schedule, Exams, Reading and Homework

-The course website is at https://gruebele-group.chemistry.illinois.edu/courses/chem-440
-**Dates:** Check below for dates of all lectures, exams, reviews!
-**Lecture**: MWF at 11-11:50 AM in 161 Noyes Lab. The title summarizes the lecture content.
-**Reading**: There is no textbook, full course notes are at the web site, covering **O** = overview, **Q** = quantum, **S** = stat mech & quantum, **T** = transport and kinetics. For example, "**Q1 p1-3"** = read Quantum notes Chapter 1, pages 1 through 3.
-**BOH**: Gruebele 'Big Office Hours' and reviews. Generally on Fridays at noon. Gruebele will stick around past noon as long as you get there by then and not all questions have been answered.
-**Homework**: All homework is listed in the course notes. Solutions are posted already, on the days most closely related to a particular homework problem. Do *all* homework, but only the **green** problems must be turned in for grading and credit. Assignments are due at the beginning of the first class of the next week. (e.g. if two green problems are assigned on various days in week 1, both are due on Monday of week 2, but you should also do the remaining problem(s) from the assigned reading).
-**Hour exam and final exam questions** 80% of questions are modified homework problems, in-class exercises, and thought experiments, listed in the course notes so *keep up with all of them every week*!

Date	Lecture	Reading	BOH	Homework
1/19 L1	The goals of pchem; averages, derivative models	O1 p1-3		Do O1.1
1/21 L2	Randomness, Bayesian inference	O1 p3-5	noon	Do O1.2, O1.3
1/24 L3	Why logarithms, complex numbers	O1 p 6-7		Do O1.4
1/26 L4	Why go 'quantum'? Music and quantum mechanics	Q1 p1-3		Do Q1.1 Play with MD demo
1/28 L5	The Postulates of quantum mechanics	Q1 p4-5	noon	Do Q1.2
1/31 L6	Some consequences of the postulates	Q1 p6-7		Do Q1.3
2/2 L7	Of molecules and springs	Q2 p8-10		Do Q2.1, Q2.2 Play with QM demo
2/4 L8	Weird properties of quantum springs	Q2 p10-12	noon	Do Q2.3, Q 2.4
2/7 L9	Other models interesting for chemistry: 'The Box'	Q3 p13-15		Do Q3.1
2/9 L10	The simplest atom	Q3 p16-17		Do Q3.2
2/11 TA-L11	The simplest molecule	Q4 p18-19		Do Q4.1 IQmol documentation
2/14 L12	The forbidden region and quantum interference: bonding and antibonding	Q4 p19-20		Do Q4.2
2/16 L13	Multi-electron molecules	Q4 p21-22		Do Q4.3
2/18 L14	Potential surfaces and absorbing/emitting light	Q5 p23-24	noon	Do Q5.1
2/23 Exam	**Hour Exam #1, covers L1-13,** Open annotated textbook and notes.			

2/25 L15	Can spectroscopy detect alien life?	Q5 p25-26	noon	Do Q5.2, Q5.3
2/28 L16	How do chemical reactions go over barriers	Q5 p27-28		Do Q5.4
3/2 L17	From mechanics to statistical mechanics	S1 p1-3		Do S1.1
3/4 L18	The Postulates of statisstical mechanics	S2 p4-5	noon	Do S2.1
3/7 L19	The microcanonical partition function	S2 p6-7		Do S2.2
3/9 L20	Entropy and deriving the 'laws' of thermodynamics	S2 p8-9		Do S2.3
3/11 L21	What is temperature?	S3 p10-12	noon	Do S3.1, S3.2
3/21 L22	Thermodynamic potentials E, F, G and H	S3 p12-14		Do S3.3, S3.4
3/23 L23	Heat flow, heat capacity and thermo calculations	S3 p14-15		Do S3.5, S3.6, S3.7, S3.8
3/25 L24	Reactions at constant temperature	S4 p16-18	noon	Do S4.1
3/28 L25	Folding proteins with stat mech	S4 p19-20		Do S4.2
3/30 L26	Solving problems with the partition function	S4 p21-22		Do S4.3, S4.4
4/1 Exam	**Hour Exam #2, covers L14-24,** In-class, open annotated textbook and notes.			
4/4 L27	Chemical equilibrium	S5 p23-24		Do S5.1, S5.2, S5.3
4/6 TA-L28	Mass action law	S5 p25-26		Do S5.4
4/8 L29	Calculating K_{eq} from first principles	S5 p27-28	noon	Do S5.5
4/11 L30	Moving molecules: brownian motion	S6 p29-30		Do S6.1
4/13 L31	Moving molecules: drift and flux	S6 p30-32		Do S6.2
4/15 L32	Chemical transport and kinetics: postulates	T1 p1-2	noon	Do T1.1
4/18 L33	Equilibrium, steady state and Boltzmann factor	T1 p2-3		Do T1.2
4/20 L34	Deriving transport: Fick's, Faraday's and Ohm's laws	T2		Do T2.1, T2.2
4/22 L35	Nernst equation, Osmosis and the 'Master Table'	T2	noon	Do T2.3, T2.4, T2.5
4/25 L36	Integrated flux and Le Châtelier's Principle	T3		Do T3.1
4/27	Activated rate theory I	T3		Do T3.2

L37				
4/29 TA-L38	Activated rate theory II	T3		Do T3.3, T3.4
5/2 Review	In-class review with Gruebele Evening review with TAs			
Final Exam: Friday May 14, 8-11 AM, covers all material				