Course Schedule, Exams, Reading and Homework

-The course website is at https://gruebele-group.chemistry.illinois.edu/Course_Notes/Chem442 Capitalization is important!
-**Dates:** Check below for dates of all lectures, exams, reviews!
-**Lecture**: MWF at 10-10:50 AM by Zoom or in 100 NL. The title summarizes the lecture content.
-**Reading**: **Q** refers to our textbook Hayward, *Quantum Mechanics for Chemists*. Do all reading assignments before lecture: the lectures *do not* just repeat the book. **N** or **T** links to handouts/notes that regularly supplement the text and lectures. **Have them handy during lecture**.
-**BOH**: Gruebele Big Office Hours and reviews. Often on Fridays at 5 PM. Gruebele will stick around past 6:15 PM as long as you get there by then and not all questions have been answered.
-**Homework**: **H** links to assignments for each lecture. The **bold** problem(s) must be turned in. 80% of hour exam and final questions are modified homework problems, so *keep up with all problems on a weekly basis*! Assignments are due at the beginning of the first class of the next week. (e.g. if three problems are assigned on MWF in week 1, all three are due on Compass Monday of week 2).

Date	Lecture	Reading	BOH	Homework
1/25 L1	Postulates of mechanics: States in classical (CM) and quantum (QM) mechanics	Q 1.1-1.3, 1.4.5, 7.1, N1, N1b		H1, S1
1/27 L2	CM of molecules I: How do *x* and *p* vary with time?	N2, L1 review		H2, S2 Play with MD demo
1/29 L3	CM of molecules II: What can it solve?		5 PM	H3, S3
2/1 L4	Why do we need QM? The problems with CM	N4		H4, S4 Play with QM demo
2/3 R1	Important math: Complex numbers	T1 Read the complex number part, and bring T1b		HT1, ST1
2/5 R2	Important math : Fourier transforms	Read the Fourier part of T1.		HT2, ST2
2/8 L5	Music: Fourier conjugate variables *t* (time) and ω (frequency)	N5	5 PM	H5 , S5
2/10 L6	QM: Fourier conjugate variables *x* and *p*: The Heisenberg principle	Q 1.3, 3.1, 3.2, 3.4 N6		H6 textbook problems! S6
2/12 L7	The Schroedinger equation: CM *vs*. QM of a vibrating diatomic molecule	Q 4.2.1, N7		H7, S7
2/15 L8	CM, QM states, probability $\|Psi\|^2$ and measurement.	Q 1.4.2-1.4.5 N8		H8, S8
2/19 L9	Time-independent Schroedinger equation: unlike CM, QM has stationary states above the lowest energy	Q 4.1, 4.2.4, 7.1, 7.2 N9	5 PM	H9, S9
2/22 L10	Stationary states of the vibrating diatomic molecule	Q 4.2.2 N10		H10, S10
2/24 L11	Connection between stationary states and wave packets, excited states and spectroscopy	Q 4.2.3, 3.6 N11		H11, S11

2/26 L12	The chain molecule as a 1-D box filled with one electron	Q 2, 3.3 N12, N12b-Math285	5 PM	H12, S12
3/1 L13	Electron in a ring, molecule rotating on surface, and angular momentum	Q 5.1, N13		H13, S13
3/3 L14	QM in more dimensions: Product wavefunctions, 3-D box	Q p. 119 (#7.1), N14		H14, S14
3/5 L15	QM in more dimensions: 3-D rotation, part 1	Q 5.2, Q p. 87-90., N15	5 PM	H15, S15
3/8 HE1	**Hour Exam #1, covers L1-12,** Open annotated textbook and notes. Solutions to be posted.			
3/10 L16	QM in more dimensions: 3-D rotation, part 2	Q 6.6.4, see N15 again, N16		H16, S16
3/12 L17	QM in more dimensions: Hydrogen atom	Q 5.2, 6 (skip 6.3), N17		H17, S17
3/15 L18	QM with more electrons: Spin, the Pauli principle (PP), and Slater wavefunctions	Q 5.3, 7.5.1-2, N18	5 PM	H18, S18
3/17 L19	QM with more electrons: Benzene as particle on a ring	N19, IQmol documentation		H19, S19, download and install IQmol on your PC
3/19 L20	Turning QM into linear algebra I: vector=function	Q 7.1-3, N20, N20a		H20, S20, play with IQmol user interface, build small molecules
3/22 L21	Turning QM into linear algebra II: matrix=operator	N21	5 PM	H21, S21
3/26 L22	Turning QM into linear algebra III: eigenvalues and the H_2^+ molecule	Q 8.4, 8.6, N22		H22, S22
3/29 L23	From matrix the bonds: H_2^+ and HeH^{2+} reviewed	Q 4.2.4, 4.3, N23		H23, S23, play with MO demo
3/31 L24	Tunneling and the chemical bond	Q 1.3-1.4, Q4.3.4, N24	5 PM	H24, S24
4/2 L25	The Hueckel model: a step up from electrons in a box	Q 8.13, N25		H25, S25
14/5 L26	Molecular orbital (MO) basis functions for Psi	Q 8.4, 8.6, 8.7, N26		H26, S26
4/7 L27	Valence bond (VB) basis functions for Psi, Lewis dots	Q 8.4, 8.6, 8.7, N27, N27a	5 PM	H27, S27
4/9 L28	The variational principle: effective nuclear charge of He	Q 7.4, 7.7, 8.2, 8.3, N28		H28, S28
4/12 L29	The Hartree-Fock energy	Q 7.8, 7.9, N29		H29, S29
4/14 L30	The self-consistent field (SCF) theory	Q 7.8, 7.9, N30, N30b		H30, S30
4/16 HE2	**Hour Exam #2, covers L13-27,** In-class, open annotaterd textbook and notes. Solutions to be posted.			
4/19	Hund rules for atoms and	Q 7.5-7.6, 7.10-	No	H31, AO energies, S31

L31	molecules	7.12, N31	BOH	
4/21 L32	Molecules: the Born Oppenheimer approximation	Q 8.5, N32		H32, S32
4/23 L33	Potential energy surfaces I: diatomics by MO theory	Q 8.8-8.10, N33	5 PM	H33, S33
4/26 L34	Potential energy surfaces II: polyatomic molecule by VB	Q 8.12, N34		H34, S34
4/28 L35	PES and orbital continuity	N35		H35, S35
4/30 L36	Orbital continuity and symmetry: Woodward-Hoffman rules	-	5 PM	Tip: See Wikipedia article on Woodward-Hoffman rules for hints on H35.
5/3 L37	Molecular spectroscopies: NMR, microwave, IR, UV-vis, to X-ray	-		No homework, but study the material
5/5	In-class review with Gruebele	-		
5/5	Evening review with TAs	-		
Final Exam: Friday May 14, 8-11 AM, covers all material				