

Chemistry 550 *Introduction to Quantum Mechanics* Autumn 2007

MWF 8:30-9:20 in Bag 108

Tutorial Th 8:30-9:20 in OUGL 101 is open to all students (475 & 550)

Instructor:	Assistant Professor David Ginger, Bagley Hall 213 ginger[at]chem.washington. <i>Address ALL subject related questions to the discussion forum below so your peers may contribute to, and benefit from, the discussion</i> (put CHEM550 or CHEM475 in the subject of <i>any</i> email directed to me)
Office Hours:	Prof.: David Ginger Mon 9:30-10:30 (Bag 213), Th 8:30-9:20 (OUGL 101), Fri. 4-5pm (Bag 213) and by appointment Grader:
Text:	Quantum Chemistry, Ira N. Levine, Prentice Hall 5 th Edition
Suggested Reading:	<i>Quantum Chemistry and Spectroscopy</i> by Tom Engel <i>Quantum Chemistry</i> by Donald A. McQuarrie <i>Introduction to Quantum Mechanics</i> by David J. Griffiths (highly recommended) <i>Molecular Quantum Mechanics</i> by Atkins and Friedman <i>Introduction to Quantum Mechanics in Chemistry</i> , M. Ratner and G. Schatz <i>Principles of Quantum Mechanics</i> , by Ramamurti Shankar <i>Quantum Mechanics</i> , by Claude Cohen-Tannoudji <i>Quantum Mechanics in Chemistry</i> , M. Ratner and G. Schatz
Discussion Forum:	https://catalysttools.washington.edu/gopost/board/dginger/2033/
Course Website:	http://faculty.washington.edu/dginger/CHEM550_A2007/index.html

TENTATIVE CLASS OUTLINE

At times, lectures may deviate significantly from the text – you should still keep reading it!

Day	Week	Reading	Day	Week	Reading
W	Sep 26	Chapters 1-3: Diff EQ, Schrod. Eqn., Particle in Box, operators, Fourier Series		Nov 5	Chapter 9 (Cont) Chapter 8: Variational Methods
	Oct 1	Chapters 1-3, Chapter 7 operators and postulates, series expansions	M	Nov 12	NO CLASS (Veteran's Day) Chapter 10: Electron Spin Chapter 11: Many electron atoms
	Oct 8	Chapter 7: tunneling Chapter 4: Harmonic oscillator and molecular vibrations		Nov 19	Chapter 11: Continued
				Nov 21	Chapter 12: Diatomic Molecules
			F	Nov 23	Thanksgiving—No Class
	Oct 15	Chapter 4: Harmonic oscillator, continued Chapter: 5 Rotations Exam 1-to be confirmed		Nov 26	Chapter 12: Born-Oppenheimer Approximation, Diatomic Molecules (Guest Lectures)
				Nov 28	Chapter 16.1-16.3: Hückel Theory
				Nov 30	Solids
	Oct 22	Chapter 5: Finish Rotations Chapter 6: Hydrogen atom		Dec 3	Bloch's Theorem/Band Structure
				Dec 5	Spectroscopy
	Oct 29	Chapter 9: Perturbation Theory Time dependent perturbations	F	Dec 7	Last day of instruction
	Nov 2	Spectroscopy			Final Exam: Take home is likely, but will be due by ~Dec 13, any in class final will be given by the university time schedule

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Exam 2
TBA
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TRANSITION TO DIFFERENT METHODS OF LEARNING

You are now, or soon will be, college graduates. This class will be one of the last times anyone will ever actively teach you anything. By the time you leave school, you won't know everything there is to know, even about one area of chemistry. The goal of education is ultimately to teach you how to think about new problems, and to make sure you are proficient at finding information by yourself, evaluating the validity of that information, and combining it with your prior experience, to apply that information to the problem at hand.

HOMEWORK

Homework will be due as announced on the website, in class or on the discussion board. Assignments will take many hours to complete. Physical chemistry is a cumulative subject, understanding the material in one week requires mastery of the material from each previous week. This is especially true of many of our computer problems—they will build on one another. Most problems will be graded for completion only—it is your responsibility to review the posted solutions and compare them with your work. Part of the homework grade is based on how clearly you allow others to follow your thinking and is non-negotiable, regardless of the correctness of the final result. All homework solutions must be your original work, even if you solved the problem in a group you should turn in your own version of the solution.

COMPUTERS

The university site license for maple allows all students free use of Maple on university owned hardware, and allows staff (graduate students are considered staff for the purposes of the license) to use Maple on private hardware.

Download your copy today: <http://www.washington.edu/computing/software/site/licenses/maple/> Undergraduates may buy a student copy of Maple at <http://www.maplesoft.com/products/Maple11/student/faqs.aspx#1> or from a reseller.

CLASS SESSIONS

Class sessions will be more useful if you 1) read the text prior to lecture and 2) attempt the homework throughout the week (even if we haven't fully covered that topic yet).

TEAMWORK

Collaboration on the problem sets is not only permitted, but is *encouraged*. However, each student **MUST** turn in their **own** completed problem set showing their own solutions, with their own maple code, their own graphs, and their own proofs. **WORD OF CAUTION:** Because this course requires both a growth in your conceptual abilities, as well as some long computations, it is possible to do well on the homework thinking you did most of the work, without realizing the key conceptual came from someone else in the group. Make SURE you work enough problems to develop your conceptual ability on your own or come exam time you will be facing a sheet of paper with 8 questions you have no idea how to start. Copying, or allowing another to copy, problems to which they have not contributed is plagiarism. Take home exams may be given. Students are NOT permitted to communicate with anyone except the instructor in any medium or manner regarding any test problems or material until after all exams have been returned. Plagiarism at any time, and giving or receiving assistance of any kind on exams is totally unacceptable and shall be regarded as academic misconduct. All cases of academic misconduct will be submitted to the registrar with an X as a final grade with a recommendation for the maximum UW sanction. Use of solution manuals, old homework keys, and similar resources are in appropriate in all circumstances.

GRADING

There will be two exams plus a final exam, as indicated on the schedule. Grading will be based on the total number of points obtained on the exams and the homework. Unannounced 'pop quizzes' may be given during lectures, and will each count as one homework grade. Lowest homework/quiz score will be dropped before computing the average.

CHEM 550	CHEM 475
Problem Sets: 50	Problem Sets: 100
Exam 1: 125	Exam 1: 100
Exam 2: 125	Exam 2: 100
Final: 200	Final: 200

Extra Credit—Bonus points up to 10% of the total hw score will be added to the homework score for correct, thoughtful replies to other students questions on the discussion board, for finding a major error in a problem answer or derivation (not just 3.14159 instead of 3.14 for pi, or a dropped – sign on one side of an equation). The awarding of any and all extra credit will rest with the non-negotiable judgement of the professor and TA/grader.