Chemistry 550 ***Introduction to Quantum Mechanics*** Autumn 2008
MWF 8:30-9:20 in Bag 260
Tutorial Th 8:30-9:20 in MGH 044

Instructor:	Associate Professor David Ginger, Bagley Hall 213 ginger[at]chem.washington. ***Address ALL subject related questions to the discussion forum below so your peers may contribute to, and benefit from, the discussion*** (put CHEM550 or CHEM475 in the subject of *any* email directed to me)
Office Hours:	Prof.: David Ginger Th 8:30-9:20 (MGH 044), Fri. 4-5pm (Bag 213) *and by appointment* Grader: Andreas Tillack
Text:	Quantum Chemistry, Ira N. Levine, Prentice Hall **6th Edition** Note: if you have an old copy of the 5th edition you can probably use that—HOWEVER it will be your responsibility to translate equation numbers, problem numbers, etc. into the new numbers
Suggested Reading:	*Quantum Chemistry and Spectroscopy* by Tom Engel *Quantum Chemistry* by Donald A. McQuarrie ***Introduction to Quantum Mechanics* by David J. Griffiths** (highly recommended) *Molecular Quantum Mechanics* by Atkins and Friedman *Introduction to Quantum Mechanics in Chemistry*, M. Ratner and G. Schatz *Principles of Quantum Mechanics*, by Ramamurti Shankar *Quantum Mechanics*, by Claude Cohen-Tannoudji *Quantum Mechanics in Chemistry*, M. Ratner and G. Schatz
Discussion Forum:	https://catalysttools.washington.edu/gopost/board/dginger/7031
Course Website:	http://faculty.washington.edu/dginger/CHEM550_A2008/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
		Chapters 1-3: Diff EQ, Schrod. Eqn.,		Nov 10	Chapter 9 (Cont)
W	Sep 24	Particle in Box, operators, Fourier			Chapter 8: Variational Methods
		Series			
	Sep 29	Chapters 1-3, continued		Nov 17	Chapter 10: Electron Spin
		Chapter 7 operators and postulates,			Chapter 11: Many electron atoms
		series expansions			
	Oct 6	Chapter 7: tunneling	M	Nov24	Chapter 12: Diatomic Molecules
		Chapter 4: Harmonic oscillator and	W	Nov 26	Chapter 12: Diatomic Molecules
		molecular vibrations	**F**	Nov 28	**Thanksgiving—No Class**
	Oct 13	Chapter 4: Harmonic oscillator, continued		Dec 1	Chapter 12: Born-Oppenheimer Approximation, Diatomic Molecules (Guest Lectures)
		Chapter: 5 Rotations			Chapter 16.1-16.3: Hückel Theory
		Exam 1-to be confirmed		Dec 8	Solids
	Oct 20	Chapter 5: Finish Rotations			Bloch's Theorem/Band Structure
		Chapter 6: Hydrogen atom			Spectroscopy
			F	Dec 12: Last day of class	
	Oct 27	Chapter 9: Perturbation Theory			
		Time dependent perturbations		**Final Exam: Take home is likely, but will be due by ~Dec 16, any in class final will be given by the university time schedule**	
	Nov 3	Spectroscopy			

~ Exam 2 TBA ~

— OVER —

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 any week requires mastery of the material from the 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

Day and night access to a computer with Maple installed will be required for both homework and exam problems. 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: https://www.washington.edu/uware/maple/ . Undergraduates should buy a student copy of Maple (discounts are offered at the same site).

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 permitted and 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 in a group without realizing the key concepts came from someone else in the group. Make SURE you work enough problems to develop your own conceptual ability 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 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. The use of solution manuals (purchased or online), old homework keys, and similar resources are inappropriate on homeworks or exams.

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 quizes' 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.