

Chemistry 442/552  
Quantum Mechanics  
Spring 2011  
Syllabus

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Office Hours: Tuesday 10-11, Wednesday 10-11 and after class meetings. Open door policy.

Text: Physical Chemistry, McQuarrie and Simon, University Science Books, 2008.

Homework: Weekly problem assignments, unless otherwise announced, will be due on Wednesdays. Homework will be posted on the D2L page. Homework is due at class time. Late homework accepted through Friday for partial credit.

Computer software: The Mathcad program is available on the chemistry commons computers, SB 1 221. You can purchase a personal student copy through OIT for \$20. Only for Windows.

For molecular modeling, Spartan software is available on the chemistry commons computers. This software is more expensive, but if you are interested in student software, you can look at the website: [www.wavefun.com](http://www.wavefun.com)

Grades: Homework: 20%  
In-Class participation: 15%  
Midterms: 15% each  
Final: 35%

The midterms are tentatively scheduled for weeks 4 and 7, but this is subject to change.

Success in this course will depend on your understanding of key concepts but also your ability to apply these concepts to solve problems. You will need to develop strong math skills and will benefit from learning a symbolic math program such as MathCad. You *must* do homework assignments to succeed. Group work on homework is encouraged. I expect about 75% of in class midterm problems to be taken from the homework. Textbook homework problems that are simply copied from the solutions manual will earn a maximum of 1/3 of possible points.

What we will be doing; Scheduled lecture time will be used in several ways. Some class meetings will follow a standard lecture format. Other meetings will be used for problem solving sessions. This will include conceptual exercises, examples and problem solving practice. It is expected that you will attend class regularly and your participation during problem solving sessions is worth 15% of your grade.

You are responsible for any information or announcements given in class. Contact me as soon as possible if you miss any exams.

Below is a rough schedule of topics that we will cover. This document will continue to evolve, for updates, check D2L. I hope to post learning objectives for each topic/chapter covered.

<b>Week</b>	<b>Chapter(s)</b>	<b>Topics</b>	<b>Objectives</b>
1	2,3 A,B	Complex Numbers Classical Wave Equation Prob and Stat Schrodinger Eq	Do diff eq problems, Manipulate complex numbers
2	3,4 C	Particle in a Box Postulates Vectors	Learn to use Mathcad Set up particle in a box problems Comfort with vectors
3	5	Harmonic Oscillator Vib spectroscopy	Be able to use HO solutions – be able to interpret IR information
4	D,5	Spherical Coordinates Rigid Rotor – rotational spectra	Be able to use rotational solutions – understand spectra model
5	E,6	H – atom Determinants	
6	7 8	Approximate Methods Multi-electron Atoms	
7	9/10, F	MO Theory – Huckel Matrices	
8	13	Molecular Spectroscopy	
9	13/14	Molecular Spectroscopy	
10	14/15	NMR / Lasers	