

## Chem 4502: Quantum Mechanics and Spectroscopy Spring 2017

**Instructor:** Prof. James Johns (331 Smith Hall, [jjohns@umn.edu](mailto:jjohns@umn.edu))

**Teaching Assistant:** John Biswakarma ([biswa052@umn.edu](mailto:biswa052@umn.edu))

Harrison Frisk ([fris0123@umn.edu](mailto:fris0123@umn.edu))

Fazel Zare Bidoky ([zareb001@umn.edu](mailto:zareb001@umn.edu))

Prerequisites: 1 year of college chemistry, 1 year of calculus, and 1 year of college physics. A 3<sup>rd</sup> semester of math (Math 2263, 2374, 2243, or 2373) is required but can be taken concurrently.

Class Location: 230 Bruinicks Hall

10:10 – 11:00 AM, M W F

Final Exam: Sat. May 13, 2017 1:30 – 3:30 AM

Course Text: Physical Chemistry by McQuarrie and Simon (**Required**)

Problems and Solutions to accompany McQuarrie and Simon, by H. Cox (Recommended)

### Goals

If atoms are composed of positive and negative charges, why don't they collapse? What size and shape are molecules? How do molecules move in a chemical reaction? Where do atomic and molecular orbitals come from and what do they really mean? Can something really be in two places at the same time?

Quantum mechanics can answer some of the deepest and most fundamental questions in chemistry. It also can be mysterious, weird, and a lot of fun. In this class, we're going to learn the fundamentals of quantum mechanics, and understand its implications on molecular structure and chemistry. We'll also learn how to measure molecular properties with light and spectroscopy.

### Academic Integrity

All students enrolled in University courses are expected to complete coursework responsibilities with fairness and honesty. Failure to do so by seeking unfair advantage over others or misrepresenting someone else's work as your own, can result in disciplinary action. The University Student Conduct Code defines scholastic dishonesty as follows:

*Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis.*

Within this course, a student responsible for scholastic dishonesty can be assigned a penalty up to and including an "F" or "N" for the course. If you have any questions regarding the expectations for a specific

assignment or exam, ask. Students should become familiar with the Regent's Policy on Student Conduct, found at: [http://www1.umn.edu/regents/policies/academic/Student\\_Conduct\\_Code.pdf](http://www1.umn.edu/regents/policies/academic/Student_Conduct_Code.pdf)

**Grading:**

**Homework: 10%**

**Midterms: 60%**

**Cumulative Final Exam: 30%**

**Homework Policy:** Quantum mechanics can defy your physical intuition, and the only way to really know it, and demonstrate that you've learned it, is to apply it. There will be approximately 10 homework assignments in this class. Homework will be due at the start of class on Friday every week we do not have an exam, except for the first week where a short assignment will be due the first Monday. Each homework will have 1 problem which will be graded in detail for 5 points. The remainder of the homework problems will be graded in a more cursory fashion, and they will be cumulatively worth 5 points, for a total of 10 points on each homework. No late homework will be accepted for any reason. If you can't make it to class, homework may be delivered by a friend or placed in my mailbox (B-19) in Smith Hall before 8:30 AM when I walk to class.

Homework Due Dates: Jan 23, Jan 27, Feb 3, Feb 17, Feb 24, Mar 10, Mar 24, April 7, April 14, April 21

**Midterms:** There are 4 midterms in this class. The goal is to break down the strange and exotic material into manageable size chunks. Each test will consist of several multiple choice questions and short answer questions, and a few longer questions that will require you to demonstrate more of your thought process. Each midterm will be focused on the more recent material, but will require proficiency and understanding of previous material. The subject material is inherently cumulative by nature.

In the event that you must miss a midterm for any excused reason (such as a proven personal emergency or a university sponsored activity), your remaining 3 midterms will be averaged together and weighted to 20% each. Failure to demonstrate that the absence should be excused will result in a zero for the midterm. No alternate or make-up midterms will be given for any reason.

Midterm Dates:

Midterm 1: Feb 8

Midterm 2: Mar 1

Midterm 3: Mar 29

Midterm 4: Apr 26

**Final Exam:** The final exam for this class is a cumulative exam, and will be given at 1:30 PM on Sat May 13 in 230 Bruinicks Hall and an additional room yet to be determined. The final exam is mandatory and will not be excused for any reason. Failure to take the final exam will result in an F for the course. N.B. The exam date is the latest exam slot, and comes after graduation ceremony for CSE students. You must still come and take the exam to pass the course.

Only non-graphing, non-programmable calculators will be allowed on midterms and the final exam. These include the one-line TI-30Xa and the two-line (non-programmable) TI-30X IIS. These calculators are available at the U of M Bookstore in Coffman Union and they are inexpensive (e.g., about \$10 for the TI-30Xa). You may want to use one of these calculators for the homework and problem sets as well, to become familiar with it. Using a programmable calculator will be considered scholastic dishonesty and can be grounds for failing a midterm or the final exam.

**Students with Disabilities:** Students with disabilities that affect their ability to participate fully in class or meet all course requirements are encouraged to contact the disability Resource Center (DRC) at 612-626-1333 to arrange a confidential discussion regarding equitable access and reasonable accommodation. If you are registered with disability services, please let the instructor know as soon as possible so that appropriate accommodations can be made. Please note that it is the student's responsibility to arrange these accommodations. Additionally, students taking midterms or final exams at the DRC must schedule them to overlap with the usual exam times.

**Class Conduct:** Harassment and behavior which excludes students from full participation will not be tolerated. For more information, refer to the University policy quoted below:

#### *Sexual Harassment*

*"Sexual harassment" means unwelcome sexual advances, requests for sexual favors, and/or other verbal or physical conduct of a sexual nature. Such conduct has the purpose or effect of unreasonably interfering with an individual's work or academic performance or creating an intimidating, hostile, or offensive working or academic environment in any University activity or program. Such behavior is not acceptable in the University setting. For additional information, please consult Board of Regents Policy: <http://regents.umn.edu/sites/default/files/policies/SexHarassment.pdf>*

#### *Equity, Diversity, Equal Opportunity, and Affirmative Action:*

*The University will provide equal access to and opportunity in its programs and facilities, without regard to race, color, creed, religion, national origin, gender, age, marital status, disability, public assistance status, veteran status, sexual orientation, gender identity, or gender expression. For more information, please consult Board of Regents Policy: [http://regents.umn.edu/sites/default/files/policies/Equity\\_Diversity\\_EO\\_AA.pdf](http://regents.umn.edu/sites/default/files/policies/Equity_Diversity_EO_AA.pdf).*

I will gladly honor your request to address you by an alternate name or gender pronoun. Please advise me of this change via the notecard I pass out at the beginning of the semester, via email or in person. Please advise me of this early in the semester so that I may make appropriate changes to how I might address you in or outside of class.

Approximate Schedule:

Week	Topics	Reading in McQuarrie & Simon
1.	Why do we need quantum mechanics? What is different than classical mechanics? Probability	Ch. 1, Math Chapter A
2.	Introduction to the Schrodinger Equation, Operators, Particle in a box,	Chapter 3
3.	Particle in a box continued, Postulates of quantum mechanics,	Chapter 4
4.	Midterm 1, Harmonic oscillator and vibrations,	Chapter 5
5.	Harmonic oscillator and vibrations continued, Rigid Rotator	Chapter 5, Chapter 13
6.	Rigid Rotator and molecular geometry, Angular Momentum, Spin	Chapter 6
7.	Start Hydrogen Atom, Midterm 2	Chapter 6
8.	Hydrogen atom, atomic orbitals, LCAO	Chapter 6
9.	Helium Atom and the variational method, Multielectron atoms, Term Symbols	Chapter 7 - 8
10.	Molecular bonding and the Born Oppenheimer Approximation, Potential Energy Surface, $H_2^+$ , $H_2$ , Molecular Orbitals	Chapter 9
11.	Molecular Orbitals, Midterm 3, Introduction to spectroscopy, Lasers,	Chapter 9
12.	Perturbation theory, vibrational spectroscopy	Chapter 7, 13
13.	Spectroscopy and Molecular shape,	Chapter 13
13.	Visible light, solar cells, and molecules	Chapter 13
14	Midterm 4 and Final Exam Review	