CHEM 4502: Introduction to Quantum Mechanics and Spectroscopy (Syllabus subject to change by instructor)
Summer 2016
Lecture: T Th 1:45-4:30 pm, 231 Smith Hall

Instructor: Dr. Steve Miller (smiller3@gustavus.edu)
Office Hours: T, Th 12:30-1:30 pm, 231 Smith Hall

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Catalogue Description

Microscopic descriptions of chemical systems. Quantum theory. Applications to atomic/molecular structure. Molecular spectroscopy. Quantum statistical mechanics. Discussion of solutions to several differential equations.

Course Goals

1) Learning the fundamental concepts of quantum mechanics
2) Application of quantum theory to the study of atoms/molecules through spectroscopy
3) Describing molecular structure and bonding from a quantum mechanical basis
4) Examining basic approximation methods

Required Materials

Textbook: McQuarrie and Simon, *Physical Chemistry: A Molecular Approach*, University Science Books (1997)

Attendance

Attendance is not required, but attending every lecture is very strongly encouraged. If you miss a lecture, **you** are responsible for getting the information and/or notes covered in class from a classmate—I will not provide it for you. Moreover, you will probably find that what is *said* during class is no less important than what is written in your notes, and there is no reliable way to hear what is said without being in class and paying attention. Also, before you miss class, consider that missing a single lecture is equivalent to missing an *entire week* of class during a normal 15 week academic semester…

Grading

Final grades will be assigned according to the following scheme:

HW	20%
In-class problems	10%
Quizzes	25%
Midterm exam	20%
Final exam	25%

The cutoffs for final course grades will be determined after the final exam. However, the maximum percentage for cutoffs will be 88% (A-), 76% (B-), 62% (C-), 55% (D), <55% (F). In other words, if

you earn a total grade of 91% for the course, you are guaranteed an A or A-; if you earn 87%, you are guaranteed some type of B, and with the final cutoffs your grade may be bumped up to the A range (the actual percentage cutoffs will be determined only after the final exam).

Note that different items may not be worth the same number of points (e.g. one assignment may be worth 25 points and another 47 points). However, I calculate total grades based on percentages, so 80% on a 25 point assignment affects your overall grade exactly the same as 80% on a 47 point assignment.

HW

Six homework assignments will be given, the tentative due dates for which are included in the schedule. Assignments are due at the beginning of class on the due date; late assignments (i.e. any not turned in immediately when they are collected) will not be accepted under any circumstances (including late arrival to class). Assignments will be designed to keep you current with the course material and provide insight into the types of problems which you are most likely to see on quizzes and exams. I will drop your single lowest homework grade; the remaining five HW grades constitute a significant portion of your overall course grade. It is very much in your best interest to complete the assignments and understand the material covered in them!

In-class problems

In-class problems will be regularly assigned (except for quiz/exam days). Each problem is to be completed and turned in before the end of the class period; you may work on the problem individually or in a group. Your lowest two scores will be dropped.

Quizzes

There will be two quizzes, which will tentatively be given in class on the dates indicated in the schedule. One hour will be allocated to complete each quiz. Quizzes will include some combination of multiple choice, short answer, and numerical/theoretical word problems and will only include information covered in class since the last quiz or exam.

You are expected to take each quiz in class on the day it is given. If you know ahead of time that you will miss a quiz, you will be allowed to take it early. If you are unable to take a quiz because of a last minute problem (e.g. illness), you must contact me as early as possible (preferably before class), and a make up quiz may be given at my discretion. Be forewarned: I will put different questions on make up quizzes; it will therefore not benefit you to see the quiz given in class before taking the make up version.

I may elect not to allow the use of calculators on quizzes. You may write in either pen or pencil on quizzes, but I will not regrade any answers written in pencil, erasable pen, or pen which has been whited out. If I make an adding error when totaling a quiz grade, I will fix it whether you used pen or pencil.

Exams

There will be one midterm exam and one final exam, tentatively given in class on the dates included in the schedule. Exams will be cumulative, and you will be given the entire class period to complete them. Exams will be like quizzes in all other ways.

General Expectations

1) I will try to treat every student with respect. In return, I expect each student to treat me and all of his/her fellow students with respect. This includes not talking during lecture or when others are speaking. For my part, I will start and finish class on time and provide ample opportunities to ask questions.
2) **All mobile devices are to be turned off during lecture.** There is nothing more distracting than a phone ringing during class or a nearby person constantly text messaging. All mobile electronic devices should be turned *off* for the entire duration of class, not just set to silent or vibrate.
3) **Academic dishonesty will not be tolerated under any circumstances.** Anyone caught cheating (copying homework, looking at a classmate's exam, etc.) will receive an automatic grade of zero for the assignment, quiz, or exam in question. A second offence will result in the student's immediate removal from the course with an automatic grade of F and referral to the University's Dean of Students.
4) If you ever have questions, ask! If I cannot answer them myself, I will try to point you to someone who can.

Tips for Success

1) **Do not wait until the night before a quiz or exam to study.** Quantum chemistry is built on a large number of abstract, conceptual ideas, and is quite math intensive. Neither of these characteristics lends itself to hurried learning of the material.
2) **Do the homework.** The homework assignments are meant to help you keep pace with the lecture material and avoid falling behind. In addition, doing the homework should be a reliable way of boosting your course grade (note that the homework contributes as much to your overall grade as the midterm exam!).
3) **When reading the textbook, re-read any passages which you do not understand.** If you see a word you do not know, look it up in a dictionary. It can also very helpful to write a summary of material you have just finished reading.
4) **Take good notes.** Quantum is a difficult course for which to study without the guidance of a good set of notes. Also remember that I will not test you on any material which I do not cover in lecture.
5) **Seek help if/when you need to.** There is no shame in being perplexed by the mysteries of quantum theory (as probably everyone who has ever studied it has been at times). If you find yourself struggling, look for assistance from an appropriate source.

Resources

I will post appropriate items (answer keys, homework assignments, etc.) on the Moodle course website; if you are looking for materials, you would do well to look there first!

CHEM 4502, Summer 2016

Tentative Schedule

Date	Topic
6/14	Course introduction, Ch. 1 (Roots of quantum mechanics)
6/16	Ch. 2 (Classical wave mechanics), MathCh. B (Probability and Statistics)
6/21	Ch. 4 (Postulates of QM)
6/23	**HW 1 due**; **Quiz 1**; Ch. 3 (Particle in a box)
6/28	Ch. 5 (Harmonic oscillator and rigid rotor)
6/30	**HW 2 due**; Ch. 5 and 13 (Molecular spectroscopy)
7/5	Ch. 5/13
7/7	**HW 3 due**; **Midterm Exam**
7/12	Ch. 6 (Hydrogen atom), Ch. 8 (Multielectron atoms)
7/14	Ch. 8, Ch. 9 (Bonding in diatomics)
7/19	**HW 4 due**; Ch. 9
7/21	Ch. 10 (Bonding in polyatomics)
7/26	**HW 5 due**; **Quiz 2**; Ch. 7, 8, 11
7/28	Ch. 7, 8, 11
8/2	Ch. 7, 8, 11
8/4	**HW 6 due**; **Final Exam**