CHE 372: Quantum Chemistry and Dynamics (Syllabus subject to change by instructor)
Spring 2009
Lecture: M T W F 12:30-1:20, OHS 103
Laboratory: W 1:30-5:20, NHS 107

Instructor

Dr. Steve Miller
Office: NHS 107A/B
Office Hours: T W 9:00 – 10:00 am

While I will be available at these times each week, I am also happy to meet with students at other times. If you would like to see me outside of my office hours, it would generally be best to contact me in advance to arrange a time. You are also welcome to stop by my office, but be aware that I may not be there or I may be unable to see you if I am occupied with other obligations.

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Catalogue Description

A continuation of CHE 371. Topics treated include elementary quantum mechanics, spectroscopy, bonding theory, atomic and molecular structure, and chemical reaction dynamics. An emphasis will be placed on the quantum mechanical foundations of molecular modeling and of molecular spectroscopy.

Course Goals

1) Learning the fundamental concepts of quantum mechanics
2) Examining the application of quantum theory to bonding and spectroscopy
3) Describing chemical behavior in terms of fundamental physical theories

Required Materials

Textbook: McQuarrie and Simon, *Physical Chemistry: a Molecular Approach*

Attendence

I do not take attendance for lecture. However, attending every lecture is 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 lecture 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. Laboratory attendance **IS** required every week. If you must miss a laboratory meeting, please inform me as soon as possible so that arrangements can be made for a make up sesssion.

Grading

Final grades will be assigned according to the following scheme:

HW	15%
Quizzes	20%
Midterm Exams	20%
Lab	30%
Final Exam	15%

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 grade of 91% for the semester, you are guaranteed an A-; if you earn 87%, you are guaranteed at least a B-; with the final cutoffs your grade may be bumped up to an A- (the actual percentage cutoffs will be determined only after the final exam).

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

Exams

There will be two midterm exams given in class on/near the dates included in the attached schedule. You are expected to take each exam in class on the day it is given. If you know ahead of time that you will be unable to do so, you may arrange another time to take a make-up exam. If you are unable to take your exam because of a last minute problem (e.g. illness), you must contact me as early as possible (preferably before the exam). Make up exams in such instances will be allowed at my discretion depending on the reason for the missed exam. Be forewarned: make up exams may contain different questions than the exams given in class; it will therefore not be beneficial to you to see the exam given in class before taking a make up exam. Exams will be meant to require the full 50 minute class period, and will contain some combination of multiple choice, true/false, matching, short answer and word problems. I may also elect not to allow the use of calculators on exams.

You may write in either pen or pencil on exams. However, I will not regrade any problems on an exam which is written in pencil, erasable pen, or pen which has been whited out. (If I make an adding error when totaling an exam grade, I will fix it whether the exam was written in pen or pencil.)

Quizzes

In class quizzes will be similar to exams, only shorter (~30 minutes each); quizzes may alternately be given as take home assignments. There will be five quizzes given throughout the semester. The policy for quizzes is the same as that for exams (with regards to make ups, calculators, etc.).

HW

Seven homework assignments will be given during the semester. Due dates for assignments are given in the tentative schedule below; note that late assignments will not be accepted under any circumstances. The 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. Also, note that HW is a significant contributor to your course grade (15%, more than either individual midterm exam). It is very much in your best interest to complete the assignments and understand the material covered in them!

Laboratory

Each student must attend every lab session and complete all of the required laboratory assignments in order to pass the course as a whole. In addition, lab is the single largest contributor to your course grade. The laboratory portion of the course is designed to apply the theory of quantum mechanics to real computational and spectroscopic experiments. No lab manual is required for the laboratory portion of the class; lab exercises and other pertinent materials will be provided. Note that CHE 372 is a WRITD approved course, and the writing component will be emphasized in the writing of lab reports.

Final Exam

The final exam will be given on Friday, 5/28 in OHS 103. All students must take the final at this time/place as mandated by the college. The final will be formatted like the midterm exams, but it will cover material from throughout the entire course.

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.
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 devices should be turned off, not just set to silent or vibrate.
3) I expect you to be honest, as per the personal code of conduct each GAC student is required to sign when registering for classes. If you have any questions/concerns about the propriety of a particular aspect of working with your fellow students, please do not hesitate to discuss it with me. **Academic dishonesty will not be tolerated under any circumstances.** Anyone caught cheating will receive an automatic grade of zero for the assignment/lab/quiz/exam in question. A second offence will result in the student's immediate removal from the course with an automatic F grade.
4) If you ever have questions, ask! If I can not 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; it is, nonetheless, quite math intensive. It is a very difficult subject to learn it in a hurry!

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.

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 to study for 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) **Come in for help if/when you need to.** I try to be available as much as possible, and do not mind lending a helping hand if need be!

Additional Resources:

I will post lots of things on the class website over the course of the semester:
homepages.gac.edu/~smiller3/courses/372-sp09.htm
If ever you need to find some information (lab handouts, homework assignments, etc.) check there first, and let me know if you can not find what you need.

If you have a learning (or other) disability which could affect your performance in this course, please see Laurie Bickett (x6286 or lbickett@gustavus.edu) in the Academic Advising Center. She will work with you to determine any accommodations which might benefit you, and I will be more than happy to implement them.