

CHE 372: Quantum Chemistry and Dynamics (Syllabus subject to change by instructor)

Spring 2012

Lecture: M W Th F 12:30-1:20, NHS 106B (the Fishbowl)

Laboratory: W 1:30-5:20, NHS 107

Instructor

Dr. Steve Miller

Office: NHS 107A/B

Office Hours: M 1:30-2:30, T 11:30-12:30

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.

Phone: x7321

Email: smiller3@gustavus.edu

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*, University Science Books (1997)

Lab manual: Gustavus Adolphus College, *Physical Chemistry Laboratory Manual* (available only through the campus bookstore)

Attendance

You are expected to attend class every day. 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 session.

Grading

Final grades will be assigned according to the following scheme:

| | |
|---------------|-----|
| HW | 15% |
| Midterm Exams | 30% |
| Lab | 35% |
| Final Exam | 20% |

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 four midterm exams given on/near the dates included in the attached schedule.

If the exam is given in class, 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, will be cumulative, and will include 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.

If a take home exam is given, you are expected to complete and turn it in by the day/time specified. You will be allowed the use of any materials (e.g. computer, book, notes, etc.) you deem necessary to complete take home exam, but will be expected not to discuss your exam with anyone else (whether or not s/he is a classmate).

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.)

HW

Rather than traditional homework assignments, you will be asked to complete one problem related to each day's new material. The assigned problem will be due the following class period, at which time each student will turn in their work and a volunteer (or randomly selected student) will present his/her solution to the problem in class. Assignments will only be accepted at the beginning of class on the due date, but you will be allowed to drop your four lowest homework scores. Note that attendance is an inherently integral part of your homework grade.

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. 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 time will be given on Monday, May 21 from 8:00-10:00 am. Depending on circumstances, part (or all) of the final exam may be given as a take home assignment. All students must take any in-class portion of the final exam at this time/place mandated by the college unless arranged with me ahead of time. The final will be formatted like the midterm exams, but 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 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) **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-sp12.htm

If ever you need to find some information (lab handouts, homework assignments, etc.) check there first, and let me know if you cannot find what you need.

Academic honesty

All students are expected and required to adhere to the Gustavus Honor Code, as embodied in the statement

“On my honor, I pledge that I have not given, received, or tolerated others’ use of unauthorized aid in completing this work.”

As per this policy, cheating can take one of three forms:

- 1) Accepting unauthorized help (e.g. copying someone else’s work)
- 2) Providing unauthorized help (e.g. letting someone copy your work)
- 3) Failing to report cheating by others (e.g. knowing someone else has cheated and not turning him/her/them in)

It will be assumed that the honor code is in effect on any graded item, whether or not signing it is actually required. Any student caught violating any part of the honor code will receive an automatic grade of zero for the assignment/lab/exam in question and will be reported to the Provost. A second offence will result in the student’s immediate removal from the course (with an automatic F) and will be reported to the Provost a second time. Further information about the Honor Code can be obtained from Assistant Provost Barbara Kaiser (kaiser@gustavus.edu or x7541).

Disability Services

Gustavus Adolphus College is committed to ensuring the full participation of all students in its programs. If you have a documented disability (or you think you may have a disability of any nature) and, as a result, need reasonable academic accommodation to participate in class, take tests or benefit from the College's services, then you should speak with the Disability Services Coordinator, for a confidential discussion of your needs and appropriate plans. Course requirements cannot be waived, but reasonable accommodations may be provided based on disability documentation and course outcomes. Accommodations cannot be made retroactively; therefore, to maximize your academic success at Gustavus, please contact Disability Services as early as possible. Disability Services (<https://gustavus.edu/advising/disability/>) is located in the Advising and Counseling Center. Disability Services Coordinator Laurie Bickett (lbickett@gustavus.edu or x6286) can provide further information.

ELL accommodations

Support for English Language Learners (ELL) and Multilingual students is available via the College's ELL Support staff person, Andrew Grace (agrace@gustavus.edu or x7395). He can meet individually with students to consult about academic tasks and to help students seek other means of support. The ELL Support person can also consult with faculty members who have ELL and multilingual students enrolled in their classes. The College's ELL staff person can provide students with a letter to a professor that explains and supports academic accommodations (i.e. additional time on tests, additional revisions for papers). Professors make decisions based on those recommendations at their own discretion. In addition, ELL and multilingual students can seek help from peer tutors in the Writing Center.

Tentative Schedule

| Week | Monday | Tuesday | Wednesday | Thursday | Friday |
|-----------|-------------------------------------|---------|------------------------------------|---------------------------------------|--------------------------------|
| 2/6-2/10 | Ch. 1 (Intro, roots of QM) | | Ch. 1 | Ch. 1 | Ch. 2, Math Ch. B (Statistics) |
| 2/13-2/17 | Ch. 2, Math Ch. B | | Ch. 3, 4 (Postulates, PIB) | Ch. 3, 4 | Ch. 3, 4 |
| 2/20-2/24 | Ch. 3, 4 | | Ch. 3, 4 | Exam 1 | Ch. 5 (HO and RR) |
| 2/27-3/2 | Ch. 5 | | Ch. 5 | Ch. 13 (Spectroscopy) | Ch. 13 |
| 3/5-3/19 | Ch. 13 | | Ch. 13 | Ch. 13 | Ch. 13 |
| 3/12-3/16 | Ch. 13 | | Exam 2 | Ch. 6 (H atom) | Ch. 6 |
| 3/19-3/23 | Ch. 6 | | Ch. 8 (Multi e ⁻ atoms) | Ch. 8 | Ch. 8 |
| 3/26-3/30 | Ch. 8 | | Ch. 9 (Diatomic bonding) | Ch. 9 | Ch. 9 |
| 4/2-4/6 | <i>No Class—Spring Break/Easter</i> | | | | |
| 4/9-4/13 | Ch. 9 | | Ch. 9 | Ch. 10 (Polyatomic bonding/HO theory) | Ch. 10 |
| 4/16-4/20 | Exam 3 | | Ch. 7, 8, 11 (Approx. methods) | Ch. 7, 8, 11 | Ch. 7, 8, 11 |
| 4/23-4/27 | Ch. 7, 8, 11 | | Ch. 7, 8, 11 | Ch. 7, 8, 11 | Ch. 7, 8, 11 |
| 4/30-5/4 | Ch. 7, 8, 11 | | Ch. 12 (Group theory) | Ch. 12 | Ch. 12 |
| 5/7-5/11 | Ch. 12 | | Ch. 12 | Ch. 12 | Ch. 12 |
| 5/14-5/18 | Exam 4 | | Review | <i>No Class—Reading Day</i> | |
| 5/21-5/25 | Final Exam 8-10 am | | | | |

Tentative Lab Schedule

| Date | Experiment | Due |
|-------------|--|--------------------------------|
| 2/8 | Introduction to Mathcad | --- |
| 2/15 | Exp 2-2: Computational chemistry | Prelab 2-2; Mathcad assignment |
| 2/22 | Exp 2-1: Absorption spectra of biological pigments | Prelab 2-1; Exp 2-2 assignment |
| 2/29 | <i>Writing day</i> | --- |
| 3/7 | Exp 2-3: Raman and infrared spectroscopy of CHCl_3 and CCl_4 | Prelab 2-3; Exp 2-1 report |
| 3/14 | <i>Writing day</i> | --- |
| 3/21 | Exp 2-4: Infrared spectra of HCl and DCl | Prelab 2-4; Exp 2-3 report |
| 3/28 | <i>Writing day</i> | --- |
| 4/4 | No class (Spring/Easter break) | |
| 4/11 | Exp 2-5: The UV-visible spectrum of Li_2 | Prelab 2-5; Exp 2-4 report |
| 4/18 | <i>Writing day</i> | |
| 4/25 | Exp 2-6: Computational determination of the ionization energy and electron affinity of SO_2 | Prelab 2-6; Exp 2-5 report |
| 5/2 | Exp 2-7: Literature review | Exp 2-6 report |
| 5/9 | <i>Writing day</i> | Literature review section |
| 5/16 | Literature review presentations | Complete literature review |