CHE 372: Quantum Chemistry and Dynamics
Spring 2007

Class Meetings: Lecture: M,T,W,F 12:30 PM, Confer-Vickner 125
Laboratory: W 2:30-6:20 PM, Nobel 107

Instructor: Prof. Amanda Nienow, Nobel 106C, 933-7327, anienow@gustavus.edu

Textbook: Donald A. McQuarrie and John D. Simon, *Physical Chemistry: A Molecular Approach.* Sausalito, CA: University Science Books, 1997.

Website: http://homepages.gac.edu/~anienow/CHE-372/che_372.html

Overview:
Physical chemistry is the quantitative interpretation of the macroscopic properties of matter informed by a detailed understanding at the atomic and molecular level. Quantum mechanics has permitted an important and exciting window into the details of atomic and molecular structure. Two important tools of modern chemistry, spectroscopy and molecular modeling, grow out of an understanding of quantum chemistry. We will explore the theories and concepts of quantum mechanics as a means to further understand the structure and properties of atoms and molecules as well as the methods used to elucidate the structures and properties.

Attendance Policy:
Class: The material presented in this course can be abstract and mathematically challenging, and seeing it in class will be helpful to your understanding. With that said, I understand that we are all busy adults, and that there may be an occasion on which you need to miss class. Therefore, you are allowed **four** absences *from class* without any negative consequences. Although I do not need any explanation for the first four absences, I do request that you discuss your absence with me in advance (even 10 minutes before class via phone or e-mail) so I am not waiting for you to begin class. Additional absences will result in a drop in your grade (5-10 absences) or an automatic failure (10 or more absences).

Lab: To get credit for laboratory assignments, you **must** be present. I will make exceptions to this rule only for emergencies and illness. If this need arises, please inform me as soon as possible.

Moodle:
Course assignments, information, and on-line quizzes/practice exams will be available on Moodle: moodle.gac.edu. If you haven't used Moodle in other courses, please see me.

Homework/Problem Sets:
In this course, there will be both required and recommended homework problems. You should do all the required and recommended problems. However, only the required problems will be graded. Problems will be posted on Moodle periodically throughout the semester, and will originate largely from McQuarrie and Simon. I will discuss the solution to a recommended problem at any time and will discuss the solutions to required problems after they have been graded (during office hours or a Friday class).

Due dates for the required problems will be discussed in class and announced on Moodle, but the problems must be turned into me by 5:00 pm on the appropriate day. There will be at least one set of required problems for each chapter discussed. Required problems are individual assignments, and should be done **alone**.

Physical Chemistry, especially Quantum Mechanics, is best learned through application. Therefore, although the recommended problems will not be graded or reviewed, I urge you to complete the problems (without the use of any study guides/solution manuals) and study them until you thoroughly understand. It is also very helpful to work on *these* problems **with your classmates**.

Friday Classes and Literature Reviews:
Each Friday, one person will prepare and present a discussion of a current paper from the Journal of Physical Chemistry A, B or C. Note that the first literature review will be this Friday, Feb 9, 2007. See attached sheet for details of this assignment. As part of the literature review, the entire class will be required to read the selected article prior to class and prepare 1 or 2 questions for the discussion. The remainder of Friday's class will be used to discuss homework problems and/or issues in the lab, to clarify any course materials, and/or to present new material.

Exams and Quizzes: (including make-up policy)
There will be three exams and a final exam. Currently, these exams are in-class exams scheduled as follows:

Exam 1: Chapters 1-4 of McQuarrie and Simon, Friday, March 2, 2007
Exam 2: Chapters 5-7 of McQuarrie and Simon, Friday March 30, 2007
Exam 3: Chapters 8-10 of McQuarrie and Simon, ***Wednesday***, May 2, 2007
Final Exam: Chapters 1-13 of McQuarrie and Simon, TBA

These dates are subject to change, and any of the in-class exams may be replaced by a take-home exam. Students must arrange **in advance** to take an exam at any other than the scheduled time, and may do so only for a valid health or school-related activity. Exams missed without pre-arrangement are entered as zero credit and cannot be made up.

Laboratory:
The laboratory work in this course is a very important portion of this course, and must be taken seriously. More information on lab requirements, schedule, etc. will be available the first day of lab. For purposes here, I will note that items to be graded will include your notebooks, your lab reports, and (potentially) any pre-lab assignments. As in any lab, **closed toed shoes** are required and other safety measures will be discussed as needed.

Lab notebooks are required for this course. This notebook should be bound with consecutively numbered pages. Each page should be dated, and a table of contents should be kept at the front of the book. Notes on the operation of instruments, summaries of the experiments, and observations made in lab must be noted in pen. Spectra, and other data, can be taped or pasted into the book. Results, in the form of tables where applicable, and any related calculations, should be included. Notebooks will be checked periodically.

Lab reports will be written in the style of a journal article and must be typewritten (if you need help with all of the symbols and equations, please see me). Further information on exact writing requirements will also be available on the first day of lab.

A key component in the publication of research articles is anonymous peer-review of the article. Thus, I will be giving you the chance to participate in both sides of peer-review (i.e., as the reviewer and as the author). Upon the electronic submission of your lab reports (to Moodle), I, as the Editor of the *Journal of Physical Chemistry G*, will send your report to other student(s) for anonymous peer-review. Reviewers' comments will be critical in grade determination, but the Editor will have the power to make the final grade decisions. In addition, the reviewers' comments

will also be evaluated and a small portion of your laboratory grade will reflect the thought put into these comments. To be considerable to your classmates, it is essential that lab reports (and reviews) are completed on time. **Late lab reports will be penalized 5% of available points *per day*.**

Grading:
Your course grade will be based on a combination of an absolute scale for exam grades, combined with a curve that may be applied at the end of the course if needed to *raise* the overall class course grade distribution. The absolute grading scale ensures that students have some sense of where they stand with respect to grades throughout the course, and may help encourage group studying without a sense that people are competing with each other. This combined absolute and curved grading method is described further below.

Grading Itemization:

Homework, Quizzes, and Literature Review:	150 pts (20%)
Exams (3 @ 100 pts each):	300 pts (40%)
Laboratory (Reports, Notebooks, etc):	150 pts (20%)
Final Exam:	150 pts (20%)
Total:	*750 pts (100%)*

Absolute exam grading scale: Grade ranges for final grades, expressed as a percentage of the maximum possible points (i.e., 750 pts) are:

	B+ 86 - 88 %	C+ 76 - 78 %	D+ 66 - 68 %
A 93 - 100 %	B 82 - 85 %	C 72 - 75 %	D 60 - 65 %
A- 89 - 92 %	B- 79 - 81 %	C- 69 - 71 %	F 0 - 59 %

Curved exam grading scale: Depending on the class performance, at the end of the semester (after the final exam) the cutoffs above may be *lowered* (but they will not be raised) if needed to *raise* the average course grade to between a B- and C+. That is, the above absolute grading scale may be modified by a curve in the favorable direction, if needed to ensure that at least half of the students receive course grades in the A or B range (including +/-).

Study Tips:
1. Your book has Math Chapters inserted between the main text. If you your math skills are lacking on a specific subject, these chapters are very useful for review and practice.
2. I highly suggest working out the 'recommended' problems as an (informal) group. In my experience, learning physical chemistry is supported by such group activities. And there is no question… you **should do** the recommended problems!
3. I also suggest staying up to date on all course reading. Although not formally outlined, you should read the appropriate chapter from McQuarrie and Simon prior to coming to class.
4. If you run into any problems, don't hesitate to see me. I will help as much as possible!

Honor Code:
In choosing to be a student of Gustavus, you implicitly agree to abide by this code. Although I will not make you sign the corresponding pledge, I will assume that your work is your own on all individual assignments. Please make yourself familiar with the honor code if you are not already. *Code*: "As a community of scholars, the faculty and students of Gustavus Adolphus College have formulated an academic honesty policy and honor code system, which is printed in the *Academic Bulletin* and the *Gustavus Guide*. As a student at Gustavus Adolphus College I agree to uphold the honor code. This means that I will abide by the academic honesty policy, and abide by the decisions of the joint student/faculty Honor Board."

Accommodations:
If you have a physical, psychiatric/emotional, medical or learning disability that may have an effect on your ability to complete the assigned work, please let me know. I will provide assistance and accommodations upon receiving verification from Laurie Bickett in the Academic Advising Center.

Tentative class schedule – subject to change

Week #: Dates	**Textbook Chapters**	**Items of Interest**
Week 1: Feb 5-9	Chapter 1, McQuarrie	
Week 2: Feb 12-16	Chapter 2 & 3, McQuarrie	
Week 3: Feb 19-23	Chapter 3, McQuarrie	
Week 4: Feb 26-March 2	Chapter 4, McQuarrie	**Exam 1**: Chap. 1-4, March 2
Week 5: March 5-9	Chapter 5, McQuarrie	
Week 6: March 12-16	Chapter 5 & 6, McQuarrie	
Week 7: March 19-23	Chapter 6, McQuarrie	
Week 8: March 26-30	Chapter 7, McQuarrie	**Exam 2**: Chap 5-7, March 30
SPRING BREAK	**N/A**	**N/A**
Week 9: April 10-13	Chapter 8, McQuarrie	
Week 10: April 16-20	Chapter 8 & 9, McQuarrie	
Week 11: April 23-27	Chapter 9, McQuarrie	
Week 12: April 30-May 4	Chapter 10, McQuarrie	**Exam 3**: Chap 8-10, ***May 2***
Week 13: May 7-11	Chapter 11&13, McQuarrie	
Week 14: May 14-16	Chapter 13, Review	
Reading Day: May 17		
Final Exam	**Cumulative: Chap. 1-13**	**TBA**