

CHE 372: Quantum Chemistry and Dynamics Spring 2008

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

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

Office Hours: I will only be on campus the following hours. I will be in labs on Mon and Tues afternoon. Feel free to find me at any time during those hours or set up an appointment (you can come find me during lab if needed).

Hours: Mon – 12 to 6:30, Tues – 12 to 5:30, Wed – 12 to 6:30,
Thur – 12 to 3:30, Fri – 12 to 4:30

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.

Homework/Problem Sets:

Homework assignments will be posted on the course website periodically throughout the semester, and will originate largely from McQuarrie and Simon. Due dates for the required problems will be discussed in class and announced on the website, but the problems must be turned into me by 3:30 pm on the appropriate day. There will be at least one set of problems for each chapter discussed. Physical Chemistry, especially Quantum Mechanics, is best learned through application.

Friday Classes and Literature Reviews:

Each Friday, two people 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, March 7,

2008. See attached sheet for details of this assignment. As part of the literature review, the entire class will be required to read one of the selected articles prior to class. Be prepared to ask the presenter questions!

Exams and Quizzes: (including make-up policy)

There will be a series of semester quizzes and exams, including a final exam. Currently, these exams are in-class exams scheduled as follows:

Quiz 1: Chapters 1-4 of McQuarrie and Simon, Thursday, March 20, 2008

Exam 1: Chapters 5-7 of McQuarrie and Simon, Thursday April 17, 2008

Exam 2: Chapters 8-10 of McQuarrie and Simon, Thursday May 8, 2008

Quiz 2: TBD

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.

As a writing intensive class, there will be several writing activities and assignments related to the lab. The largest of these is a review article summarizing your data and other work on molecular spectroscopy. This will cover the data from the majority of our labs and will be discussed in detail at a later date. To help prepare for this article, there will be short lab writing exercises on each lab. There will also be several editing-related activities presented to you to help prepare the final draft. Finally, the lab on computational chemistry will be in full journal style.

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. You **MUST** pass the lab portion of the class to pass the class.

Grading Itemization:

Homework, Quizzes, and Literature Review:	(30%)
Exams:	(30%)
Laboratory (Reports, Notebooks, etc):	(20%)
Final Exam:	<u>(20%)</u>
Total:	(100%)

Absolute exam grading scale: Grade ranges for final grades, expressed as a percentage of the maximum possible points 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 chapters of 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 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.
3. 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: March 3-7	Chapter 1 & 2, McQuarrie	
Week 2: March 10-14	Chapter 2 & 3, McQuarrie	
Week 3: March 17-20	Chapter 4, McQuarrie	Quiz: Chap 1-4, March 20
SPRING BREAK	N/A	N/A
Week 4: March 31-April 4	Chapter 5 & 13, McQuarrie	
Week 5: April 7-11	Chapter 6, McQuarrie	
Week 6: April 15-18	Chapter 7, McQuarrie	Exam: Chap 5-7,13, April 17
Week 7: April 21-25	Chapter 8, McQuarrie	
Week 8: April 28-May 2	Chapter 8 & 9, McQuarrie	
Week 9: May 5-9	Chapter 9 & 10, McQuarrie	Exam: Chap 8-10, May 8
Week 10: May 12-16	TBA	
Week 11: May 19-21	TBA	Possible Quiz