Chemistry 381
Quantum Chemistry
(Advanced Physical Chemistry)
Second Semester 2001-2002
SYLLABUS

Instructor

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Office hours: 7:15-7:50 AM M-F or by appointment

Class schedule

Lecture	8:00-8:50 MWF	(GSC 241)
Lab	8:00-9:50 TTh	(GSC 240)

Texts

Mark A. Ratner and George C. Schatz, *Introduction to Quantum Mechanics in Chemistry*, Prentice Hall, 2001. (Lecture: required, cloth).

Solutions Manual for Mark A. Ratner and George C. Schatz, *Introduction to Quantum Mechanics in Chemistry*, Prentice Hall, 2001. (Lecture: required, paper).

James B. Foresman and Æleen Frisch, *Exploring Chemistry with Electronic Structure Methods*, .2nd ed., Gaussian, Inc., 1996. (Laboratory: required, paper). Cited as **SG**N.

Supplies

A scientific calculator (not necessarily programmable) is important. Each student should have a couple of floppy disks available for her/his work in this course.

Time expectations

Plan to spend about 8 hours per week efficiently studying text and lecture material and working problems. On the average, another 2-3 hours a week will probably be needed for preparation of lab reports.

Attendance

Attendance is required for laboratories, and is encouraged for lectures. Students absent from lecture are responsible for obtaining lecture notes from a classmate. Principal examples of excused absences: illness, family emergency, or an activity officially excused by Augustana.

Nature of the course

Advanced topics in physical chemistry, with emphasis on quantum chemistry, symmetry, and spectroscopy. Starting from solid textbooks, students will also do some work with other sources in the chemical literature. The course is problem-oriented, and will use computer resources as appropriate. This course may be taken as lecture only (Chemistry 381A, 3 credits), or as lecture and lab (Chemistry 381A , 3 credits and Chemistry 381L A lab, 1 credit). For students taking both lecture and lab, normally both grades will be the same, based on total semester %, unless the student specifically arranges with the instructor for separate grading of the two courses. Corequisite: Chemistry 302.

Time expectations

Plan to spend about 6 hours a week efficiently studying lecture material and working problems. Students taking Chem 381L A lab will probably need another 2-3 hours a week for preparation of lab reports.

Attendance

Students are responsible for announcements and for understanding material discussed in class, whether present or not. Attendance is required at exams (and lab periods, if you are taking Chem 381L A lab. In case of unavoidable absence, speak with the instructor promptly. The final exam will replace points on an exam missed due to illness.

Disabilities

Any students with disabilities who need reasonable accommodation in this course are encouraged to speak with the instructor as soon as possible.

Problems

Mark A. Ratner and George C. Schatz, *Introduction to Quantum Mechanics in Chemistry*, Prentice Hall, 2001.

Chapter	**Problems**
1	2, 4, 6
2	1, 3, 4, 5, 7, 9
3	1, 3, 4, 7, 9
4	1, 2, 3, 5, 7, 9
5	1, 3, 6, 7
6	1, 2, 3, 6, 8
7	1, 2, 3
8	1, 2, 7, 8, 11
9	2, 3, 4, 7, 10, 13, 14
10	1, 3, 4, 5, 6, 9, 11
11	1, 2, 3, 4, 6
12	1, 2, 3, 4, 6, 8, 9, 10, 12, 14, 16
13	1, 2, 4, 6, 7
14	1, 2, 4, 8, 9, 12, 13
15	3, 4, 5, 6, 8

As a required part of your **381 Portfolio Web Pag**e, post thoughtful solutions to a reasonable representative sample of problems, that you consider to be the most interesting and significant. To work some problems not assigned here, speak with the instructor.

Term Paper

This assigned paper will deal with the life and work of a scientist with interesting and significant work in a field related to this course, such as: quantum chemistry/physics, theoretical treatment of atoms, molecules, nuclear structure and processes, solid state electronic structure, molecular modeling, spectroscopy, lasers, philosophical interpretation of quantum mechanics (and related controversies), DFT, related software development, and the like. The term paper should place roughly equal emphasis on the person and on the scientific work.

A number of Nobel Prizes in Chemistry and Physics have been related to some of these topics. Some relevant links are provided on the links page of our class web site at http://inst.augie.edu/~viste/381s2002/links.html
A few such names include Heisenberg, Schrödinger, Bohr, G. N. Lewis, Einstein, Dirac, Pauling, Slater, Mulliken, Bohm, J. S. Bell, Hückel, Maria Goeppert-Mayer, Lise Meitner, Fermi, Pople, Kohn, Wigner, Herschbach. This list is intended to be illustrative, certainly not exhaustive. Please discuss your initial plans with the instructor. The term paper should use printed literature and classic papers, as well as web sites. Appropriate length is the equivalent of 5-10 pages, double-spaced. However the term paper will be posted as part of your Chemistry 381 Portfolio Web Page.

Point distribution

Chem 381 A Lecture

Take-home unit exams (2 @ 150)	300
Homework problems on 381 Portfolio Web Page	100
Journal sharing on 381 Portfolio Web Page	75
Quantum Chemistry software use on web page	25
Term Paper on 381 Portfolio Web Page	100
Final exam (in class)	150
Subtotal	750

Chem 381L A Lab

Lab Reports on 381 Portfolio Web Page	250
Total	1000

For students taking both lecture and lab, normally both grades will be the same, based on total semester %, unless the student specifically arranges with the instructor for separate grading of the two courses.

Grade lines

A/B	90 %
B/C	80
C/D	60
D/F	50

+ and - grades normally extend ±3% from each grade line. Thus 87-89.9% for B+, 90-92.9% for A-.

However there is room for some flexibility, particularly if the 381 Portfolio Web Page is sensational.

What grade do you think you have earned in this course? Take into account the scope and quality of your overall work. Submit this statement to the instructor individually, either at the end of the 381 Portfolio Web Page, or privately. As the instructor assigns final grades for the course, such a statement of your own realistic self-assessment will provide important input in the process.

Quantum Chemistry software use

All students in the course, even those taking the course without the lab, are require to use one of the major quantum chemistry software packages to carry out a significant calculation on an interesting molecular system. This might be related to one of the assigned problems, such as one of those in Chapter 14, or a calculation related to your Journal Sharing. Other options are possible. Select your calculation(s) in consultation with the instructor. Post the results on your web site.

Chemistry Seminar Presentation

Each student in Chemistry 381 is required to present a Chemistry Seminar. In most cases the seminar presentation will be related to other work in this course, and a web version should be included on the Chem 381 Portfolio Web Page. For grading purposes, the seminar will be considered as part of the Chem 381 work which it presents, and which is reflected on the web site. If a student is also obligated for a seminar in relation to another chemistry course (Chem 341), the student should meet simultaneously with both instructors, to agree on the nature of the seminar presentation and its grading.

Chem 381 Portfolio Web Page

The general idea is to post on your web site a comprehensive and mature representation and summary of your work in this course.

Particularly since this is an advanced chemistry course, we want to encourage a good deal of creativity and initiative in this regard. The development of an appropriate Chem 381 Portfolio Web Page should reflect your own personality and strengths. Quality and insight are more important than sheer bulk.

Post lab reports of your work on your web site, steadily as you go along. For cooperative reports, distribute them among the web pages of group members, rather than all of them on one group member's web site.

Although the Chem 381 Portfolio Web Page is not intended to be a matter of recipe or a routine algorithmic activity, it may be useful to review guidelines provided for such work recently in Chemistry 301 and 302, in these syllabi (pdf documents).
http://inst.augie.edu/~viste/301f2001/CH301f2001.pdf
http://inst.augie.edu/~viste/302s2002/CH302s2002.pdf

Chemistry 381 home page

Your home page will be linked to the Chem 381 home page for our class at this URL.
http://inst.augie.edu/~viste/381s2002/

Along with other information, a number of potentially useful links are provided on the links page of our class web site at
http://inst.augie.edu/~viste/381s2002/links.html

Such links are relevant especially to software and term paper.

Journal sharing

Three times during the semester **(deadlines March 1, April 3, and May 3**) we will have the sharing of a journal article by each student in the class on their own web site.

1. Locate and digest a journal article which interests you. Current or recent journal articles related to quantum chemistry, symmetry, and computer graphics are recommended, but earlier classic papers are also appropriate and welcome.

2. Journals: Browse in the *Journal of Chemical Physic*s, and in the *Journal of Computational Chemistr*y. A lot of worthwhile articles in the topic areas also appear in other sources, such as *Journal of the American Chemical Society*, *Journal of Physical Chemistr*y, *Inorganic Chemistr*y, and *Journal of Organic Chemistr*y, and in back files of the *International Journal of Quantum Chemistr*y.

3. One of the three journal articles shared may be a review article if you wish, perhaps from *Chemical Review*s, *Chemical Society Reviews* (formerly *Quarterly Review*s, *Accounts of Chemical Researc*h, or *Annual Review of Physical Chemistr*y. At least two of these three articles shared should be primary research publications.

4. Once you have selected your journal article, prepare a photocopy for yourself, and one to be on reserve in the Seminar Room. If the article is quite long, consult with the instructor concerning how much to copy.

5. Prepare a brief written summary and discussion of the article. Include a full bibliographic citation for the article, including its title. The summary will probably be the equivalent of two pages, printed, double spaced. **Post this on your web site by the deadline**.

6. At the end of your summary write (ask, but don't answer) a question which you think might be appropriate as an exam question in this course.

7. The three journal article summaries, presented on your web site, will be worth 100 points total.

Chem 381L A
Quantum Chemistry (Advanced Physical Chemistry)
Laboratory
Second Semester 2001-2002

Initial sources of computational lab work

James B. Foresman and Æleen Frisch, *Exploring Chemistry with Electronic Structure Method*s, 2nd ed., Gaussian, Inc., Pittsburgh, PA, 1996 (paperback).

Types of calculations

- Molecular Mechanics
- Atomic orbitals
- Semiempirical MO
- *ab initio* MO
  - HF
  - CI
  - MP2
- Valence bond
- DFT
- AIM (Atoms In Molecules)
- Molecular vibrations
- NMR
- Transition state and IRC
- Band structure

Computational software

- HyperChem
- Spartan
- Gaussian 94 and 98
- GAMESS
- WebMO implementation of Gaussian 94 and GAMESS
- Jaguar
- ADF (Amsterdam Density Functional Theory)
- CAChe (MOPAC, DGAUSS)

Utility software tools

Mathcad
Xvibs
Batchman
Visual Basic
Quattro Pro, Excel
Crystallographic software
Tcl/Tk

Visualization

GaussView
gOpenMol
Slicer
Chime
JCamp-DX spectral display in Chime

Experimental work

FTIR
Raman

Chemical systems

Atoms
Molecules
Vibrations
Crystals
Macromolecules
Reactions

Getting started on lab work

We encourage you to shape your own body of lab work within broad limits of available resources and tools. The suggestions below simply provide advice on possible ways to get started.

Post your lab reports on your Chem 381 Portfolio Web Page (p. 6). Try to provide a visually interesting presentation, one that reflects and fosters insight.

James B. Foresman and Æleen Frisch, *Exploring Chemistry with Electronic Structure Method*s, 2nd ed., Gaussian, Inc., Pittsburgh, PA, 1996.

We use Gaussian 94 on the IBM RS/6000 (sometimes with Spartan visualization, and sometimes with a WebMO interface), and Gaussian 98W under Windows NT. This includes the Example and Exercise input files referred to in Foresman and Frisch. Explore related types of calculations with other software packages, such as Spartan, Jaguar, ADF, HyperChem, and CAChe.

Chapter	Topic	Key Pages
	Introduction	
	Tutorial for Gaussian for Windows	xxxviii
	Convert PDB file	xlv
	Gaussian output	xlix, App B
	Table of input files	xiv
	Theoretical Background	App A
	Essential Concepts and Techniques	
1	Computational models and model chemistries	3
2	Single point calculations	22
3	Geometry optimizations	49
4	Frequency calculations	70
	Model Chemistries	93
5	Basis set effects	103
6	Selecting an appropriate theoretical method	124
7	High accuracy energy models	159
	Applications	
8	Studying chemical reactions and reactivity	185
9	Modeling excited states	218
10	Modeling systems in solution	242

This lab book and associated Gaussian documentation include and support a very wide range of examples, exercises, and potential research projects. Particularly consider including work along the following lines.

DFT	p. 119
NMR	p. 21, 29, 53, 104
Vibrations, Transition state, IRC	p. 72, 76, 176, 191, 199; Xvibs with Chime or gOpenMol
AIM	p. 198, Gaussian 98 User's Reference p. 41
Cube density & visualization	Gaussian 98 User's Reference p. 66
Visualization	with gOpenMol, Slicer, or integrated with Spartan [p. 167]

Chem 381 A
Quantum Chemistry: Advanced Physical Chemistry
Lecture Schedule
Second Semester 2001-2002

Date	Topic	Chapter
Feb 11, 13	Intro and background to Quantum Mechanics	1
15,18,20	Quantum Theory	2
18	Library instruction -- Lisa Brunick	
22, 25,27	Particle in a box	3
Mar 1, 4, 6	Rigid rotor and angular momentum	4
8,11.13	Molecular vibrations, perturbation theory	5
Mar 13 (W)	Receive Exam 1 (take home, due Wed Mar 20, 8:00 AM)	
15, 18	Hydrogen atom	6
20, 22	Helium atom	7
	[Spring Break: Mar 25-Apr 1]	
Apr 3, 5*	Electron spin	8
8,10	Many-electron atoms	9
12,15	Homonuclear diatomic molecules	10
17,19,22	*Ab initio* and DFT	11
24,26	Semiempirical methods	12
29, May 1, 3	Applications of group theory	13
May 6, 8	Applications of electronic structure theory	14
May 8 (W)	Receive Exam 2 (take home, due Wed May 15, 8:00 AM)	
10,13	Time dependence and spectroscopy	15
15, 17	Topics - student term paper / presentations	
May 20 (Mon, 8:00-10:00)	Final Exam	

* Apr 5 SD Academy of Science