Class Web Site: http://www.uwosh.edu/faculty_staff/gutow/Chem_371_S09/P-Chem Home.html

Course Overview: This course concentrates on learning to use 20th and 21st century developments in chemical theory to model and understand reactivity and structure. We will begin with macroscopic models of kinetics. Then molecular structure will be described using quantum mechanics. The theoretical results will be compared to evidence from measurements of molecular spectroscopy and physical properties. We will finish by considering microscopic models of kinetics that include quantum mechanical information. The experiments in lab will follow this same pattern.

You should be able to use these models to predict the behavior of matter. This means both estimating the range in which a measurement will fall and solving mathematical story problems, using approximations where valid. A summary list of the models and the types of systems to which you should be able to apply them is at the end of this syllabus.

As part of a good liberal arts curriculum this course has a number of goals. The primary goal, as described above, is to introduce you to modern chemical theory. This topic fits well into the liberal arts curriculum because it teaches skills which are generally useful and specific models that are widely applicable. Learning to use these theories is extremely good practice at solving difficult and unfamiliar problems as well as thinking analytically, critically and creatively. The models of chemical reactivity (kinetics) and structure (quantum mechanics) are fundamental to understanding much of what happens to matter in the universe. These models are used to understand the chemical reactions involved in living, to predict the shapes of biomolecules, to develop new drugs, design solid-state electronics, and understand environmental issues such as global warming. Lasers and photosynthesis are quantum phenomena. In lecture and lab you will practice using these widely applicable models and consider their limitations (more critical thinking), because in many cases simpler models or direct experimentation can provide high accuracy results with significantly less effort. A secondary, but very important goal of the course, is to help you develop effective communication skills. You will work on communication skills primarily in lab where you will produce written, web-based, and oral reports on your work.

Required Texts: Atkins & de Paula, Physical Chemisty, 8th Edition
Barrante, *Applied Mathematics for Physical Chemistry,* 3rd edition.

Required Equipment: bound duplicating laboratory notebook, pen (for writing in lab notebook), scientific calculator and goggles.

Prerequisites: Physical Chemistry I (Chem 370), calculus III and calculus-based physics II.

Class times: *Lectures*: MWF 10:20-11:20 (HS 456); *Lab*: T 1:20 - 4:30 (sec 1, HS-428).W 1:50 - 5:10 (sec 2, HS-428),

Office Hours: Dr. Gutow (HS-412): M 3-4, TTh 9:10-10:10, WF 8:30-9:30 or by appointment.

Reading Assignments: A study sheet will be distributed approximately weekly, listing the specific reading assignments.

Critical Thinking Exercises: Short assignments designed to help you learn how to use the textbook and other reference sources to prepare for class. For example, you might be asked to find definitions, compare two models and explain when it is appropriate to use each or work through some 'what if' calculations. Some in-class group worksheets will also be used. In general a group of these will be handed out with the reading and homework assignments. Each exercise is to be finished for a specific class. The primary goal of these exercises is to help you learn how to prepare for class. A copy is due at the beginning of the class for which they are assigned. They will be graded on a pass/fail basis and are worth 5 points each. Up to 50 points may be received for these exercises. A minimum of twelve such assignments will be given during the semester. You are encouraged to discuss these assignments with your classmates as well as the instructor.

Homework: Homework will be distributed with the reading and critical thinking assignments. Homework will consist of "discussion" and "exercise" questions, which are straightforward practice with definitions and equations, plus "problem" questions, which require more involved application of concepts and problem solving. The "discussion" and "exercise" questions will be graded as attempted/not attempted out of 5 pts total. The "problems" will be graded out of 20 pts total. Discussion of the homework with your classmates and instructor are encouraged. If you are having trouble with particular types of problems try additional questions of a similar type. Numerical answers to many of the "exercises" and "problems" are available in the textbook appendices. Detailed solutions to most "problems" will be provided on the class web site two days after the homework due date. The best 10 out of 12 homeworks will count for your grade. Doing **ALL** the homework is the best way to prepare for exams in this class.

Homework is due in class on the day specified when handed out. Late homework will be marked down 10%/day. No homework will be accepted after the detailed answer key has been posted on the class website two days after the due date.

Exams: There will be three exams worth 200 points (plus 20 pts extra credit). The exams will be written to be completed in one hour, but you will be given unlimited time. The exams will be administered in the testing center. The material requires that exams be cumulative, but primary emphasis will be on the chapters covered since the previous exam. The goal of this course is not to memorize formulas, but to learn how to use models to make predictions. You will be provided with an equation sheet for each exam consisting of the fundamental equations of each model. Additionally, you will be allowed to bring a 3” x 5” card of ***handwritten*** notes to the exam. There will also be a 90 minute laboratory exam (see the lab section of the syllabus for more details).

Grading:

Critical Thinking Exercises:	10 x 5 pts =	50 pts
Graded Homework:	10 x 25 pts =	250 pts
Exams:	3 x 200 pts =	600 pts
Lab	300 pts	300 pts
Total:		1200 pts

Additional Resources:

WEB RESOURCES: The course web site may be accessed by starting at the instructor's home page: http://www.uwosh.edu/faculty_staff/gutow/. Problem sets and answer keys will be password protected. The username for login into the protected part of the web site is: chem371S09. The password will be supplied the first day of class.

SYMBOLIC MATH PACKAGES: The open source SAGE math package is available on the Chem SAGE Server or can be downloaded from the SAGEmath web site. MAPLE™ is available on the computers in the P-Chem lab and the open access labs in Halsey.

WEB INTERFACE TO GAMESS QUANTUM PACKAGE: The GAMESS package is available on the UWO Quantum Server.

TEXTS: The following books are on reserve in in the Halsey Resource Center (HS-289). You may find it useful to see difficult concepts described a number of ways. Homework assignments will suggest sections of these texts to look at for additional help.

Atkins, *Molecular Quantum Mechanics*, QD462.A84 1997. This text expands on the quantum mechanics discussed in the course text.

Atkins, *Quanta*. This is essentially a dictionary of quantum mechanical terms. You may find it useful because it explains the significance of most things with very little mathematics. A good way to get an overview.

Barrante, *Applied Mathematics for Physical Chemistry* QD455.3.M3 B37. A good review of chemical applications of graphing and calculus.

Jorgensen and Salem, *The Organic Chemist's Book of Orbitals*, QC461.J68. This book has lots of nice electron density maps for the various orbitals of common molecules calculated using molecular orbital theory.

Warren, *The Physical Basis of Chemistry*, QD475.P47. This book has nice simplified, but accurate, descriptions of many of the quantum, spectroscopic and thermodynamic concepts we will discuss.

Lecture and Homework Schedule:

Chapter	Lectures	Homework Due*
I. Chemical Kinetics		
22: Reaction Rates	2/2, 2/4, 2/6, 2/9	2/9
25: Surface Kinetics/Isotherms	2/11, 2/13	2/16
23: Complex Reactions	2/16, 2/18, 2/20, 2/23	2/20, 2/25
Review	2/25	
Exam 1 (Unit I)	**Friday, February 27, 2009**	
II. Theory of Molecular Structure		
8: Introduction to Quantum Mechanics	3/2, 3/4, 3/6	3/9
9: Mechanics of Quantum	3/9, 3/11, 3/13, 3/16	3/16
10: Quantum of Atoms	3/18, 3/20, *Spring Break*, 3/30	4/1
11: Molecular Structure	4/1, 4/3, 4/6	4/8
Review	4/8	
Exam 2 (Unit II)	**Friday, April 10, 2009**	
III. Macroscopic Manifestations of Quantum Mechanics		
13: Rotational & Vibrational Spectroscopy	4/13, 4/15, 4/17, 4/20	4/17, 4/22
14: Electronic Spectroscopy/Lasers	4/22, 4/24, 4/27	4/29
18: Molecular Interactions	4/29, 5/1, 5/4	5/6
24: Reaction Dynamics	5/6, 5/8, 5/11	not due
Review	5/13	
Exam 3 (Unit III)	**Friday, May 15, 2009**	

*The homework will generally be handed out during the first lecture on each chapter.

Laboratory

Laboratory Notebooks: Notebooks should be records of everything a scientist does. They are used as legal evidence that an experiment was performed in patent claims and are often referred to by other scientists working on related experiments. Entries should be made in permanent ink. *Notes from pre-lab lectures should <u>not</u> be recorded in your notebook*, but all calculations and data analysis should be. A minimum checklist of what should be in your notebook is available on the class web site. Pages should be numbered consecutively and a table of contents included. Date each page as it is used and start a new page on each day; do not tear out pages, simply draw a line through errors. Lab notebooks will be checked each day and initialed by your instructor. You will turn in your duplicate pages for grading with each lab report.

Pre-lab preparation: Read the description of the experiment and any additional assignment. The experiments are not described as a list of steps to be followed, so careful reading and reflection before lab will be required to develop a plan for the project.

In your notebook record a brief outline of the procedure you expect to follow and construct two tables of information: 1) reagents; 2) equipment. In the reagents table write the chemical name, chemical formula, a drawing of the structure, the state in which it will be found (solid, liquid, gas, or in solution), and hazard information from the Material Safety Data Sheet(s), which are available online or in the stockroom. If solutions are to be prepared, calculate the amounts needed. Each row in the equipment table should contain the property to be measured, the equipment used for the measurement, and the sample(s) that will be measured.

During lab: Procedures actually followed should be described in your laboratory notebook. Do not rely on a summary written before the lab, although you may just note deviations from your planned procedure. List lab partners. Include all experimental observations, data and calculations; you should tape in computer printouts and spectra (cut or fold to fit). If data is stored in computer files accurately record the data file names. Goggles and appropriate clothing (no sandals or shorts) must be worn at all times. Failure to wear safety goggles may result in ejection from lab and an F in the course.

Lab Reports: Because scientists use many formats for communicating information, we will practice a variety of report styles this semester.

1. <u>Proposal:</u> You will prepare a proposal for additional research beyond the preliminary work done in lab. The proposal will contain a summary of the background available in the literature, a justification of why the work is interesting, a hypothesis to be tested, preliminary results showing that you can work with the proposed system, and a description of the proposed experiments explaining how they will test the hypothesis.

2. <u>Formal laboratory reports:</u> Your reports should be written as if for publication in *The Journal of Physical Chemistry*. Assume that your readers have studied physical chemistry but are not familiar with your handouts. A sample lab report is available on the class web site. Additional recommendations on word choice, grammar, reference format, notation and nomenclature may be found in *The ACS Style Guide*, J. S. Dodd, Ed. (QD8.5.A25) which is on reserve in the Halsey Resource Center.

3. <u>Web poster presentation:</u> You will prepare a web page or pages to be posted on the Internet. Posters should be eye-catching and informative. You must have: a title, authors' names, an abstract, an introduction, a body (consisting mostly of tables and figures with appropriate captions), a conclusion and references. This is a web version of a formal report.

4. <u>Poster presentation:</u> This is the way most scientific work is communicated at meetings.

Posters must be eye-catching and informative. Keep text to a minimum. You must have: a title, author's name, an introduction, a body (consisting mostly of tables and figures with appropriate captions), a conclusion and references.

5. Peer Review: All articles published in the literature are reviewed by anonymous reviewers. They are only published after the reviewers are satisfied that they are accurate, well written and a new contribution to the scientific body of knowledge. Most articles are rewritten at least once in response to reviewers' comments. Often additional experiments are also done. You will review two of your peers' formal lab reports for each formal report that is due and rewrite your reports based on the reviews returned to you.

Students may discuss the write-up and calculations with each other but every student must turn in an individual report. Reports must be typed or computer word processed. Use of computers for data plotting and analysis is encouraged as is reference to the chemical literature for accepted values.

Reports will be graded as follows: 10 points on writing, 10 points on calculations including error analysis, 2 point for literature search/comparison with the literature. A copy of the grading cover sheet for formal reports is attached to this syllabus. The criteria are:

1. Does the report contain all the sections (abstract, introduction, experimental method, results, discussion)? Is the information logically distributed among the sections?
2. Is sufficient information given in experimental methods for another physical chemistry student to repeat the experiment without referring to your handouts?
3. Have all the discussion questions been answered?
4. Are the spelling and grammar correct? Is verb tense consistent (present or past)? In general past is appropriate unless referring to data presented in the report. Is the voice correct? Most scientific articles are in the passive voice. For example: instead of, "we did the experiment three times," write, "the experiment was done three times." Note that the implied "by _____" is left out.
5. Are the equations used in calculations included? Are there any errors in the calculations? Are the significant figures carried correctly? Are the error estimates reasonable?
6. Was a literature search performed? Is a copy of the title/author/abstract found in the search attached. You may use the references supplied in handouts or the text for actual comparison, but you must perform a literature search using SciFinder™ and provide at least one abstract found this way from an appropriate reference.

The reviews will be due the lab day after the reports were originally due. You may rewrite reports based on the reviews. If you turn in the rewritten report within one week of getting the reviews, the grade will be recalculated as the mean average of the original and rewritten reports. A copy of one of your reports, the best, will be kept for your student portfolio. Thus you should rewrite at least one report. Turn in **three** copies of the initial version of your formal reports and **two** copies of rewritten reports **with the original graded version attached**. Reviews of classmates' reports are worth 3 points each.

Reports are due in class the week following completion of the project. Late reports will be marked down 10%/day. Incomplete reports will be returned and the late penalty assessed.

Laboratory Exam: There will be a 90 minute final exam based on work done in lab. You will be able to refer to your textbooks, lab reports, and lab notebooks on the exam. The 90 minutes alloted for the exam will not be enough to figure out what you did from your text and your lab reports. You will only have enough time to use them as references to get constants, formuli and relationships correct. You will need to review your laboratory reports and correct any mistakes you made in order to do well on this exam. You will also be responsible for material from the prelabs and assigned reading. Two non-graded problem sets will be distributed during the semester to assist your preparation for the exam.

Grading:

6 x 6	=	36	pre-laboratory preparation
6 x 6	=	36	laboratory notes
6 x 3	=	18	reviews of reports
6 x 22	=	132	laboratory reports (formal, poster and web poster)
		78	final exam
		300	points total

Lab Schedule:

Week of	Project	Written	Review	Rewrite
2/2	Surface Adsorption/Analysis	-	-	-
2/9	Surface Adsorption/Analysis	-	-	-
2/16	Surface Adsorption/Analysis	2/23 (proposal)	3/2	3/9
Quantum Calculations				
2/23	Quantum Calculations A	-	-	-
3/2	Quantum A(continued)	3/9 (formal)	3/16	3/30
3/9	Quantum B	-	-	-
3/16	Quantum B (continued)	3/30 (web poster)	-	-
3/23	*no lab/Spring Break*			
Rotate through 2 labs (HCl rovibrational and dye electronic spectroscopy)				
3/30	Spectroscopy A	-	-	-
4/6	Spectroscopy A	4/13 (formal)	4/20	4/27
4/13	Spectrocopy B	-	-	-
4/20	Spectrocopy B	4/27 (poster)	-	-
Fluorescence and Fast Kinetics				
4/27	Fluorescence (Lasers)	-	-	-
5/4	Fluorescence (continued)	5/11(formal)	-	-
5/11	90 min Lab Exam (exact time to be arranged)			

Assessment of Learning: As part of the department's assessment of its majors program, evidence will be added to your portfolios to demonstrate your ability to do a number of things.
From Lecture:

1. describe the structure and composition of matter;
2. apply theoretical and mechanistic principles to the study of chemical systems employing both qualitative and quantitative approaches;
3. use theories of microscopic properties to explain macroscopic behavior;
4. explain the role of energy in determining the structure and reactivity of molecules;

5. use mathematical representations of physical phenomena.

From Lab:

1. read and follow experimental protocols;
2. properly set up and safely manipulate laboratory equipment;
3. plan and execute experiments, including the use of the chemical literature;
4. maintain accurate records of experimental work;
5. analyze data statistically and assess reliability of results;
6. prepare effective written scientific reports;
7. use mathematical representations of physical phenomena;
8. use and understand modern instrumentation;
9. use computers for chemical applications;
10. retrieve specific information from the chemical literature;
11. work cooperatively in problem solving situations.

Models you will learn to apply:

Model	Be able to apply to
Quantum Mechanics -Schršdinger equation -Born-Oppenheimer -Rigid-Rotor -Franck-Condon principle	Molecular and atomic structure Molecular and atomic energy levels Spectroscopy of gas phase molecules (electronic, vibrational, rotational and ro-vibronic) Liquid phase spectroscopy (electronic, vibrational) Fluorescence Spectroscopies (UV-Vis, Raman, IR, photoelectric) Physical properties (dipole moments)
Electrical Properties of Molecules -Coulomb's law -Capacitance/Dielectric Constant -Scattering -Mie Potential -Lennard-Jones Potential	Molar polarization Dipole moments Bond moments Ionic character Polarizability Radial distribution functions Molecular interactions (attractions and repulsions)
Kinetics -Macroscopic (mechanistic) -Microscopic --Collision Theory of Reaction Rates --Collision Theory of Solution Reactions --Transition State Theory	First order reactions Mechanisms made of first and second order reactions Unimolecular gas phase reactions Michaelis-Menten (be aware of limited experimental conditions for applicability) Surface processes Potential energy surfaces Modeling of simple reactions (liquid and gas phase) Radiation processes (photochemical reactions, lasers, fluorescence)

ASSESSMENT GOAL #2

Laboratory Report Cover Sheet

Student: ____________________________

Course: _____________________________ Semester/Year: __________

Skill Level Indicators

N Novice: requires explicit guidance of instructor
I Intermediate: performs with minimal guidance
A Advanced: exhibits independence; may modify protocols to new conditions, instruct others
ne No Expectation in this area
number in parentheses indicates maximum deduction if in error.

Performance of experiment N I A

____ Follow experimental protocols (N needs list of steps to follow; I plans steps from a general description; A uses the literature to develop procedure)

Laboratory Notebooks N I A ____ / 6

____ Record data accurately (I numbers recorded; A additional observations)

____ Record procedures followed (N none; I minimal; A work could be reproduced from notes)

Laboratory Report N I A ____ / 10

____ Spelling/grammar (some -1, many -2, unreadable -3); vocabulary (-1/2); tense consistency (-1/2); voice passive (-1/2)

____ Organize material into standard sections (minor problems -1/2, major problems -1)

____ Abstract: system studied; method used; important results (-1 if absent, no other deductions)

____ Introduction: what experiment will tell us (-1); balanced equations for chemical reactions (-1)

____ Experimental: reagents (-1/2); equipment specifications/name (-1/2); procedures followed (only refers to text -2, N)

____ Results: data is complete; displayed as table or graph when appropriate (up to -1)

____ Discussion: significance of experiment (-1); comparison to literature; answers to text questions (-1); discussion of error sources (-1/2)

____ Equations: complete description including definition of variables (some missing -1/2, many missing -1, most -1.5)

____ References: complete; correct format

Data Analysis and Interpretation N I A ____ / 6

____ Performs algebraic calculations: includes equations;units (-1/2); sample calculations (-1); accuracy (up to -4)

____ Graphs data (N simple graph, I regression/curve fitting) (up to -2 if missing)

____ Uses computer simulations/molecular modeling

Assess reliability of results N I A ____ / 4

____ Estimates error in measurements (N gives sources of error (-2), I propagates errors-- includes equations, sample calculations (-2))

____ Significant digits (-1/2)

Literature Search N I A _____ / 2

____ Finds appropriate references (provide abstract) (-1)

____ Compares literature results with own (-1)