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 (chapters 25, 26, 28). Then molecular structure will be described using quantum mechanics (chapters 11-14). The theoretical results will be compared to evidence from measurements of molecular spectroscopy and physical properties (chapters 16, 17, 21). We will finish by considering microscopic models of kinetics that include quantum mechanical information (chapter 27). The experiments in lab will follow this same pattern.

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.

As you progress through the course you should develop the ability 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.

Lectures: 11:30 - 12:30 MWF (HS 367) **Lab**: 1:20-4:30 TUESDAYS (HS 428)

Required Texts: Atkins & de Paula, Physical Chemisty, 7th Edition
Barrante, *Applied Mathematics for Physical Chemistry,* 2nd edition.
No text required for lab, but reading assignments will be provided prior to each experiment.

Required Equipment: Calculator, bound duplicating laboratory notebook, water insoluble pen (Pentel Hybrid model available at the bookstore is acceptable) and goggles, which must be worn during lab.

Prerequisites: Physical Chemistry I (Chem 370/347), calculus III and calculus-based physics II.

Office Hours: Dr. Gutow (HS-412): MF 8:30-9:30, TTh 9-10, W 1-2, or by appointment. Phone: 424-1326. E-mail: gutow@uwosh.edu. Web site: http://www.uwosh.edu/faculty_staff/gutow

Lecture

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 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 ungraded exercises to be worked and one graded problem (10 pts each) provided by the professor. Numerical answers will be provided for the exercises so that you may check your work. Treat the graded exercise as an open book, take-home quiz, which can be discussed with the instructor but not classmates. The lowest two scores will be dropped when calculating your grade. The goal of the graded homework is to provide a measure of individual student mastery of problems and skills that are too involved to be included on an exam. Please do not collaborate on these graded problems. You are encouraged to work together on all other homework and exercises.

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 answer key has been posted on the class web site two days after the due date.

Exams: There will be three exams worth 100 points (plus 10 pts extra credit). The exams will be written to be completed in one hour, but you will be given unlimited time. The first two exams will be administered in the testing center and the last exam will be administered in a classroom at a time to be arranged. 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.

Lecture Class Schedule:

Chapter	Lectures	Homework Due*
I. Chemical Kinetics		
25: Reaction Rates	9/7, 9/9, 9/12, 9/14	9/14
28: Surface Kinetics	9/16, 9/19	9/21
26: Complex Reactions	9/21, 9/23, 9/26, 9/28	a:9/26, b:9/30
Review	9/30	
Exam 1 (25, 26, 28)	**Monday, October 3**	
II. Theory of Molecular Structure		
11: Introduction to Quantum Mechanics	10/5, 10/7, 10/10	10/12
12: Mechanics of Quantum	10/12, 10/14, 10/17, 10/19	10/19
13: Quantum of Atoms	10/21, 10/24, 10/26	10/26
14: Molecular Structure	10/28, 10/31, 11/2	11/4
Review	11/4	
Exam 2 (11-14)	**Monday, November 7**	
III. Macroscopic Manifestations of Quantum Mechanics		
16: Rotational and Vibrational Spectroscopy	11/9, 11/11, 11/14, 11/16	a:11/14, b:11/18
17: Electronic Spectroscopy/Lasers	11/18, 11/21, (Thanks giving break), 11/28	11/30
21: Molecular Interactions	11/30, 12/2, 12/5	12/7
27: Reaction Dynamics	12/7, 12/9, 12/12	not due
Review	12/14	
Exam 3 (16, 17, 21, 27)	**Friday, December 16**	

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

Laboratory

Lab experiments are meant to illustrate concepts being discussed in lecture and to familiarize you with many of the tools used by physical chemists. The tools you will learn to apply include the chemical literature, written and oral communication, mathematical functions, molecular modeling software, error analysis, and mechanical and electronic equipment.

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 is not enough time to figure out what you did from your text and 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.

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. 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. Copies of your entries will be collected at the end of each lab period for grading.

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. List lab partners. Include all experimental observations, data and calculations; you may staple or tape in computer printouts and spectra. 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) Formal laboratory reports: 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.

2) Web poster presentation: 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.

3) Poster presentation: 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.

4) Oral report: Over the course of the semester groups of students will work to prepare a 10 minute presentation on one laboratory. The instructor will assign a topic and a date for the oral presentation for each group. Each group member will present a part of the report (Introduction, Experimental, Results/Discussion) The time limit means it will be a summary of the material in a formal report. Overhead transparencies or PowerPoint™ should be used as visual aids. IF YOU WISH TO USE PowerPoint™ PLEASE INFORM THE INSTRUCTOR A WEEK AHEAD OF TIME AS A PROJECTOR WILL HAVE TO BE ORDERED FOR THE LAB CLASSROOM.

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 points 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 preferred. 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 STN/CAS and provide an abstract found this way for 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 <u>one week</u> 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. <u>Turn in **three** copies of the initial version of your formal reports and **two** copies of rewritten reports **with the original graded version attached**.</u> Reviews of classmates' reports are worth 2 points each.

<u>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.</u>

Lab Schedule:

Date	Project	Written	Review	Rewrite	Oral*
9/13	Kinetics of Surface Adsorption	-	-	-	-
9/20	Surface Adsorption (continued)	-	-	-	-
9/27	Surface Adsorption (continued)	Wed! 10/5 (formal)	10/11	10/18	10/11

10/4	Quantum Calculations A	-	-	-	-
10/11	Quantum A(continued)	10/18 (formal)	10/25	11/1	10/25
10/18	Quantum B	-	-	-	-
10/25	Quantum B (continued)	11/1 (Web Poster)	-	-	11/8

11/1 - 11/22 Rotate through 2 labs (HCl Rovibrational and Dye Electronic Spectroscopy)

11/1	Spectroscopy A	-	-	-	-
11/8	A continued	11/15 (formal)	11/22	11/29	11/22
11/15	Spectrocopy B	-	-	-	-
11/22	B continued	11/29 (poster)	-	-	-

11/29	Fluorescence (Lasers)	-	-	-	-
12/6	Fluorescence (continued)	12/13 (formal)	-	-	-
12/13	Cleanup/Lab Exam				

*Oral presentations will occur at the beginning of the laboratory class session. If you intend to use PowerPoint™, please inform the instructor, as a projector will have to be ordered for the lab classroom.

Grading

Lecture Grading:	Critical Thinking Exercises:	10 x 5 pts =	50 pts
	Graded Homework:	10 x 10 pts =	100 pts
	Exams:	3 x 100 pts =	300 pts
	Lecture Total:		450 pts
Lab Grading:	Pre-laboratory preparation:	6 x 5 =	30 pts
	Laboratory notes:	6 x 6 =	36 pts
	Reviews of reports:	6 x 2 =	12 pts
	Lab reports(one poster and one web poster):	6 x 22 =	132 pts
	Oral report:	1 x 10 =	10 pts
	Lab exam:	1 x 80 =	80 pts
	Lab Total: (÷2 before adding to Lecture score)		300 pts
Grand Total:	450 + 150 = 600 pts		

The total points necessary to receive a particular grade are listed below. The instructor reserves the right to change the point total downward.

A: 542 AB: 512 B: 482 BC: 447 C: 425 CD: 382 D: 339 F: <339

Additional Resources:
WEB RESOURCES: This syllabus, copies of homework assignments and answer keys will be available at the course web site. 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 web site is: pchemf05. The password will be supplied the first day of class.

TEXTS: The following books are on reserve in the Halsey Resource Center (HS-259). 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.

> *The ACS Style Guide*, J. S. Dodd, Ed. QD8.5.A25. This book explains the standard format used in ACS journals.
>
> Atkins, *Molecular Quantum Mechanics*, QD462.A84. 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.

Model	Be able to apply to
Quantum Mechanics -Schrödinger 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 ____ / 5

____ 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)