Class Web Site: http://www.uwosh.edu/facstaff/gutow/physical-chemistry-2 contains some publicly available class content (syllabus) and useful links. Most class content will be in D2L: http://www.uwosh.edu/d2lfaq/d2l-login/.

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 at the microscopic level using quantum mechanics to describe molecular structure. The theoretical results will be compared to evidence from measurements of molecular spectroscopy and physical properties. We will finish by considering kinetics at both the macroscopic and microscopic levels. 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.

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 and web-based reports on your work.

Required Texts: Chang & Thoman, *Physical Chemistry for the Chemical Sciences*.
WebAssign for Chang's Physical Chemistry for the Chemical Sciences.
Barrante, *Applied Mathematics for Physical Chemistry,* 3rd edition.
Chemistry 371 Lab Manual available at the University Bookstore.

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

Prerequisites: Physical Chemistry I (Chem 370), calculus III.

Class times: *Lectures*: MWF 9:10-10:10 (HS 457); *Lab* (HS 428): M 1:50-5:10

Instructor:

Name (Office)	E-mail	Class Sections	Office Hours
Dr. Gutow (HS 412)	gutow@uwosh.edu	Lecture & Lab	MWF 10:20 – 11:20; TTh 9 – 10 *or by appointment*.

Homework, in-class exercises and exams will be used to assess your chemical knowledge and document your ability to:

- describe the structure and composition of matter;
- apply theoretical and mechanistic principles to the study of chemical systems employing both qualitative and quantitative approaches;
- use theories of microscopic properties to explain macroscopic behavior;
- explain the role of energy in determining the structure and reactivity of molecules;
- use mathematical representations of physical phenomena.

Reading Assignments and Homework will cover a week or two and will have parts due at the beginning of most class meetings. Assignments will not be accepted late.

Reading Assignments will come primarily from the textbook. Other sources will be used as necessary.

Homework will be due for each class and usually have an online and written component. Online parts will be due at 8 A, written parts at the beginning of lecture. You will see three different types of questions. The first two types will focus on material we will be discussing during the class meeting for which the assignment is completed.

Critical Thinking Exercises/Discussion Questions: The questions are 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.

Practice Exercises: These will be primarily online and similar to the end of chapter problems in the text. The goal is to help you figure out what you need to ask about in class. WebAssign questions are answered and graded online; you will have five attempts to get a correct answer, and can ask for hints. You will need to register for the class at <**https://www.webassign.net/login.html**>.

Instructor	Class	Section	Class Key
Jonathan Gutow	Chem 371	[No Name]	uwosh 6025 2084

Problems: The problems will be a little more challenging and based on material discussed in the previous classes.

Exams: There will be 220 available points on each exam. However, exams will be scored out of 200 points (20 pts of extra credit distributed throughout the exam). 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:

Homework & in class worksheets:		25%
Exams:	3 x 200 pts	50%
Lab:		25%
Total:		100%

Grade Cutoffs: A/A- > 87%, B+/B/B- > 77%, C+/C/C- > 67%, D+/D > 60%, F ≤ 60%. The cutoffs will not be adjusted upwards, but the instructor reserves the right to lower them.

Additional Resources:

WEB RESOURCES: This syllabus, copies of homework assignments and answer keys will be available at the course D2L site. Useful links will be provided within D2L, but can also be accessed from the instructor's home page: http://www.uwosh.edu/facstaff/gutow.

SYMBOLIC MATH PACKAGES: These can help you do algebra and calculus. The open source SAGE math package is available on the Chem SAGE Server or can be downloaded from the SAGEmath web site and installed on your personal computer. Information on user accounts on the Chem SAGE Server will be provided in class.

GAMESS QUANTUM PACKAGE: The GAMESS package is available on the computers in P-Chem lab.

TEXTS: The following books are on reserve at Polk Library. You may find it useful to see difficult concepts described a number of ways. Homework assignments may suggest sections of these texts to look at for additional help.

- Atkins, *Molecular Quantum Mechanics*, QD462.A84 1997. Graduate level presentation.
- Karplus & Porter, *Atoms and Molecules*, QD461.K33. A more detailed presentation of quantum mechanics.
- Barrow, *Physical Chemistry*, 6th ed. Alternative introduction to quantum mechanics.
- Barrante, *Applied Mathematics for Physical Chemistry* QD455.3.M3 B37. A good review of chemical applications of graphing and calculus.
- Warren, *The Physical Basis of Chemistry*, QD475.P47. This book has nice simplified, but accurate, descriptions of many of the quantum, and spectroscopic concepts we will discuss.

Tentative Lecture Schedule (S18):

Topic (#.# refers to chapter sections in Chang & Thoman)	Lectures
I. Theory of Molecular Structure	
Introduction to Quantum Mechanics (10.1 – 10.12, 11.2)	1/29, exercises in lab, 1/31, 2/2, 2/5, 2/7
Atoms (12.1 – 12.11)	2/9, 2/12, 2/14, 2/16
Molecules (13.1 – 13.9)	2/19, 2/21, 2/23
Review	2/26
Exam 1 (Unit I)	**February 28, 2018**
II. Spectroscopy and Bulk Properties	
Vibrational & Rotational Spectroscopy (11.1 – 11.3, 11.5)	3/2, 3/5, 3/7, 3/9, 3/12
Electronic Spectroscopy/Lasers (14.1 – 14.5)	3/12, 3/14, 3/26
Spring Break	
Liquid (17) and Solid Properties (18.1, 18.4)	3/26, 3/28
Kinetics Intro (15.1 – 15.2) NOT ON EXAM 2	3/30
Review	4/2
Exam 2 (Unit II)	**April 4, 2018**
III. Kinetics	
Kinetics Concepts and Fundamental Models (15.1 – 15.7, 20.6)	3/30, 4/6, 4/9, 4/11
Experimental Kinetics (15.8 – 15.10)	4/13, 4/16
Catalysis (15.12 + handouts/web reading)	4/18
Photochemistry [greenhouse, smog, ozone] (16.1 – 16.5)	4/20, 4/23. 4/25, 4/27
Kinetic Modeling (handouts)	4/30, 5/2, 5/4, 5/7
Review	5/9
Exam 3 (Unit III)	**May 11, 2018**

Laboratory

This laboratory emphasizes the use of tools to study properties of chemicals. The tools you will learn to apply include: the chemical literature; mechanical and electronic equipment, such as vacuum lines and lasers; mathematical functions; error analysis; and written and oral communication.

The laboratory will used to assess your chemical knowledge and document your ability to:

- read and follow experimental protocols;
- properly set up and safely manipulate laboratory equipment;
- plan and execute experiments, including the use of the chemical literature;
- maintain accurate records of experimental work;
- analyze data statistically and assess reliability of results;
- prepare effective written scientific reports;

- use mathematical representations of physical phenomena;
- use and understand modern instrumentation;
- use computers for chemical applications;
- retrieve specific information from the chemical literature;
- work cooperatively in problem solving situations.

What will happen in lab? We will begin the semester with a review of mathematical principles needed for quantum mechanics.

Six experiments have been chosen to illustrate principles studied in lecture.
quantum mechanics: Conjugated Dyes, Quantum Calculations
spectroscopy: Infrared Spectroscopy and Laser Spectroscopy
kinetics: Iodination of Ketone, Laser Induced Fluorescence

Laboratory Notebooks: Details of what is required and grading are included in the lab manual. NOTE: there is an extra requirement for pre-lab preparation beyond last Fall. You must also include a brief outline of expected procedures in addition to the reagent and equipment tables. Completed pre-labs should be initialed by the instructor at the beginning of lab. Duplicates of the pre-labs and notes made during data collection and analysis will be turned in for grading when the lab report is due.

Lab Reports: You will be writing some formal reports, sections of reports and one group report (in the form of a website). See the Lab manual for details. You will be able to rewrite one formal report and the website based on instructor comments and peer reviews.

Peer Reviews: You can get credit for doing peer reviews of the formal reports and the website.

SciFinder Searches: You can get credit for searches on any 5 of the 6 labs.

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 allotted 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.

Lab Schedule S18

		Due on lab day		
Week of	**Project**	**Written**	**Review**	**Rewrite***
1/29	Math and Quantum Mechanics	-	-	-
2/5	Spectroscopy of Conjugated Dyes	2/12 (formal)	2/19	2/26
2/12	Quantum Calculations	-	-	-
2/19	Quantum Calculations (continued)	-	-	-
2/26	Quantum Calculations (continued)	3/5 (web poster)	3/12	3/26
Rotate through 2 labs: HCl rovibrational spectroscopy and Raman/Laser Spectroscopy.				
3/5	Spectroscopy A	-	-	-
3/12	Spectroscopy A	3/26 (formal)	4/2	4/9
3/19	*no lab/Spring Break*			
3/26	Spectroscopy B	-	-	-
4/2	Spectroscopy B	4/9 (Res&Disc)	-	-
4/9	Solution kinetics (Iodination)	-	-	-
4/16	Solution kinetics (Iodination)	4/23 (formal)	4/30	-
4/23	Laser Induced Fluorescence	-	-	-
4/30	Laser Induced Fluorescence	5/7 (Res&Disc)	-	-
5/7	90 min Lab Exam (exact time to be arranged)			

*** You may only rewrite one formal report: either the Dye lab or Spectroscopy A.**

Why this is a Liberal Arts Course: As part of a good liberal arts curriculum this course has a number of goals. The primary goal, as described in the course overview, 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). 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 and web-based reports on your work.

Models you will learn to apply:

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, intermolecular forces, bulk electrical properties)
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) Potential energy surfaces Modeling of simple reactions (liquid and gas phase) Radiation processes (photochemical reactions, lasers, fluorescence)