Chemistry 4507 - Physical Chemistry 1

Syllabus Fall 2015

Instructor - Michael S Sommere-mail - sommer@uwyo.edu

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Phone - 1-307-766-2812

Office Hours - Mondays and Wednesdays, 2-4 pm

Class - Classroom Building, CR 103

Mon., Wed., Fri. 10:00 am - 10:50 am,

Textbooks - Quanta, Matter, and Change, 2nd Edition, by Atkins, de Paula, and

Friedman (Oxford or Freeman, 2014)

Course URL - http://w3.uwyo.edu/~sommer/Chem4507/Ch4507-main.html

Purpose - The purpose of this course is to introduce the concepts and methods of physical chemistry to junior-level undergraduates. The prerequisites for this course are the first year of general chemistry, two semesters of college physics, and three semesters of calculus. Knowledge of differential equations, probability theory, and linear algebra would be helpful, but not absolutely necessary.

Outline - The course begins by introducing some of the early results that lead to the need for quantum mechanics. The time-independent Schrödinger equation – the central equation in quantum mechanics – is presented as along with a series of postulates. Examples of the usage of the equation start simple – e.g. particle in a box – and move onto more complicated cases – e.g., harmonic oscillator. Along the way, physical interpretations and applications are introduced – e.g. the uncertainty principle – and the necessary math will be presented.

Once this basis is established, the quantum mechanics of atoms is tackled. The simplest case - the hydrogen atom - is used as the starting point, and the complications due to multiple electrons are then introduced. One of the systems to be looked at in detail will be the helium atom. Molecular bonding will be discussed, and approximate methods – e.g. molecular orbitals –will prove to be invaluable.

Finally, rudiments of molecular symmetry will be covered.

Grades - The grades for the course will be based on the mid-term exam, homework, quizzes, and the final exam. The assignment schedule is given in the lecture schedule.

The quizzes, which will be given at the beginning of class, are short assignments designed to ensure that you are keeping up with the lectures. They will be given out sporadically during the course, and if you miss one you will <u>NOT</u> be allowed to make it up. If you show up late to class while a quiz is being given, you will <u>NOT</u> be given extra time to complete it. Therefore, it is in your best interest to always attend class and to arrive on time.

<u>Several</u> homework sets will be handed out in lecture, and will due ON the date listed on the problem sheet. These will be turned in at the beginning of class. <u>Late homework will NOT be accepted</u>. If you are planning to be absent, it is up to you to make arrangements to get the assignment in on time. There are NO exceptions to this rule.

The beakdown of points is as follows:

Several Homework Assignments (variable points)	=	200 pts
Midterm Exam	=	200 pts
Quizzes	=	50 pts
Final Exam		200 pts
Course Total	=	650 pts

The letter grade cutoffs will be *roughly* as follows:

$$94\% - 100\% = A$$
 $89\% - 93\% = A$
 $84\% - 88\% = B$
 $80\% - 83\% = B$
 $77\% - 79\% = B$
 $70\% - 76\% = C$
 $65\% - 76\% = C$
below $54\% = F$

The exact cutoffs for the grades will be determined at the end of the semester.

Academic Dishonesty - As a student at the University of Wyoming, you are expected to observe high standards of intellectual integrity and honesty. Plagiarism of the work of a fellow student or another author and cheating on exams constitutes cheating, and is a discredit to you and the University. Students caught cheating are subject to dismissal from the course with a grade of **F**. A second offense may result in dismissal from the University.

<u>Students with Disabilities</u>: Students requiring special arrangements for exams should contact the Office for Students with Disabilities. Together, we will make the necessary accommodations.

<u>Working Together</u>: Effective learning requires a constructive relationship between the teacher and the student. Guidelines that detail the responsibilities of <u>both</u> the teacher and student can be found at:

 $\frac{\text{http://uwadmnweb.uwyo.edu/a\&s/Current/2005Stud\&TeachersWorking\%20Together(7-29-05).doc}{05).doc}$

A link to this site is available on our course page.

<u>Tentative Lecture Schedule</u>: Subject to change, so come to class to find out!

DAY	DATE	TOPIC	Topics	HW
Mon.	Aug. 31	Introduction, Policies, Etc.; Background	1-3	
Wed.	Sept. 2	The Postulates of QM	4-6-	
Fri.	Sept. 4	Orthonormality and Uncertainty	7-8	
Mon.	Sept. 7	Labor Day - No School.		
Wed.	Sept. 9	Free Particle in 1 –D	9	
Fri.	Sept. 11	Particle in a 1-D Box	9	HW1
Mon.	Sept. 14	Rosh HaShana I – no lecture		
Wed.	Sept. 16	Particle in a Well, Tunneling	10	
Fri.	Sept. 18	Particle in a 2-D and 3-D Box	11	
Mon.	Sept. 21	Simple Harmonic Oscillator	12	
Wed.	Sept. 23	Yom Kippur – no lecture		
Fri.	Sept. 25	The Not-So-Simple H.O.	12	HW2
Mon.	Sept. 28	Succoth II – no lecture		
Wed.	Sept. 30	Particle on a Ring	13	
Fri.	Oct. 2	Angular Momentum	13-14	
Mon.	Oct. 5	Shemini Atzereth – no lecture		
Wed.	Oct. 7	Particle on a Sphere	14	
Fri.	Oct. 9	Spherical Harmonics	14	HW3
Mon.	Oct. 12	Spin Angular Momentum	19.2	
Wed.	Oct. 14	MIDTERM EXAM		
Fri.	Oct. 16	Bohr Model	17-18	
Mon.	Oct. 19	Radial Function	17-18	
Wed.	Oct. 21	Hydrogenic Orbitals	17-18	
Fri.	Oct. 23	Perturbation Theory	15	HW4
Mon.	Oct. 26	More Perturbation Theory	15	
Wed.	Oct. 28	Multi-Electron Atoms	19	
Fri.	Oct. 30	Aufbau and Pauli Principles	20	
Mon.	Nov. 2	Hund's Rules	20	
Wed.	Nov. 4	Term Symbols	21	
Fri.	Nov. 6	Atomic Transitions	16	HW5
Mon.	Nov. 9	Selection Rules	21	
Wed.	Nov. 11	Valence Bond Theory	22	
Fri.	Nov. 13	Hybrid Orbitals	22	
Mon.	Nov. 16	LCAO-MO Theory	23	
Wed.	Nov. 18	Diatomic Molecules	23-24	113376
Fri.	Nov. 20	Homonuclear Diatomics	24	HW6
Mon.	Nov. 23	Heteronuclear Diatomics	25	
Wed.	Nov. 25	Thanksgiving Break - No School		
Fri.	Nov. 27	Thanksgiving Break - No School	0.5	
Mon.	Nov. 30	Variational Principle	25	
Wed.	Dec. 2	Hückel MO Theory	26	
Fri.	Dec. 4	Aromaticity	26	
Mon.	Dec. 7	Molecular Shape and Symmetry	31	
Wed.	Dec. 9	Application of Group Theory	32	11337.7
Fri.	Dec. 11	Symmetric MOs	33	HW 7
Wed.	Dec. 16	Final Exam, 10:15 am – 12:15 pm		