

**CHEMISTRY 452**  
**Physical Chemistry**  
**Fall 2004**

**MWF 12:20 – 1:10pm**

**117 Osmond**

**Instructor:** Professor A. W. Castleman, Jr., 309 CHEM Bldg., 865-7242  
Professor Mark Maroncelli, 408 CHEM Bldg., 865-0898, [mpm@chem.psu.edu](mailto:mpm@chem.psu.edu)

**Office Hours:** As announced in class or by appointment

**The Course:** This course consists mainly of an introduction to quantum chemistry, atomic and molecular spectroscopies, and chemical kinetics.

**Prerequisites:** Chemistry 13 and 451, Math 141 and Physics 202. Students with questions about their readiness for this course should consult the instructor.

**Text:** Atkins & DePaula, *Physical Chemistry* – (W.H. Freeman & Co.), required  
Atkins & DePaula, *Student Solutions Manual* – (W.H. Freeman & Co.), optional  
J. P. Lowe, *Chemistry 452 Supplementary Materials*, required  
(Sold through the Penn State Book Store.)  
And electronic calculator with logarithm/exponential capability is essential.

**Examinations:** There will be three evening examinations as shown in the course schedule. Examination dates and times are listed below. You are expected to inform the instructor in writing during the first two weeks of classes of any conflicts you have with this examination schedule. A comprehensive final examination will be given during the final examination period at the time and place scheduled by the University. There will be 8 quizzes given on selected Fridays, unannounced; 5 will be selected at random for grading. Unless otherwise instructed, all examinations will be closed book. For examinations only, one sheet of notes will be allowed. You must bring your student I.D. card and a calculator to each examination. You are not allowed to share a calculator.

Questions about grading of an exam must be submitted in writing to the instructor within one week after the graded exams are returned.

**Problems:** Problem assignments will be made regularly in class. These will not be collected (see below). If you cannot solve these problems, seek help from either the instructor, the chemistry department tutoring room (211 Whitmore, 6:30pm – 10:30pm Sunday-Thursday) or a fellow student. We will also keep weekly office hours, so do come by for help.

**Examination Dates:**

I	September 30	6:30 – 7:45 pm
II	October 26	6:30 – 7:45 pm
III	November 22	6:30 – 7:45 pm
Final	Will be available on October 4 <sup>th</sup> .	

**Grading:** Each exam will be worth 100 points, the 5 quizzes selected for grading will be assigned 50 points, and the final exam will count 200 points. The final course grade will be assigned on the basis of 450 of these possible 550 points, weighted in such a manner that your course grade will be maximized. Hence, no make-up exams will be given.

**References:** The following material is on two-hour reserve for this course in the Physical Sciences Library, 230 Davey:

P. Atkins, *Physical Chemistry*, 6<sup>th</sup> edition  
Daniels, *Mathematical Preparation for Physical Chemistry*  
Avery and Shaw, *Basic Physical Chemistry Calculations*  
Avery and Shaw, *Advanced Physical Chemistry Calculations*  
Metz, *Schaum's Outline: Theory and Problems of Physical Chemistry*  
Castellan, *Physical Chemistry*  
Levine, *Physical Chemistry*  
Lowe, *Quantum Chemistry*  
Barrow, *Physical Chemistry*, 6<sup>th</sup> edition

**Academic Ethics:** Possession of unauthorized material during exams, alteration of exams prior to submission for regrading, plagiarism, or any other forms of cheating will be regarded as serious violations of academic ethics and may result in a failing grade in the course. Such incidents may also be referred to the University's disciplinary system. All Penn State policies (<http://www.psu.edu/ufs/policies/>) regarding ethics and honorable behavior apply to this course.

**Study Groups:** Many students like to form small study groups. Educational research suggests that active participation in a small study group can be very helpful in mastering course material and improving problem-solving skills.

**Course Schedule:** Estimated and subject to change

<u>Lectures</u> <sup>#</sup>	<u>Lowe</u>	<u>Text</u> <u>Chapter*</u>	<u>Topic</u>
1-5	B-1		Review of Physics and Math, Introduction to Quantum Theory
6-8	B-2	11	Quantum Mechanics of Linear Motion
9-11	B-3	12	Circular Motion in Two and Three Dimensions
12-15	B-4	13	The Hydrogen-Like Atom
16-19	B-5	13	The Orbital Model for Many Electron Atoms
20-23	B-6	14	Electronic Structure of Homonuclear Diatomic Molecules
24-26	B-8	16	Spectroscopy of Atoms and Rotating Diatomic Molecules
27-28	B-9	16	Spectroscopy of Polyatomic Molecules
29-31	B-10	17	Molecular Electronic Spectroscopy
32-36		25, 26	Rates and Mechanisms
37-41		27	Elementary Reactions

# The exact lecture when a given topic is covered could vary slightly

\* Chapter sub-sections to be announced.