

Physical Chemistry (Graduate) Tentative Lecture Schedule

Spring 2009

Course Number: CHEM 6525
Course Title: Physical Chemistry II 3 Credits
Day: Wednesday
Time: 10:25 pm – 1:00 pm Room: EWC 201
Instructor: Dr. Arthur R. Murphy
Office: DH 4456 Office Hours: M 10:00 AM – 12:00 PM , F – 10:00AM – 11:00AM
and by appointment
Telephone No: 201-692-2322
e-mail: arthur_murphy@fdu.edu

Required Text: Physical Chemistry (6th Edition) by Ira Levine ISBN 0-07-231808-2

Catalog Description for Physical Chemistry II.

Principles of thermodynamics, kinetics, quantum chemistry, statistical mechanics, spectroscopy, and molecular structure. Assumes prior knowledge of MATH 2202 Calculus II or equivalent.

Policies and Procedures:

- 1) All cell phones, beepers, and pagers must be turned off during lecture.
- 2) Students are expected to arrive for class on-time so as not to disrupt a lecture in progress.
- 3) All homework assignments will have a due date on them: Typically a student will have two weeks in which to complete an assignment. Late homework assignments will not be accepted.
- 4) Last Day for dropping the course with a grade of "W" is April 3th.

Grading Policy

Homework 40 %
Exams: 40 %
Term Paper 20 % (Term paper Rules are described in a separate document).

Introduction:

Chemists, and other scientists are interested in the properties and behavior of chemical systems, and these systems show patterns and regularities that can be analyzed using quantitative physical principles. Physical Chemistry provides us with a powerful organizational tool to study phenomena encountered in many areas of chemistry, biology, and physics. Schematically:

Physical Chemistry Principles (both the macro and micro worlds and the relationships between them)	Explanations, Insights ===== >	Phenomena encountered in Organic Chemistry, Inorganic Chemistry, Analytical Chemistry, Biochemistry, and other fields.
--	-----------------------------------	--

Physical Chemistry is one of the corner stones of science, and it is composed of many sub-areas among which are:

- 1) Classical and non-classical Thermodynamics (macroscopic approach) including phase chemical and phase equilibria.
- 2) Statistical Mechanics (microscopic approach to thermo)
- 3) Quantum Chemistry (atomic and molecular structure)
- 4) Spectroscopy (Ex. Vibr., Rot., electronic, NMR etc.)
- 5) Kinetics (Reaction rates, mechanisms)
- 6) Electrochemistry
- 7) Biophysical Chemistry
- 8) Computational Chemistry

Objectives:

In the Graduate Physical Chemistry course , we will focus on the following:

- a) Selected topics in thermodynamics.
- b) The postulates and use of Introductory Quantum Chemistry.
- c) Applications of quantum theory to atoms, molecules, and spectroscopy will be explored. Various mathematical and computer techniques will be presented as needed.
- d) Introductory Chemical Kinetics will be investigated.
- e) If time permits, various aspects of one or more of the following will be investigated: statistical mechanics, chemistry of solids, electrochemistry.

Course objectives and outcomes:

Objective 1: Introduction to Mathcad and other software as needed.

Outcome 1.1 Students will learn to use the basic features of Mathcad. This software can be used to perform arithmetic and symbolic calculations as well as graphical analysis.

Objective 2: To learn the structure of Quantum Mechanics and how it is applied to systems of chemical interest.

Outcome 2.1: Students should have reviewed the mathematics associated with elementary Quantum Mechanics including certain aspects of linear algebra

Outcome 2.2: Students should understand the postulates of Quantum Chemistry and how to apply this knowledge to atomic and molecular structure. Students should be comfortable applying this knowledge to chemical bonding and spectroscopy.

Objective 3: Student should learn key concepts associated with introductory Statistical Mechanics

Outcome 3.1: Students will have reviewed some basic mathematics needed to study statistical mechanics.

Outcome 3.2: Students will review the fundamental laws of

Outcome 3.3: Students should understand what a partition function is and how this information is applied to translational, rotational, vibrational, and electronic aspects of molecules.

They should be able to apply this information to the study of various monatomic and

polyatomic ideal gases .

If time permits, one or more of the following objectives will be explored.

Objective 4: To learn basic aspects of both experimental and theoretical chemical kinetics and how this information is applied to problems of chemical interest.

Outcome 4.1: Students will have reviewed and deepened their understanding of differential rate laws, integrated rate laws, temperature dependence of reaction rates, and reaction mechanisms.

Outcome 4.2: Students should understand how parallel, and consecutive reactions are handled. They should also have a rudimentary knowledge of nuclear decay and enzyme kinetics.

Objective 5: To learn basic aspects of both experimental and theoretical electrochemistry, and how this information is applied to problems of chemical interest.

Outcome 5.1: Students will have reviewed and deepened their understanding of galvanic and electrolytic cells.

Objective 6: Students should learn some basic aspects of crystal structures.

Outcome 6.1: Students should know about the types of bonding encountered in solids

Outcome 6.2: Students should know about the various common crystal structures and how these are determined.

ADDITIONAL “OUTCOMES”

Students who successfully complete this course should have a good background for pursuing other courses in chemistry and other sciences that require knowledge of the material addressed in this course.

TEACHING METHODOLOGIES / ACTIVITIES

- 1) The fundamental method of transmitting material to the students is by means of traditional lectures.
- 2) Web resources will be used where appropriate.
3. Students will receive instructions on how to use Mathcad. Knowledge of this software should greatly help students with their homework assignments.
- 4) In order to assess student's understanding of the material, major hourly exams as well as homework assignments will be given.

TENTATIVE LECTURE SCHEDULE

Week #	Topic
1	Introduction to Mathcad. Postulates of Quantum Chemistry
2	Mathcad (continued) + Completion of Postulates and useful Theorems
3	Quantum Chemistry (Exactly solvable systems)
4	Rotation and Vibrational Spectroscopy
5	Exam #1
6	Approximate methods. Atomic and molecular Electronic Structure
7	Huckel Theory, Qualitative MO theory

- 8 Spring Recess
- 9 Qualitative MO theory, Molecular Mechanics (Perhaps Hyperchem)
- 10 Exam #2
- 11 Spin and NMR
- 12 Topics in one of the following: Kinetics/ Statistical Mechanics
- 13 Topics in one of the following: Kinetics/ Statistical Mechanics
- 14 Topics in one of the following: Kinetics/ Statistical Mechanics
- 15 Final Exam

Expectations:

- 1) In order to be successful in this course, students are expected to be proficient in the use of calculus. A good background in the scientific applications of microcomputers is also very desirable. However, use of pertinent software will be reviewed as needed.
- 2) Students will be expected to become familiar with the primary Physical Chemical literature. This includes current books, current Journals, monographs, and Web sites devoted to Physical Chemistry.
- 3) One of the keys to success in a Physical Chemistry Course is to do lots of problems. In addition to Physical Chemistry textbooks, P. Chem. problem solving books exist, and a short list of those most likely to be of use to students is given in the "Literature" section of this syllabus.

The Physical Chemistry Literature – a First Look.

- I. Books containing many solved problems are:
 - A. Adamson, Arthur W., Understanding Physical Chemistry, Benjamin-Cummings 3rd Ed., 1980. This paperback has been placed on reserve in the library.
 - B. Labowitz, Leonard, Arents, J., Physical Chemistry Problems and Solutions. Academic Press, 1969. This paperback has been placed on reserve in the library.
 - C. Metz, Clyde, Schaum's Outline of Physical Chemistry, 2nd edition, McGraw-Hill, 1988. (paperback).
 - D. Fogiel, M., Ogden, J. The Physical Chemistry Problem Solver: a complete solution guide to any textbook. Research and Education Assn. 1994 (paperback.)
- II. Textbooks
 - A. Silbey, R., Alberty, R., Physical Chemistry, 3rd Edition, Wiley, 2000 This book has some good problems as well as a nice discussion of standard states used in Biochemistry.
 - B. McQuarrie, D., Simon, J., Physical Chemistry: A molecular approach, University Science Books, 1997. This is an excellent advanced text. High quality problem too! Earlier printings of this book omitted discussions of the thermodynamics of solutions. The later printing included this information.
 - C. Atkins, Peter, Physical Chemistry 6th Edition, Freeman, 1998. I prefer some of the earlier editions of this textbook. Graphics are good and there is a large selection of problems at the end of each chapter.
 - D. Noogle, J., Physical Chemistry 2nd Edition, Scott Foresmen and Co. This is a very good P. Chem textbook. It deserved more recognition than it received. Lots of good problems.

- E. Laidler, K., Meiser, J., Sanctuary, B. Physical Chemistry 4th Edition, Houghton Mifflin Co, 2003. This is a good introductory text. Beginning students should find the material accessible. Many end of the chapter problems.
- F. Lesk, A. , Physical Chemistry, Prentice Hall, 1982. This is another textbook that deserved more recognition than it received. Many of the subjects were given a fresh look. More problems could have been included.
- G. Barrow, G. Physical Chemistry 6th edition, McGraw-Hill 1996. This books has numerous problems, and the beginning student may find the presentation style very accessible.

III. Useful Math textbooks

- A. Boas, M. Mathematical Methods in the Physical Sciences 2nd Edition, Wiley, 1983. This is a excellently written book. Crisp, clear descriptions and lots of problems. Highly recommended.
- B. Barrante, James, Applied Mathermatics for Physical Chemistry, Prentice Hall, 1998. Very concise. Beginners may find it of interest. Fairly expensive for a thin paperback. I'll donate my copy to the library and place it on reserve.
- C. Daniels, Farrington, Mathematical Preparation for Physical Chemistry, McGraw-Hill 1956. This book is somewhat dated, but beginning students may find some of the discussions of interest.

IV. Physical Chemistry and Computers

- A. Noogle, J. , Physical Chemistry Using MathCad, Pine Creek Pub., 1997. This book provides a nice introduction to computer applications in many areas of Physical Chemistry. I only wish that more advanced applications were included.

V. Physical Chemistry and the Web

Throughout this course, URL's will be given to interesting P. Chem. Sites.

VI. Some Physical Chemistry Journals of interest.

- A. The ACS Journal of Physical Chemistry Parts A,B, C are available on line as part of FDU's e-journals. Years ago, this journal was not divided into three sections.
- B. The Journal of Chemical Physics. Older issues of this journal are available at FDU's library. For current issues, consult libraries at other institutions.
- C. Physical Chemistry related e-journals available at FDU are
 - (i) Theochemica Acta
 - (ii) Electrochemica Acta
 - (iii) Electrochemistry Communications
 - (iv) Chemical Physics
 - (v) Chemical Physics Letters
 - (vi) Journal of Computational Chemistry
 - (vii) Journal of Molecular Structure (TheoChem)