

# Physical Chemistry II (Undergraduate)

## Tentative Lecture Schedule

Spring 2008

Course Number: CHEM 3242.51  
Course Title: Physical Chemistry II 3 Credits  
Day: Monday  
Time: 5:25 pm - 8.00 pm Room: TBA  
Instructor: Dr. Arthur R. Murphy  
Office: DH 4456 Office Hours: M W F 10:00 AM – 11:00 AM and by appointment  
Telephone No: 201-692-2322  
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**Required Text:** Physical Chemistry (5th Edition) by Ira Levine ISBN 0-07-231808-2

### Catalog Description for Physical Chemistry I and II.

The principles of physical chemistry from the molecular and microscopic aspects: kinetic theory, quantum mechanics, spectroscopic studies and statistical concepts; thermodynamics, chemical and phase equilibria, electrolytes and electrochemistry..

### 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 March 31<sup>st</sup>.

### Grading Policy

Final Grade = 50 % Exam Grades + 50 % Homework Grades

### 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.
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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 Physical Chemistry II, we will focus on the following:

- a) The thermodynamics of ideal and non-ideal systems.
- b) The postulates and use of Introductory Quantum Chemistry. Applications to atoms, molecules, and spectroscopy will be explored. Various mathematical and computer techniques will be presented as needed.
- c) Introductory Electrochemistry will be presented
- d) Introductory Chemical Kinetics will be investigated.
- e) If time permits, various aspects of statistical mechanics or solids will be introduced

### **Course objectives and outcomes:**

**Objective 1:** To learn basic concepts of phase equilibria involving one as well as multi-component systems and the will learn the basic concepts associated with ideal and real solutions.

*Outcome 1.1:* Students will learn the phase rule and study colligative properties.

*Outcome 1.2:* Students will review and understand Raoult's and Henry's Law.

*Outcome 1.3:* Students should learn the concepts of fugacity coefficients, activity coefficients and how these are applied to the study of real solutions and chemical equilibria.

**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.

*Outcome 2.3:* Students should understand the zeroth, first, second, and third laws of thermodynamics.

**Objective 3:** To learn basic aspects of both experimental and theoretical chemical kinetics and how this information is applied to problems of chemical interest.

*Outcome 3.1:* Students will have reviewed and deepened their understanding of differential rate laws, integrated rate laws, temperature dependence of reaction rates, and reaction mechanisms.

*Outcome 3.2:* Students should understand how parallel, and consecutive reactions are handled. They should also have a rudimentary knowledge of nuclear decay and enzyme kinetics.

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

*Outcome 4.1: Students will have reviewed and deepened their understanding of galvanic and electrolytic cells.*

**Objective 5:** (If time permits students should learn some basic aspects of statistical mechanics and how this information is utilized by chemists.

*Outcome 5.1: Students will have reviewed some basic mathematics needed to study statistical mechanics.*

*Outcome 5.2: 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 .*

**Objective 6:** (If time permits 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 Physical Chemistry II.

### **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**

<b>Week #</b>	<b>Topic</b>
1	Chemical Potential Review. Material Equilibrium in ideal and real systems of gases and solutions.
2	“ “ “ + Multicomponent phase equilibria. One component and multicomponent phase equilibria
3	“ “ “ “
4	Quantum Chemistry Postulates.
5	Exam #1.
6	Quantum Chemistry (Exactly solvable systems)
7	Rotation and Vibrational Spectroscopy
8	Approximate methods. Atomic and molecular Electronic Structure
9.	Huckel Theory, Qualitative MO theory and electronic structure
10.	Exam #2
11.	Molecular Mechanics, semi-empirical and ab-initio methods

- 12. Kinetics
- 13. Kinetics
- 14. Statistical Mechanics or Solids
- 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 Chemistry 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 3<sup>rd</sup> 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, 2<sup>nd</sup> 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, 3<sup>rd</sup> 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 6<sup>th</sup> 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 2<sup>nd</sup> 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 4<sup>th</sup> 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 6<sup>th</sup> 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 2<sup>nd</sup> Edition, Wiley, 1983. This is a excellently written book. Crisp, clear descriptions and lots of problems. Highly recommended.
- B. Barrante, James, Applied Mathemratics 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

- A. Throughout this course, URL's will be given to interesting P. Chem. Sites. For now, I mention only a few of these.
- (i) [www.monmouth.edu/~tzielins/mathcad/](http://www.monmouth.edu/~tzielins/mathcad/)  
This site is a repository for many documents that use MathCad in Physical Chemistry.
- (ii) <ftp://wsu.edu/pub/chem/scicomp> This is another site containing applications of MathCad to P. Chem. An index to the various documents would have made it easier to locate applications of interest.
- B. Thermodynamic Data:  
<http://webbook.nist.gov/chemistry/> This is a wonderful site for obtaining a great deal of current thermodynamic data. The National Institute of Science and Technology is the successor to the National Bureau of Standard.

### VI. Physical Chemistry Journals

- A. The ACS Journal of Physical Chemistry A, B, and C are available on-line from FDU's network. In prior times, this Journal was not divided into parts.
- 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).