Physical Chemistry II (Undergraduate) Spring 2014

Course Number:	CHEM 3242.21	
Course Title:	Physical Chemistry II	3 Credits
Day:	Monday	
Time:	2:00 pm - 4.30 pm	Room: TBA
Instructor:	Dr. Arthur R. Murphy	
Office: DH 4456	Office Hours: M W F 1:00 PM – 1:50 PM and by appointment	
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Required Text: Physical Chemistry (6th Edition) by Ira Levine

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 April 7.

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.

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 Chemical 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 Chemical Kinetics will be investigated.
d) 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. (Programmatic Objective #1,3,4,5,6)

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. Objective #1,3,4,5,6)

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. Objective #1,3,4,5,6)

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

If Time Permits one or more of the following may be explored.

Objective 4: To learn basic aspects of both experimental and theoretical electrochemistry, and how this information is applied to problems of chemical interest. Objective #1,3,4,5,6)

Outcome 4.1: *Students will have reviewed and deepened there 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. Objective #1,3,4,5,6)

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 .*

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

Week #	Topic
1	Chemical Potential Review. Activities, fugacities, Ideal and Real Solutions. Debye Huckel Theory.
2	Review of some math topics. Probability Distributions. Simple DE's. Postulates of Quantum Chemistry
3	Quantum Chemistry Postulates continued. Exactly solvable simple systems.
4	Exactly solvable systems. Important Theorems. Angular Momentum.
5	Exam #1.
6	Rotation and Vibrational Spectroscopy
7	Approximate methods. Atomic and molecular Electronic Structure
8.	Linear Algebra. Huckel Theory, Qualitative MO theory and electronic structure
9.	Molecular Mechanics, semi-empirical and ab-initio methods
10.	Exam #2
11.	NMR
12.	Kinetics
13.	Kinetics (continued)
14	TBA. Perhaps some Statistical Mechanics, or Aspect of the solid state, etc.

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 additional 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. The 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., Santuary, 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

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/
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).

Academic Integrity Policy

Students enrolled at Fairleigh Dickinson University are expected to maintain the highest standards of academic honesty. Students have the responsibility to each other to make known the existence of academic dishonesty to their course instructor, and then, if necessary, the department chair, or the academic dean of their College. Course instructors have the added responsibility to state in advance in their syllabi any special policies and procedures concerning examinations and other academic exercises specific to their courses. Students should request this information if not distributed by the instructor.

Academic dishonesty includes, but is not necessarily limited to, the following:

1. *Cheating*—Giving or receiving unauthorized assistance in any academic exercise or examination. Using or attempting to use any unauthorized materials, information, or study aids in an examination or academic exercise.

2. *Plagiarism*—Representing the ideas or language of others as one's own. A more complete description is listed below in the section titled "Plagiarism Described."

3. *Falsification*—Falsifying or inventing any information, data, or citation in an academic exercise.

4. *Multiple Submission*—Submitting substantial portions of any academic exercise more than once for credit without the prior authorization and approval of the current instructor.

5. *Complicity*—Facilitating any of the above actions or performing work that another student then presents as his or her assignments.

6. *Interference*—Interfering with the ability of a student to perform his or her assignments.

Plagiarism Described*

As defined by the Council of Writing Program Administrators, plagiarism "occurs when a writer deliberately uses someone else's language, ideas, or other original (not common-knowledge) material without acknowledging its source." ("Defining and Avoiding Plagiarism: The WPA Statement on Best Practices."<http:// www.wpacouncil.org/positions/WPAplagiarism.pdf>)

Plagiarism can occur in the following ways:**

- Using text from another source (e.g. websites, books, journals, newspapers, etc.) without documenting the source;
- Using direct quotation from a text without quotation marks, even if the source has been cited correctly;
- Paraphrasing or summarizing the ideas or text of another work without documenting the source;
- Substituting a word or phrase for the original while maintaining the original sentence structure or intent of the passage;
- Using graphics, visual imagery, video or audio without permission of the author or acknowledgment of the source;
- Translating text from one language to another without citing the original work;
- Obtaining packaged information, foreign language translation or a completed paper from an online source and submitting it as one's own work without acknowledgment of the source; and
- Presenting the work of another student as one's own.

Fairleigh Dickinson students are responsible for authenticating any assignment submitted to an instructor should the instructor request it. Students must be able to produce proof that the assignment they submit is actually their own work. Therefore, students must engage in a verifiable work process on all assignments:

- Keeping copies of all drafts of work;
- Making photocopies of research materials (including downloads from websites);
- Writing summaries of research materials;
- Keeping Writing Center receipts;
- Keeping logs or journals of their work on assignments and papers; and
- Saving drafts or versions of assignments under individual file names on a computer, external drive or other source.

In addition to requiring students to authenticate their work, Fairleigh Dickinson University instructors may employ various other means of ascertaining authenticity—such as using search engines to detect plagiarism, using external plagiarism detection services, creating quizzes based on student work, and requiring students to explain their work and/or process orally. The inability to authenticate work is sufficient grounds for a charge of plagiarism.

If subsequent evidence of plagiarism should be found after a grade has already been assigned, instructors have the right to lower the grade and/or apply one of the sanctions listed below.

Sanctions: Any student violating academic integrity will, for the first offense, receive one or a combination of the following penalties imposed by the faculty member:

1. *No credit (0) or Failure* for the academic exercise.

2. *Reduced grade* for the course.

3. *Failure* in the course.

4. Recommendation for *Academic Probation* to the dean of the college in which the student is registered.

The instructor shall file a notice of the penalty in the student's file maintained in the campus Office of Enrollment Services.

In cases of interference and complicity, whether or not the student is registered in the affected course, the incident and penalty shall be recorded in the student's file maintained in the campus Office of Enrollment Services.

For a subsequent violation of academic integrity, a student will be subject to any combination of the above sanctions, and, after due review by the academic dean according to the procedure below, one of the following:

1. *Suspension* from the University for one year. Readmission will be contingent upon the approval of the academic dean.

2. *Dismissal* from the University.

3. *Dismissal from the University identified on the student's academic transcript* as a result of a violation of the Academic Integrity Policy.

Procedure: When a faculty member believes that a student has violated the Academic Integrity Policy, the faculty member shall discuss the incident with the student as soon as possible. If after the conference, the faculty member determines that an act of academic dishonesty has occurred, the faculty member may impose the appropriate sanctions. Within five days of the faculty member's action, the faculty member shall notify his or her department chair/school director in writing of the circumstances of the violation and the imposed sanctions. Within five days the academic department/school shall notify the student via certified mail/return receipt of the sanctions and the appeals' procedures. Copies of the notice shall be sent to the chair of the department or director of the school of the student's major, the dean of the college in which the course is offered and the campus Office of Enrollment Services. The student may appeal the instructor's decision as outlined below. Upon completion of the appeals process, the dean shall notify the student of the final disposition of the matter and the sanctions to be imposed, if any, via certified mail with copies to the faculty member, the department chair/school director and the campus director of enrollment services.

Appeals Process: A student who is charged with violating the Academic Integrity Policy by an instructor may appeal in writing to the chair of the department or the director of the school in which the alleged incident took place. The letter must state the specific grounds for the appeal. The student must submit a written appeal to the department chair or school director within 14 days of the receipt of the notification of the imposed sanctions. Failure to make an appeal within this 14-day period shall constitute a waiver of the appeal right. Within 10 working days of the receipt of the student's appeal, the chair/director will review the circumstances of the alleged violation with the student and the instructor and recommend upholding, modifying, or dismissing the sanctions imposed by the instructor. The chair/director, within five working days, shall notify the student in writing via certified mail of the outcome, with copies to the instructor, the chair/director of the student's major, the academic dean of the college in which the course is taught and the campus director of enrollment services. If it is determined that a violation of academic integrity did not occur, the student's final grade in the course cannot be based on the assumption of such violation. If the differences between the instructor and the student are not resolved by this review, the student may appeal the outcome to the dean of the college in which the course is offered.

Within 10 working days of the department chair/school director's notification, the student may submit a written appeal to the dean of the college in which the alleged dishonesty took place. The letter must state the specific grounds for the appeal. Upon receipt of the student's appeal, the dean shall provide the faculty member and his or her chair/director with a copy of the student's appeal. Within 10 working days the dean shall convene a five-person hearing committee consisting of a faculty member at large from the college in which the course is offered, the dean or his or her designee, the campus dean of students or his or her designee, a faculty member from the department or school of the student's major, and a student, selected by the campus dean of students, from the college in which the alleged dishonesty took place. The hearing will be chaired by the college dean or his or her designee. The role of the appeals committee is to review the record of the matter and determine whether a finding of academic dishonesty is founded and whether a sanction is consistent with the terms of this policy. The committee shall base its decision upon a review of the record but may meet with the student and the faculty member to secure additional information to help it in making a determination about the merits of the appeal. The committee can uphold, modify or dismiss the sanction imposed by the instructor. The college dean shall notify the student of the committee's decision within five working days of the hearing. For a second offense of academic dishonesty, the academic dean can suspend or dismiss the student as indicated above.

For a sanction of suspension or dismissal imposed by the academic dean, the student may file a written appeal to the University Provost/Senior Vice President for Academic Affairs within 10 working days of

receiving the notification of the dean's decision. The University Provost, or his or her designee, shall review the case within 10 working days of the receipt of the appeal. The University Provost shall make the final decision, using any appropriate resource to assist in deciding the appeal. The University Provost shall then notify all parties in writing of his or her final decision within five working days of his or her decision.

Reviewed: August 2011