004:132:00A PHYSICAL CHEMISTRY II. FALL 2014

INSTRUCTOR: Prof. Claudio J. Margulis

Office: 118 IATL
Phone: 335-0615
Office Hours: MWF 9:25-10:15 AM in 118 IATL. All other meetings are by appointment only.
E-mail: claudio-margulis@uiowa.edu

TA: TBA
Phone: TBA
Office Hours: to be announced during discussion section or by appointment only.
Location TBA
E-mail: TBA

Grader: TBA
Email: TBA
Phone: TBA

LECTURES: 8:30A - 9:20A MWF 125 106 GILH. Attendance is mandatory.

PROBLEMS SECTION: M 5:30P - 6:20P E203 CB and W 11:30A - 12:20P E203 CB
Attendance is highly recommended. These sessions are provided to assist you, so take advantage of the opportunity to discuss any questions concerning lecture material, problems from your text or exam question material.

COURSE DESCRIPTION: This course will cover the subject of chemical kinetics, which provides a quantitative framework for examining the rates of chemical reactions. Students will learn about the connection between the detailed reaction mechanism and the experimentally observed rate law. The rest of the course will be devoted to a discussion of the fundamental principles of quantum mechanics, atomic and molecular structure and spectroscopy.

1) To prepare and be successful for the close book tests, you must become proficient in solving problems and understanding the underlying theory behind them.

2) Some times a particular topic is more clearly explained in one book than in some other. Read other textbooks if you have trouble understanding a particular concept from the required class textbook. A list of other books on the topic appears later on this syllabus.

3) This course is demanding; we will cover a large amount of material this semester. You must spend enough time to keep up with the lectures. If you fall behind it will be very hard to catch up because topics are interconnected. You will not be able to study for this class the night before an exam and expect to do well.
4) As **calculus is a prerequisite** for this class, knowledge of calculus will be assumed. If you find that you are having trouble with the math consult a calculus text book.

Basic concepts of linear algebra and differential equations will be taught and used in class in order to understand the material. Students are expected to learn and use these tools.

**TEXT AND MATERIALS:**

**PHYSICAL CHEMISTRY, 9th edition, by Peter Atkins and Julio de Paula (required).**  
**Student Solution Manual (highly recommended).**

Optional physical chemistry books that you might find useful at times (not required):

- Physical Chemistry, Ira N. Levine  
- Physical Chemistry, Silbey and Albery (I like this one)  
- Physical Chemistry, Castellan  
- Physical Chemistry, Berry, Rice and Ross

Many other excellent physical chemistry books exist. Please check with the library.

More advanced books on quantum chemistry (more mathematics is required to read these, but the reward is that concepts will become clearer)

- Molecular Quantum Mechanics, Atkins and Friedman. (I like this one very much)  
- Quantum Chemistry, Levine.  
- Quantum Mechanics, The Feynman Lectures on Physics. (The beginning of this book introduces some of the most difficult concepts in quantum mechanics in a beautiful way, but the book is oriented towards quantum physics not quantum chemistry)

Please use the library to your advantage.

**GRADING:** The final course grade will be based on the following components:

Problem sets 15 %  
3 Exams  20 % each (total 60%)  
Final  25%

While the distribution of grades will generally be similar to that of previous semesters, variations between classes are common. Plus/minus grades will be assigned within each range.

**EXAMINATIONS:** There will be **3 exams and a comprehensive final.** Exams are closed-book. **Exams will be held on 9/23, 10/28 and 12/2 between 6:30 and 8:30 pm in**
LR2 VAN. The final is comprehensive (i.e. covers all the material studied). See CLAS Final Examination Policies section below for information regarding scheduling of the final.

For each exam, emphasis will be placed on material covered since the preceding exam, however it is very important to understand that the material covered later in the course requires the application of concepts learned earlier. Announcements will be made in class regarding the material to be covered on each exam. All exams will most likely require you to be able to solve problems. All exams must be written in ink, but not red or erasable ink. Exams on which white-out was used or exams written in pencil, red or erasable ink will not be regraded. Exams will be graded as soon as possible. I will attempt (this is not guaranteed) to give you a lecture day off for every night exam you must attend. The day off will not necessarily be the one following the exam.

Make-up exams must be arranged with the instructor and are only available in the event of a University recognized excuse (e.g. a documented medical emergency). Under no circumstances will a make-up exam be given to take the place of a regular exam taken earlier.

If you feel that an error was made in the grading of an exam, you may request a regrade by notifying the instructor within one week of receiving the graded material. The request should be in writing and indicate the section of the exam that is in question. Please note that the entire examination will be subject to a regrade. No regrades after one week.

HOMEWORK: There will be weekly (or otherwise announced) graded problem sets. Unless otherwise announced in class, a problem set will be due in class exactly one week after it was assigned (i.e. If the homework is assigned on Monday it will be due the following Monday, if it is assigned on Wednesday it will be due the following Wednesday, and if it is assigned on Friday it will be due the following Friday). Late assignments and assignments submitted by email will not be accepted. The homework assignments must be securely fastened with a staple. The problem sets are subject to the same regrade policy as for examinations, as described above.

A NOTE ON COLLABORATION

Homework in this course is assigned to better prepare you for the closed-book exams. In this spirit, brain storming sessions and collaborative work in order to figure out how to solve problems is highly encouraged and not penalized. However, after these collaborative sessions are finished, I expect each of the participants to independently write in their own words (and equations) the solutions for the assigned problems. This is the only way to make sure you fully understood what was discussed collectively. Identical or nearly identical assignments solutions are not acceptable.
College of Liberal Arts and Sciences: Policies and Procedures (insert from http://clas.uiowa.edu/faculty/teaching-policies-resources-syllabus-insert)

Administrative Home
The College of Liberal Arts and Sciences is the administrative home of this course and governs matters such as the add/drop deadlines, the second-grade-only option, and other related issues. Different colleges may have different policies. Questions may be addressed to 120 Schaeffer Hall, or see the CLAS Academic Policies Handbook at http://clas.uiowa.edu/students/handbook.

Electronic Communication
University policy specifies that students are responsible for all official correspondences sent to their University of Iowa e-mail address (@uiowa.edu). Faculty and students should use this account for correspondences (Operations Manual, III.15.2, k.11).

Accommodations for Disabilities
A student seeking academic accommodations should first register with Student Disability Services and then meet privately with the course instructor to make particular arrangements. See www.uiowa.edu/~sds/ for more information.

Academic Honesty
All CLAS students or students taking classes offered by CLAS have, in essence, agreed to the College's Code of Academic Honesty: "I pledge to do my own academic work and to excel to the best of my abilities, upholding the IOWA Challenge. I promise not to lie about my academic work, to cheat, or to steal the words or ideas of others; nor will I help fellow students to violate the Code of Academic Honesty." Any student committing academic misconduct is reported to the College and placed on disciplinary probation or may be suspended or expelled (CLAS Academic Policies Handbook).

CLAS Final Examination Policies
The final examination schedule for each class is announced by the Registrar generally by the tenth day of classes. Final exams are offered only during the official final examination period. No exams of any kind are allowed during the last week of classes. All students should plan on being at the UI through the final examination period. Once the Registrar has announced the date, time, and location of each final exam, the complete schedule will be published on the Registrar's web site and will be shared with instructors and students. It is the student's responsibility to know the date, time, and place of a final exam.

Making a Suggestion or a Complaint
Students with a suggestion or complaint should first visit with the instructor (and the course supervisor), and then with the departmental DEO. Complaints must be made within six months of the incident (CLAS Academic Policies Handbook).

Understanding Sexual Harassment
Sexual harassment subverts the mission of the University and threatens the well-being of students, faculty, and staff. All members of the UI community have a responsibility to uphold this mission and to contribute to a safe environment that enhances learning. Incidents of sexual harassment should be reported immediately. See the UI
Comprehensive Guide on Sexual Harassment for assistance, definitions, and the full University policy.

Reacting Safely to Severe Weather
In severe weather, class members should seek appropriate shelter immediately, leaving the classroom if necessary. The class will continue if possible when the event is over. For more information on Hawk Alert and the siren warning system, visit the Department of Public Safety website.

Student Classroom Behavior
The ability to learn is lessened when students engage in inappropriate classroom behavior, distracting others; such behaviors are a violation of the Code of Student Life. When disruptive activity occurs, an instructor has the authority to determine classroom seating patterns and to request that a student exit the classroom, laboratory, or other instructional area immediately for the remainder of the period. One-day suspensions are reported to Departmental, Collegiate, and Student Services personnel (Office of the Vice President for Student Services and Dean of Students).

TENTATIVE COURSE OUTLINE

The following is the tentative sequence of material to be covered this semester. Any changes in the course material will be announced in class.

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<thead>
<tr>
<th>CHAPTER</th>
<th>TITLE</th>
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<tbody>
<tr>
<td>21</td>
<td>The rates of chemical reactions</td>
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<tr>
<td>22</td>
<td>Reaction Dynamics</td>
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<td>23</td>
<td>Catalysis</td>
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<td>7</td>
<td>Quantum Theory: Introduction and Principles</td>
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<tr>
<td>8</td>
<td>Quantum Theory: techniques and applications</td>
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<tr>
<td>9</td>
<td>Atomic structure and atomic spectra</td>
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<td>10</td>
<td>Molecular structure</td>
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<td>11</td>
<td>Molecular symmetry</td>
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<tr>
<td>12</td>
<td>Spectroscopy 1: rotational and vibrational spectra</td>
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<tr>
<td>13</td>
<td>Spectroscopy 2: electronic transitions</td>
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<tr>
<td>14</td>
<td>Spectroscopy 3: magnetic resonance</td>
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Apart from the graded problem sets a list of suggested problems by chapter may be given by the instructor. These will not be graded but may be helpful in preparing for the exams.