Chemistry 4531 – Physical Chemistry 2  
Course Syllabus Spring 2011  
(see also http://jilawww.colorado.edu/weberlabs/course-CHEM4531.html)

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Prerequisites:  
Formal: CHEM 4511 or 4411 and PHYS 1120 or 2020.  
Recommended: Firm grasp of algebra, complex numbers, calculus, and differential equations.

Course Overview:  
- **Lectures**  
  Physical chemistry is a very broad subject, and we will need to be rather selective about the topics and details that will be covered. We will discuss basic principles of quantum mechanics and their application to atomic and molecular structure. These principles can be applied in molecular spectroscopy to gain information about structure and energy states of molecules. In the last part of the course, the principles of statistical mechanics and their applications to macroscopic properties of matter will be introduced. You will find a tentative list of topics at the end of this syllabus.

  **Please do not come late to class, because this disrupts the attention of your classmates.** The lectures are a critical component of this course, and you are expected to attend. Students who attend classes perform on average much higher than those who do not (who would have thought that ...). Your participation in class both in asking and discussing relevant questions will be welcomed.

- **Additional Class Meetings**  
  In addition to the regular lectures, there will be several additional class meetings, typically on Thursday nights, between 6 pm and 7 pm. Participation is completely voluntary, but the additional meetings will be lectures or problem solving sessions that are thought to improve your learning in particular areas e.g. by reviewing some of the math, computer experiments, etc. These additional meetings will be announced in class and by email, typically a few days in advance.

- **Clickers**  
  To facilitate your engagement (which will increase your learning success), and to provide feedback to you and me about where you are in your thinking, we will use the iClicker system in class. Each student must purchase an iClicker to participate in clicker questions presented in lecture. The number of clicker questions will vary, but you should expect up to 6 questions per class period. Clicker questions are presented in multiple-choice format. Depending on the purpose for asking a particular question, you may be asked to answer on your own or to discuss possible reasoning with students around you. Sometimes you may be asked a question about a topic you haven’t yet encountered in class; often, you’ll be asked to apply what you have just learned. In any case, it’s important that you answer honestly as this provides the most accurate assessment of the class’s thinking to me, and what comes next in lecture may depend on how the class responds. **You should always be prepared to discuss your reasoning or your group’s reasoning for your answer.**

Please register your iClicker. Instructions are provided at:  
http://www.colorado.edu/its/cuclickers/students/register.html
Homework Assignments
Homework assignments (problem sets and reading assignments) are an important part of the course as they should enhance your understanding of the material. You will have to use computer programs to generate function graphs, calculations, etc. for some of the homework assignments. Unless otherwise noted, you may use the programs of your choice to do this, provided you can achieve the objective with them. Assignments will usually be posted on Wednesdays on the course web site. They are usually to be returned the following Wednesdays before class, but the due dates will be listed on each assignment. Problem sets will be graded by a graduate teaching assistant whose contact information will be given to you at a later date. In addition to homework assignments you are expected to read the relevant textbook chapters and sometimes additional material.

Office Hours
Office hours will be Mondays, 5 pm to 6 pm, and Tuesdays/Fridays 10:30 a.m. – 11:30 a.m. These office hours are thought as an opportunity for you to ask any questions to clarify your understanding of the material. Always remember that there is no such thing as a dumb question! Please use the office hours, not email, for questions. If you email questions, I will only be able to answer them if I have time to do so during the office hours. If you cannot make the scheduled office hours, I will try to arrange an alternative time for you. If you come to me for help with your homework, I expect that you have already tried to solve the problems yourself for a few hours.

Exam Schedule:
There will be three two-hour-exams and a final exam. It may be that at least one of the exams will be a take-home exam, but currently they are scheduled as follows:

Scheduled dates for two-hour exams:
- Exam 1: February 10, 2011, 6 p.m. – 8 p.m. or 5 p.m. – 7 p.m., location to be announced
- Exam 2: March 10, 2011, 6 p.m. – 8 p.m. or 5 p.m. – 7 p.m., location to be announced
- Exam 3: April 14, 2011, 6 p.m. – 8 p.m. or 5 p.m. – 7 p.m., location to be announced

If there are problems with these exam dates, you must indicate these conflicts before Friday January 14, 2011! There will be no makeup exams. The grade on an excused exam will be replaced by your average of the other exams, scaled by the class average on the missed exam. Exams missed without excuse will count as an F.

Final exam: time and location will be announced at a later date.

Stand-In Lectures:
Due to conference and seminar travel, the lectures on Wednesday, February 2, Monday, February 28, and Wednesday, March 2 may be given by another instructor in my stead. Alternatively, one or both of these lectures may be cancelled (see below). Details will be announced in class.

Dates without Class Meetings:
As the two-hour exams are held outside of class hours and count as contact hours, some class hours may be cancelled without losing class time. If so, cancellations may be announced at a later date.
Grades:

- During the semester, you will accumulate credits through your homework that will determine your homework performance grade. If an answer is unintelligible or illegible, you will lose some or all credits for the problem. Late homework will not be graded and counts as zero credits, unless the late return is excused. Everyone may drop one homework assignment without penalty. Your total homework performance will count 40% towards the final grade.

- At the end of the semester, a student's clicker points are summed and increased by 10% to allow for absences, malfunctioning clickers, and all other possible problems. These clicker points are then normalized to the maximum of achievable points. You will receive 1 clicker point per question, based on participation. However, recall that your honest and best response is what will help you and me – never click in just to click in. You’ll learn much more – even if you’re wrong – if you’ve given it your best effort. The participation in clicker questions will count 5% towards the final grade.

- The average of the two-hour-exams will count 30% towards the final grade.

- The final exam will count 25% towards the final grade.

Textbooks:

- Donald A. McQuarrie, John D. Simon “Physical Chemistry”. We concentrate mostly on Chapters 1 – 18.

- Optional: James R. Barrante “Applied Mathematics for Physical Chemistry”

Science Education Research:

For the past years, education research has been in the process of transforming the traditional paradigms of teaching and learning. During this course, a graduate student and I will use various education research techniques to measure the effectiveness of teaching methods, focusing on the quantum mechanics part of the course. Our research effort is sponsored in part by the National Science Foundation. In the course of this research, you will be asked to help us by answering questionnaires and by participating in interviews. Your participation is entirely voluntary, but we greatly value your help. Your performance on any of these questionnaires or interviews will not affect your grade. I will not see your individual scores, only the aggregate scores of the class as a whole. Your participation will not only help us, but contribute to improve learning for generations of students in the future.
Students with Disabilities:
If you qualify for accommodations because of a disability, please submit to me a letter from Disability Services in a timely manner so that your needs may be addressed. Disability Services determines accommodations based on documented disabilities. Contact: 303-492-8671, Willard 322, and www.Colorado.EDU/disabilityservices

Religious Observances:
Campus policy regarding religious observances requires that faculty make every effort to reasonably and fairly deal with all students who, because of religious obligations, have conflicts with scheduled exams, assignments or required attendance. In this class, please indicate any such conflicts to me at least two weeks in advance of the conflicting date for a homework assignment, and before January 14, 2011 for scheduled exams. Religious observances on regular class dates do not constitute a problem, but please notify me as well about such occurrences. See full details at http://www.colorado.edu/policies/fac_relig.html

Classroom Behavior:
Students and faculty each have responsibility for maintaining an appropriate learning environment. Students who fail to adhere to such behavioral standards may be subject to discipline. Faculty have the professional responsibility to treat all students with understanding, dignity and respect, to guide classroom discussion and to set reasonable limits on the manner in which they and their students express opinions. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with differences of race, culture, religion, politics, sexual orientation, gender variance, and nationalities. Class rosters are provided to the instructor with the student's legal name. I will gladly honor your request to address you by an alternate name or gender pronoun. Please advise me of this preference early in the semester so that I may make appropriate changes to my records. See polices at http://www.colorado.edu/policies/classbehavior.html and at http://www.colorado.edu/studentaffairs/judicialaffairs/code.html#student_code

Discrimination and Harassment:
The University of Colorado at Boulder policy on Discrimination and Harassment (http://www.colorado.edu/policies/discrimination.html, the University of Colorado policy on Sexual Harassment and the University of Colorado policy on Amorous Relationships applies to all students, staff and faculty. Any student, staff or faculty member who believes s/he has been the subject of discrimination or harassment based upon race, color, national origin, sex, age, disability, religion, sexual orientation, or veteran status should contact the Office of Discrimination and Harassment (ODH) at 303-492-2127 or the Office of Judicial Affairs at 303-492-5550. Information about the ODH and the campus resources available to assist individuals regarding discrimination or harassment can be obtained at http://www.colorado.edu/odh

Honor Code:
All students of the University of Colorado at Boulder are responsible for knowing and adhering to the academic integrity policy of this institution. Violations of this policy may include: cheating, plagiarism, aid of academic dishonesty, fabrication, lying, bribery, and threatening behavior. All incidents of academic misconduct shall be reported to the Honor Code Council (honor@colorado.edu; 303-725-2273). Students who are found to be in violation of the academic integrity policy will be subject to both academic sanctions from the faculty member and non-academic sanctions (including but not limited to university probation, suspension, or expulsion). Other information on the Honor Code can be found at http://www.colorado.edu/policies/honor.html, http://www.colorado.edu/academics/honorcode/
Topics (tentative):
The exact topics are not quite set in stone and may evolve during the course. Below you find a tentative list of topics as I currently plan to cover them.

Quantum mechanics and spectroscopy:
1) Origins of quantum mechanics
2) Wave mechanics and wave functions
3) Operators, eigenfunctions, eigenvalues
4) Quantum mechanical principles
5) The free particle and the particle in a box
6) The harmonic oscillator and vibrational spectra of molecules
7) Angular momentum, the rigid rotor and rotational spectra of molecules
8) Approximations in quantum mechanics: Variational theory and perturbation theory
9) The Hydrogen atom
10) Multielectron atoms
11) Atomic Spectra
12) The Born-Oppenheimer approximation
13) Valence-bond theory
14) LCAO-MO theory
15) Bonding in polyatomic molecules
16) Electronic spectra of molecules
17) Interaction of electromagnetic radiation and matter

Statistical mechanics:
18) Distribution of molecular states
19) Internal energy and entropy
20) Partition functions
21) Thermodynamic functions
22) Applications of statistical thermodynamics