

SYLLABUS

Physical Chemistry II 3322 – Spring 2014
Quantum Chemistry, Spectroscopy, and Structure
Monday, Wednesday, Friday 10:00 a.m. – 10:50 a.m.
Science Hall 205 (SH 205)



Instructor: Peter Kroll

Office: Chemical and Physics Building, Room 353

Office hours: Mon, Wed, Fri 11-noon (or upon appointment). Please check CPB 315 (Computational Lab) as well.

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Required Course Materials:

1. *Physical Chemistry* by Engel & Reid (Prentice Hall, Pearson), 3rd edition

2. Mastering Chemistry Access (available with the Engel&Reid textbook and from <http://masteringchemistry.com>)

The course ID at MasteringChemistry is MCPCHEMSRING2014KROLL9876.

3. *Mathematica* from Wolfram Research: You may consider purchasing Mathematica (see

<http://www.uta.edu/oit/cs/software/wolfram/mathematica-8-win/index.php>). Mathematica is also installed on many campus computer labs, as well as on some computers in the modeling lab (CRB 317).

You are advised to read the text before you come to class!

You find a list of topics that will be next in lecture on the course Wiki

The Engel/Reid book (3rd edition) defines the standard level of difficulty for assigned homework problems and exams. Other textbooks are quite good as well, and might – for your personal taste – even be better. You can try and take a look into Atkins, Levine, McQuarrie. Many of them are available at bargain prices. So take them all for studying. Having a different text provides the same material from a different view using some other style and language. It often helps the process of understanding the content – especially if you share the information with others.

Content and Objectives:

Quantum theory, introduction, principles. Schrödinger Equation, wavefunction; particle in a box, uncertainty; postulates of quantum mechanics; hydrogen atom, orbitals, structure of multi-electron atoms, atomic spectra and selection rules; molecular structure of diatomic molecules; introduction to molecular spectroscopy; materials and structure: lattices, diffraction methods, properties of solids.

In this class you will learn to understand the principles of Quantum Chemistry and how it applies to atoms, molecules, and solids. We emphasize conceptual understanding and will become skilled in quantitative descriptions. The goal is that at the end of the course every student can outline the basic principles of Quantum Chemistry, both qualitatively and quantitatively. Students will obtain a sound understanding of probability, wavefunctions, orbitals, and spectroscopy, and can apply the learned concepts and tools to engage in self-driven investigations.

Expected Student Learning Outcomes:

By the end of the semester you should be able to:

- apply the Schrödinger equation to a variety of standard case
- analyze atomic spectra and assign term symbols
- use approximate descriptions for bonding in molecules

- understand basic metallic, ionic, and covalent structure and their properties.

Prerequisites:

- Please bring with you the spirit to engage, the eagerness to learn, and the professionalism to build your career in Chemistry.
- I expect “fluency” in all concepts of physical chemistry as taught in General Chemistry courses (1441 and 1442). This includes basic principles of quantum chemistry, bonding, and spectroscopy.
- Likewise, you master the problems of Quantitative Chemistry (2335&2285). This, in particular, refers to spectroscopy.
- You are “at ease” with differentiation and integration at the level of Calculus III. Lecture and homework only appear to be math intensive, due to a lack of practice of math – let this not hamper your understanding of Chemistry.
- PChem I is not a pre-requisite. However, I expect you to be or to become familiar with the Boltzmann statistics.

PChem Blog: We will continue the PChem Blog and Wiki this semester. The blog will include discussion of topics of the lecture. Contributions to the wiki may be made from homework assignments or through extra-credit work.

Grading:

Grading is based on class participation (10%), homework (25%), four exams (40%), and a final exam (25%).
Letter Grade assignments: 100-90: A ; 89-76: B ; 75-60: C ; 59-50: D ; below 49: F

Class Participation:

You are supposed to attend every class. “Class participation” refers to more than just physical presence, however. It includes active participation with questions and answers, discussion and problem solving. Quick “stand-up” problems may be used to check the learning progress. I expect that you are able to reproduce the next lecture what I did in the previous lecture (drawings, explanations). Class participation includes Quizzes and, if started, participation in the class blog.

Homework:

We follow a two-fold path in Homework:

1. MasteringChemistry: the homework system that comes along with the textbook contains a variety of tutorials, short answer questions, and will provide a sound foundation for succeeding in exams. Although the computerized system lacks the complexity necessary and required for many problems dealing with concept understanding and “theoretical” content, it nevertheless provides a basic “training” that every student should master easily. Please welcome all the points you can achieve that way.

Expect: 2-3 times a week about 1 hour (by MSChem indicated time) homework via Mastering Chemistry.

2. Additional homework will be assigned in class. Expect one page with exercises each week, requiring on average 2-3 hours of time to work. Due days are indicated and the homework will be collected in class and graded. I expect readable and tidy hand-writing and drawings on clean paper. No computer-printed homework will be accepted until explicitly noted otherwise!

Note: some homework problems will include the use of Mathematica (see Course Material).

Study groups with up to 4 (four!) students are acceptable. Indicate with whom you worked together and who contributed. All (!) students of a study group share equally the responsibility for the work. Hence, do not let your work to copy (this becomes most visible in Mathematica problems)

Written exams:

We will have four exams. All exams will be written at Tuesday evening, starting at 7 pm (lasting 2 ½ h). Dates are set to Tuesday, Feb 11th, Mar 4th, Apr 1st, and April 29th (note that this exam is set into the last week of lecture time). All exams are comprehensive, though the emphasis will be on the most recent material covered in lecture. You will have to be present for the exams – you must contact me during the first two weeks of the semester if you see that you will have time conflicts and bring along proof that you are enrolled and occupied in another class at that time.

Otherwise, no make-up will be given for a written exam.

Exams are composed from homework problems (in variation, of course) and will include transfer problems as well. The final will be written during Final week, most probably scheduled for Monday, May 5th, 8-10:30 a.m. I reserve the possibility to substitute parts of the written exams with an oral examination (10- to 15-minutes instructor-student colloquium).

Expectations for Out-of-Class Study:

A general rule of thumb is this: for every credit hour earned, a student should spend 3 hours per week working outside of class. Hence, a 3-credit course has a minimum expectation of 9 hours of reading, study, etc..

Beyond the time required to attend each class meeting, students enrolled in this course should expect to spend at least an additional 3-4 hours per week working outside of class for every credit hour earned. This is of their own time in course-related activities, including reading required materials, completing assignments, preparing for exams, etc.

You will experience weeks during which you find that the Physical Chemistry class requires even more time.

However, this depends not at least on your experience with quantitative problems in general.

Extra Credit:

You have the chance to receive extra credit (up to 5 grading points during the semester) for work that you contribute to the Wiki or for the general benefit of the class. I will usually award one grading point for well carried out extra work, for most outstanding work up to two grading points. You can strive for this extra credit reward only once between exams, giving you 5 opportunities. Your work must reflect the current content of the lecture, and shall not address a topic of a previous exam. I will not accept a back-log on extra-credit work.

March 28th is the last day to drop this class. Please see UTA's drop policy for this.

Students may drop or swap (adding and dropping a class concurrently) classes through self-service in MyMav from the beginning of the registration period through the late registration period. After the late registration period, students must see their academic advisor to drop a class or withdraw. Undeclared students must see an advisor in the University Advising Center. Drops can continue through a point two-thirds of the way through the term or session. It is the student's responsibility to officially withdraw if they do not plan to attend after registering. **Students will not be automatically dropped for non-attendance.** Repayment of certain types of financial aid administered through the University may be required as the result of dropping classes or withdrawing. For more information, contact the Office of Financial Aid and Scholarships (<http://www.uta.edu/ses/fao>).

Spring break: Mar 10-14

Written examination needs: Non-programmable calculator. Document-ready fountain pen or ball-pen in either blue or black (never use red color except for special drawings). Do not use a pencil for writing your exam.

Communications: Classroom announcements represent the sole source of official information for this course. For requests on additional advices, please visit me in my office. If you send me an e-mail, UTA policy requires students to use their MyMav account and discourages instructors to respond to e-mails sent by other accounts.

You must include the course number "CHEM 3322" into your subject line.

UT Arlington has adopted MavMail as its official means to communicate with students about important deadlines and events, as well as to transact university-related business regarding financial aid, tuition, grades, graduation, etc. All students are assigned a MavMail account and are responsible for checking the inbox regularly. There is no additional charge to students for using this account, which remains active even after graduation. Information about activating and using MavMail is available at <http://www.uta.edu/oit/cs/email/mavmail.php>

Attendance Policy: Attendance is part of class participation and, hence, part of your grade.

Bomb Threat Policy: In the event of a bomb threat to a specific facility, University Police will evaluate the threat. If required, exams may be moved to an alternate location, but they will not be postponed. UT-Arlington will prosecute those phoning in bomb threats to the fullest extent of the law.

Academic Integrity:

All students are expected to pursue their scholastic careers with honesty and integrity. Academic dishonesty will not be tolerated by the Department of Chemistry and Biochemistry. Academic dishonesty includes (but is not limited to) cheating, falsification of data, plagiarism, and contracting/collusion with others to take your test or do your work.

All students enrolled in this course are expected to adhere to the UT Arlington Honor Code:

I pledge, on my honor, to uphold UT Arlington's tradition of academic integrity, a tradition that values hard work and honest effort in the pursuit of academic excellence.

I promise that I will submit only work that I personally create or contribute to group collaborations, and I will appropriately reference any work from other sources. I will follow the highest standards of integrity and uphold the spirit of the Honor Code.

Per UT System *Regents' Rule* 50101, §2.2, suspected violations of university's standards for academic integrity (including the Honor Code) will be referred to the Office of Student Conduct. Violators will be disciplined in accordance with University policy, which may result in the student's suspension or expulsion from the University.

Americans with Disabilities Act:

The University of Texas at Arlington is on record as being committed to both the spirit and letter of all federal equal opportunity legislation, including the *Americans with Disabilities Act (ADA)*. All instructors at UT Arlington are required by law to provide "reasonable accommodations" to students with disabilities, so as not to discriminate on the basis of that disability. Any student requiring an accommodation for this course must provide the instructor with official documentation in the form of a letter certified by the staff in the Office for Students with Disabilities, University Hall 102. Only those students who have officially documented a need for an accommodation will have their request honored. Information regarding diagnostic criteria and policies for obtaining disability-based academic accommodations can be found at www.uta.edu/disability or by calling the Office for Students with Disabilities at (817) 272-3364.

Student Feedback Survey:

At the end of each term, students enrolled in classes categorized as lecture, seminar, or laboratory are encouraged to complete a Student Feedback Survey (SFS). Instructions on how to access the SFS for this course will be sent directly to each student through MavMail approximately 10 days before the end of the term. Each student's feedback enters the SFS database anonymously and is aggregated with that of other students enrolled in the course. UT Arlington's effort to solicit, gather, tabulate, and publish student feedback is required by state law; students are strongly urged to participate. For more information, visit <http://www.uta.edu/sfs>.

Final Review Week:

A period of five class days prior to the first day of final examinations in the long sessions shall be designated as Final Review Week. The purpose of this week is to allow students sufficient time to prepare for final examinations. During this week, there shall be no scheduled activities such as required field trips or performances; and no instructor shall assign any themes, research problems or exercises of similar scope that have a completion date during or following this week *unless specified in the class syllabus*. During Final Review Week, an instructor shall not give any examinations constituting 10% or more of the final grade *unless specified in the class syllabus*, except makeup tests and laboratory examinations. In addition, no instructor shall give any portion of the final examination during Final Review Week. During this week, classes are held as scheduled. In addition, instructors are not required to limit content to topics that have been previously covered; they may introduce new concepts as appropriate. Following this guideline, I announce that there will be one regular exam (the 4th) in the Final Review week.