

SYLLABUS

Physical Chemistry II 3322 – Spring 2010
Quantum Chemistry, Spectroscopy, and Structure
Monday, Wednesday, Friday 10:00 a.m. – 10:50 a.m.
Chemistry Research Building 114 (CRB 114)



Instructor: Peter Kroll

Office: Chemical and Physics Building, Room 353

Office hours: Mon to Thu 11-noon, other times upon appointment. Please check room 315 (Computational Lab) as well.

Telephone: (817) 272 3814

E-Mail: pkroll@uta.edu

Textbook/Course Material: *Atkins' Physical Chemistry* by Atkins & de Paula, 9th edition

You are advised to read the text before coming to class !

Atkins' book is the standard textbook for physical chemistry. It doesn't matter much, if you use the 9th or 8th or even 4th edition (and any other in-between). For studying, these are equally good. Moreover, other textbooks are quite good as well, and might be – for your personal taste – even better. You can try and take a look into Engel/Reid, 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. However, the 9th edition of Atkins' defines the standard level of difficulty for assigned homework problems and exams.

Mathematica from Wolfram Research: You may consider purchasing Mathematica (currently \$30 for UTA students, 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). It can be used there on Windows PC's. However, I can not guarantee you access to a computer in this room all day and night, especially the day before homework is due.

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, has a sound understanding of probability, wavefunctions, orbitals, and spectroscopy, and can apply the 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 you to be “fluent” in all concepts of physical chemistry as taught in General Chemistry courses (1441 and 1442). Lectures and homework may sometimes appear to be math intensive, and so you should not be afraid of differentiation and integration at the level of Calculus III – meaning, you should be at ease with this so that it doesn’t hamper the understanding of Chemistry.

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:

Homework will be assigned in class. Expect one page with exercises each week. One or two homework sheets will be for a 2-week period. Due-days are indicated. Homework will be taken up and graded. You are also strongly encouraged to attempt end-of-chapter exercises and problems. I expect readable and tidy hand-writing and drawings on clean paper. No computer-printed homework will be accepted until explicitly noted otherwise! You are encouraged to form study groups, so I don’t mind if solutions look quite identical. However, indicate with whom you worked together and, above all, don’t cheat on yourself! Simply copying other students work will have its end in the written exams.

Note: some homework problems will include the use of Mathematica. You do not need to purchase Mathematica, since it is installed on some computers in the modeling lab (CRB 317) and can be used there on both Windows and PC’s. Mathematica is also available for your personal computer (currently \$30 for UTA students, see <http://www.uta.edu/oit/cs/software/wolfram/mathematica-8-win/index.php>)

Written exams:

We will have four exams. All exams will be written at Tuesday evening, starting at 6 pm (lasting 2-3 h). Dates are set to Tuesday, Feb 9th, Mar 9th, Apr 13th, and May 4th. 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, probably scheduled for Monday, May 9th, 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).

April 1st is the last day to drop this class. Please see UTA’s drop policy for this.

Spring break: Mar 14-18

Written examination needs: Non-programmable calculator and No. 2 pencil with eraser.

Communications: Classroom announcements represent the sole source of official information for this course. For requests on additional advices, please visit me in my office.

Attendance Policy: I do not take attendance, but I see who misses class.

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 Dishonesty:

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.

Americans with Disabilities Act:

The University of Texas at Arlington is on record as being committed to both the spirit and letter of federal equal opportunity legislation; reference Public law 93112-The Rehabilitation Act of 1973 as amended. With the passage of new federal legislation entitled Americans with Disabilities Act - (ADA), pursuant to section 504 of The Rehabilitation Act, there is renewed focus on providing this population with the same opportunities enjoyed by all citizens.

As a faculty member, I shall accommodate students with disabilities, so as not to discriminate on the basis of that disability. Student responsibility primarily rests with informing faculty at the beginning of the semester and in providing authorized documentation through designated administrative channels.

Please inform me immediately, in private, of any ADA accommodations you want to request. Your requests and any actions taken will be kept confidential.