SYLLABUS

Physical Chemistry II 3322 – Spring 2018 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. Telephone: (817) 272 3814 E-Mail: <u>pkroll@uta.edu</u>

Required Course Materials:

1. *Physical Chemistry* by Engel & Reid (Prentice Hall, Pearson), 3rd edition 2. *Mathematica* from Wolfram Research. There are several options to get Mathematica for an enrolled UTA student,

2. *Mathematica* from Wolfram Research. There are several options to get Mathematica for an enrolled UTA student, see <u>http://www.uta.edu/oit/cs/software/wolfram/mathematica-10-win/index.php</u>; 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 covered in lecture on the course's Blackboard site

The Engel/Reid book (3rd edition) defines the standard (breath, level of difficulty, expectations) 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 familiar with **Boltzmann statistics in the way it refers to occupation numbers**.

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; I will take attendance occasionally. "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:

Expect one page with exercises each week, requiring <u>on average</u> 3-5 hours of time to work. Times may be longer, in particular if math skills are not properly developed. Homework will be available on Blackborad and due days are indicated. The homework will be collected in class and graded. I expect readable and tidy <u>hand-writing</u> and drawings on clean paper. No computer-printed homework will be accepted until explicitly noted otherwise! All homework must be written by yourself. Copying homework from another student is not acceptable. Since the homework is the base of all the written exams [about 75% of exam questions correspond to homework questions], it is imperative that you deliver correct and full solutions. Only this way it will be possible to use your homework solutions for studying towards exams. There will be no credit for "effort", but only for correct and comprehensive solutions.

Written exams:

We will have four exams. All exams will be written at Tuesday evening, starting at 7 pm (lasting $2\frac{1}{2}$ h). Dates are set to Tuesday, Feb 20^{th} , Mar 6^{th} , April 3^{th} , and May 1^{st} (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, <u>no make-up</u> will be given for a written exam.

Exams are composed from homework problems (in variation) and will include transfer problems as well. The final will be written during Final week, Monday, May 7th, 8-10:30 a.m. I reserve the possibility to augment parts of a written exam 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.

Spring break: Mar 12-16

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). Pencils are NOT allowed for writing your exam. (simple) ruler with scale.

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 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.

March 30th is the last day to drop this class. Please see UTA's drop policy for this.

Drop Policy: 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://wweb.uta.edu/aao/fao/).

Disability Accommodations: UT 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), The Americans with Disabilities Amendments Act (ADAAA), and Section 504 of the Rehabilitation Act. 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 disability. Students are responsible for providing the instructor with official notification in the form of a letter certified by the Office for Students with Disabilities (OSD). Students experiencing a range of conditions (Physical, Learning, Chronic Health, Mental Health, and Sensory) that may cause diminished academic performance or other barriers to learning may seek services and/or accommodations by contacting: The Office for Students with Disabilities, (OSD) www.uta.edu/disability or calling 817-272-3364. Counseling and Psychological Services, (CAPS) www.uta.edu/caps/ or calling 817-272-3671.

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.

Title IX: The University of Texas at Arlington does not discriminate on the basis of race, color, national origin, religion, age, gender, sexual orientation, disabilities, genetic information, and/or veteran status in its educational programs or activities it operates. For more information, visit uta.edu/eos. For information regarding Title IX, visit www.uta.edu/titleIX.

Academic Integrity: Students enrolled all UT Arlington courses 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.

UT Arlington faculty members may employ the Honor Code as they see fit in their courses, including (but not limited to) having students acknowledge the honor code as part of an examination or requiring students to incorporate the honor code into any work submitted. 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.

Electronic Communication: 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.

Student Feedback Survey: At the end of each term, students enrolled in classes categorized as "lecture," "seminar," or "laboratory" shall be directed to complete an online 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, 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.

Emergency Exit Procedures: Should we experience an emergency event that requires us to vacate the building, students should exit the room and move toward the nearest exit, *which is located at the bottom of the staircase to the right outside the classroom*. When exiting the building during an emergency, one should never take an elevator but should use the stairwells. Faculty members and instructional staff will assist students in selecting the safest route for evacuation and will make arrangements to assist individuals with disabilities.

Student Support Services: UT Arlington provides a variety of resources and programs designed to help students develop academic skills, deal with personal situations, and better understand concepts and information related to their courses. Resources include tutoring, major-based learning centers, developmental education, advising and mentoring, personal counseling, and federally funded programs. For individualized referrals, students may visit the reception desk at University College (Ransom Hall), call the Maverick Resource Hotline at 817-272-6107, send a message to resources@uta.edu, or view the information at http://www.uta.edu/universitycollege/resources/index.php

Emergency Phone Numbers: In case of an on-campus emergency, call the UT Arlington Police Department at **817-272-3003** (non-campus phone), **2-3003** (campus phone). You may also dial 911. Non-emergency number 817-272-3381