Department of Chemistry
The University of Texas at El Paso
Physical Chemistry II: Quantum Chemistry

CHEM 3352 (CRN 20909**)** Spring Term, 2022

Instructors:
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This class may be *technology enhanced*. This class is scheduled to have in-person meetings, yet we may have virtual sessions if necessary depending on the COVID-19 situation. Lectures will be held in person Tuesdays and Thursdays from 9:00 AM – 10:20 AM at Main 211 *or* through zoom/teams. Links will be provided when appropriate. **We should expect to have face-to-face examinations.** If those are not possible, we will have them online using Respondus Lockdown browser. When meeting online, lectures will be recorded, and they will be available through the Microsoft Teams or Zoom applications, accordingly.

Course Description
The objective of this course is to describe the fundamentals of quantum theory as applied to chemistry problems. We will discuss the historical development and the theories that describe much of current chemistry. We will cover the fundamentals of atomic structure and spectroscopy by first discussing hypothetical situations that will build up in complexity leading towards the hydrogen atom. We will also cover basic bonding theories focusing on the simplest molecule, H_2. If time permits molecular symmetry and fundamentals of group theory will be discussed. We will try to cover chapters 12 to 27 from the textbook.
This is a mathematics intensive course, and understanding of integral, differential and multivariable calculus is required. Understanding of the basics of matrix algebra may be necessary for the latter topics. Despite these requirements, this course will attempt to focus on the conceptual understanding of the quantum mechanic theories in which chemistry is based upon.

Textbook:
Physical Chemistry; Thomas Engel, Philip Reid, 3rd. Edition; *Pearson*. If needed, additional handouts will be uploaded to Blackboard which can be accessed through http://my.utep.edu.

We will follow the book closely starting at Chapter 12. Reading of the assigned chapter prior to the lecture is *mandatory*. The concepts in this course may be difficult since quantum mechanics lacks the intuitive foundation that classical physics does. Thus, each chapter must be read at least three times! Prior to the lecture, immediately after the lecture, and a final review prior to any examination.

Additional reading:
Physical Chemistry; Peter Atkins, Julio de Paula, Ronald Friedman, 2nd. Ed.; *Freeman*.
Physical Chemistry Study Guide. *Pearson*.

Software:
Please have Microsoft Teams and Zoom installed in your devices. Make sure you have the possibility of using a computer that can launch Respondus Lockdown browser, in case it is needed.

Grading:

The grade for this course for will be determined by three exams (30% each) and problem sets (10%). Grades will be determined according to the typical sliding scale 90% and above, A; 80-89%, B; 70-79%, C; 60-69%, D; below 60%, F.
Each exam is comprehensive. Every topic covered will be subject for each exam (i.e. the first exam will consists of every topic covered, the second exam will cover every new topic and those already examined, and the third exam will be, in essence, about everything covered in the course, hence comprehensive).
The final exam date will be set according to the office of the registrar office.

Problem sets will be assigned throughout the course. Once again, this is a difficult course. Most of the material will be learned outside class. *Just attending lecture will not be enough to pass this course*. It is in your best interest to fully understand the assigned homework. This homework will be graded with heavy emphasis in the effort shown. Students are encouraged to work collaboratively in these problem sets, but the work **must** show individual work. **Sets of identical solutions by two or more students will not be tolerated.** Late homework will be accepted with a 10% penalty per late day. Additionally, it is in your best interest to do all the problems in the back of each chapter. Hint: obtaining the student homework manual may be very useful! Random quizzes will be given throughout the semester and the percentages will be applied to the homework percentage.

Attendance: Attendance will not be taken nor it will directly factor towards your grade. It is, however, your responsibility to come to lecture and ask questions. It is highly unlikely that a chronic absentee will do well in this course. Your absence most likely will be noted, though. Lectures will be recorded and you are encouraged to review the material as often as you need.

Syllabus.
The topics to be covered will closely follow the book order starting from chapter 12. These include:

1. Classical mechanics and its limitations
2. The Schrödinger equation
3. Quantum mechanical postulates
4. Particle in a box (1D, 2D) (Exam 1? Tentative, Ch12-Ch16)
5. Heisenberg Uncertainty Principle
6. The Harmonic Oscillator (Classical and quantum mechanical descriptions)
7. Vibrational and rotational models on diatomic molecules
8. Particle in a Sphere: The hydrogen atom
9. Many Electron Atoms: The helium atom and beyond (Exam 2? Ch16-Ch20)
10. Quantum States and Atomic Spectroscopy
11. The Chemical Bond
12. Electronic Spectroscopy
13. Molecular Orbital Theory. Linear Combination of Atomic Orbitals (LCAO) approximation (Exam 3? Ch20-Ch23)

Course Drop Policy All grades of Incomplete must be accompanied by an Incomplete Contract that has been signed by the instructor of record, student, departmental chair, and the dean. Although UTEP will allow a maximum of one year to complete this contract, the College of Science requests it be limited to month based upon completion data. A grade of Incomplete is only used in extraordinary circumstances confined to a limited event such as a missed exam, project, or lab. The course drop deadline is April 1th 2022.
Other considerations: Please turn your cell phones off and keep them away during lectures and practices.

Disability: If you believe you may qualify for special accommodations due to disability contact the Center for Accommodations and Support Services Office: http://sa.utep.edu/cass; 915-747-5148.