

Department of Chemistry
The University of Texas at El Paso
Quantum Chemistry (graduate level)

CHEM 5352/6352 (CRN 11736)

Spring Term, 2017

Instructor: Prof. Lela Vuković
Classroom Building, CRBL C202
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Lectures will be held on Mondays and Wednesdays 10:00 AM – 11:20 AM. Office hours will be held on Tuesdays from 12:00 PM – 13:00 PM (tentative) or by appointment; in case of changes, the class will be informed in time.

Course Description Fundamentals of quantum mechanics in chemical systems.

Textbook:

I. N. Levine, **Quantum Chemistry** (7th edition)

Additional reading:

D.A. McQuarrie, **Quantum Chemistry** (University Science Books);

Grading:

The grade for this course will be determined by three or four exams (90%) and problem sets (10%).

Problem sets will be assigned throughout the course. This is a difficult course. Most of the material will be learned by you outside of class. *Just attending lecture will probably 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 on the effort, and understanding the concepts**. 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. It is in your best interest to do all the problems in the back of each chapter.

Each exam will build upon the previous one, and all material covered will be considered for each exam. (i.e. you should be aware that Exam 2 may include content covered before Exam 1, etc.). In particular, Exam 4 will be a cumulative exam for the whole course.

Syllabus (tentative)

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| 1. Introduction, math and apparatus of QM | Week 1 |
| 2. Simple QM systems (quantum wells) | Week 2 |
| 3. Wave packets, tunneling, oscillators | Week 3 |
| 4. Angular momentum and related stuff | Week 4 |
| 5. The H atom | Week 5 |
| * The first exam (covers Weeks 1-4) | |
| 6. Linear algebra and operator representations | Week 6 |
| 7. Variational and perturbation methods | Week 7-8 |
| 8. Spin and systems of identical particles | Week 8 |
| 9. Many-electron atoms | Week 9 |
| * The second exam (covers Weeks 5-9) | |
| 10. Electronic structure of diatomic molecules | Week 10 |
| 11. Presentation of calculations with Gaussian | Week 11 |
| 12. Theorems in molecular QM | Week 11-12 |
| * The third exam (covers Weeks 10-12) | |
| 13. Advanced electronic structure methods | Week 12-13 |
| 14. Review of the course | Week 14-15 |
| The fourth exam (cumulative) | |

Text book: I. N. Levine, Quantum Chemistry (7th edition)

Course Drop Policy: Drop date deadline is of March 30th, 2017.

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.

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 Disabled Student Services Office: <http://sa.utep.edu/dsso>; 915-747-5148.