Chemistry 210A: Quantum Chemistry: Introduction and Stationary–State Properties Winter, 2009

Instructor: C. William McCurdy
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Office Hours: 163 E Chemistry MW 10 – 11:30 AM or by appointment

Description: CHE 210A introduces the principles of quantum mechanics and its application to simple, stationary state problems dealing with atoms and molecules. Topics include postulates and general principles; Schrodinger equation; translational motion and penetration of barriers; particle in a well; harmonic oscillator; rotational motion; angular momentum; hydrogen atom; variational method; perturbation theory; many–electron atoms; molecular orbital theory; and a brief introduction to the Hartree-Fock and Density Functional computational approaches to the calculation of electronic structure.

Prerequisites: CHE 110A.

Lecture: MWF 8:00–8:50 a.m., 263 Olson – until otherwise announced in class.

Text: P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 4th ed., Oxford University Press, 2005.

Other useful texts and references:

Ira Levine, *Quantum Chemistry*, 5th ed., Prentice Hall, 2000. – Excellent discussions of bonding and the methods of quantum chemistry including variational and perturbation approaches.

Eugen Merzbacher, *Quantum Mechanics*, 3rd ed. Hamilton, 1998 – A physics text, one of the best references for learning time-dependent QM, in which full detail is on view.

Grading: Grading will reflect performance on homework sets (33%), one midterm exam (33%) and a final exam (34%).

Assignments: Reading and homework assignments will be from the text by Atkins and Friedman. The course will cover Chapters 1–4 , Chapter 6 through section 6.10, Chapter 7, Chapter 8 through section 8.6 and Chapter 9 through section 9.8. Roughly one chapter will be covered per week, but later chapters will be given more time at the expense of earlier chapters. Solutions to the assigned problems will be available after the due date on the course website accessible through http://My.UCDavis.edu/

Lecture Topics and Reading Assignments

Week 1— Chapter 1.1-1.21: QM operators, the postulates of QM, uncertainty principle and Matrices in QM.

Week 2 — Chapter 2.1-2.18: Free particle, particle-in-a-box, transmission and reflection by 1-D barrier, harmonic oscillator

Week 3 — Finish chapter 2, begin chapter 3: One-electron central force problems

Week 4 — Chapter 3: Angular motion and spherical harmonics, states of the hydrogen atom

Week 5 — Finish chapter 3: begin Chapter 4.1-4.8: Angular momentum for one particle

Midquarter exam – open book

Week 6 – finish sections 4.6 -4.8, begin Chapter 6 sections on perturbation theory

Week 7 — Chapter 6.1-6.10 Perturbation theory and the variational principle

Week 8 — Chapter 7: Electronic structure of many-electron atoms, the Pauli Principle, Slater determinants, introduction to term symbols, and the Zeeman and Stark effects.

Week 9 — Chapter 8.1 - 8.6 Introduction to molecular electronic structure, molecular orbitals, details of bonding the H_2 molecule, MO description of bonding in diatomics.

Week 10 — Chapter 9.1-9.8: Electronic Structure Calculations: the Hartree-Fock approximation, Configuration Interaction, and the idea of Density functional theory

Final Exam – two hour, in class, at the scheduled time.