

Chemistry 531
Quantum Chemistry
Fall Semester 2006

- Instructor:* Dr. Spiridoula Matsika,
Office: Beury 242, Phone: 1-7703, e-mail: smatsika@temple.edu
Office Hours: Mon 1-2pm, Wed 1-2pm, Th 1-2pm or stop by anytime.
- Lecture:* Monday Evening 6:10 pm - 9:00 pm, Beury Hall 413
- Text:* "Quantum Chemistry" (fifth Edition) by I. Levine
- References:* "Introduction to Quantum Mechanics: with Applications to Chemistry" by Pauling and Wilson (QC174.1.P38 1935)
"Principles of Quantum Mechanics" by R. Shankar (QC174.12.S52 1994)
"Quantum Mechanics" by Cohen-Tannoudji, Diu, and Laloe (QC174.12.C6313)
"Modern Quantum Mechanics" by Sakurai (QC174.12.S25 1994)

Topics:

- I. Background
 - Review of Classical Mechanics
 - Wave/particle behavior of electrons
- II. Fundamentals of Quantum Mechanics
 - Schrodinger Equation/ Wavefunctions/ Operators/ QM Postulates
- III. Particle in a Box
- IV. Harmonic Oscillator
- V. Angular Momentum
- VI. The Hydrogen Atom
- VII. Approximate Methods
 - Variational approaches
 - Perturbation Theory
- VIII. Many Electron Atoms
- IX. Born-Oppenheimer Approximation/Bonding/ Molecules

Course Description:

Introduction to the principles of Quantum Mechanics and applications of them to the study of atoms and molecules

- Grading: Weekly Homework: 20%
Midterm: 40%
Final: 40%

Homework and Exams:

Weekly homework problems will be collected in class on the due date. Late homework will not be accepted without prior consent of the instructor.

There will be one midterm exam on the week of 10/30/06 and the final exam on 12/11/06.

Students with disabilities:

Any student who has a need for accommodation based on the impact of a disability should contact me privately to discuss the specific condition as soon as possible. Contact Disabilities and Services at 215-204-1280 in 100 Ritter Annex to coordinate reasonable accommodations for students with documented disabilities.

Freedom to teach and freedom to learn are inseparable facets of academic freedom. The University has adopted a policy on Student and Faculty Academic Rights and Responsibilities (Policy # 03.70.02) which can be accessed through the following link:

http://policies.temple.edu/getdoc.asp?policy_no=03.70.02.

First class: Monday, August 28.

Labor Day (no class) Monday, September 4.

Last day to drop (tuition refund available): Monday, September 11.

Last day to withdraw (no refund): Monday, October 30.

Thanksgiving Holiday: November 23-26

Last Class: Monday, December 4.