CHEM 586 Syllabus (Fall 2005)
TTh 9:25 – 10:40 a.m.
Mellon Hall 308 Conf.

Course Title: *Quantum, Structure & Dynamics*
Instructors: *Drs. Jeffry D. Madura*
e-mail: *madura@duq.edu*
Office: *Mellon Hall, Madura (308 or 320)*
Office Hours: *MWF 9:00 –10:00 a.m. or by appointment*

Textbook: *Introduction to Quantum Mechanics in Chemistry* by Mark A. Ratner and George C. Schatz. Prentice-Hall ©2001. ISBN: 0-13-895491-7. Library of Congress call number QD462.S328 2000.
Quantum Mechanics in Chemistry by George C. Schatz and Mark A. Ratner. Dover ©2002. ISBN: 0-486-42003-5. Library of Congress call number QD462.S33 2001.
Mathematical Methods for Scientists and Engineers by Donald A. McQuarrie. University Science Books ©2003. ISBN: 1-891389-29-7. Library of Congress call number QA37.3.M36 2003.

In addition to the required textbook for this class the following books are suggested as reference books.

- Fayer, Michael D.: Elements of Quantum Mechanics
  - An introduction into the area of quantum mechanics.
- Craig, D. P. and Thirunamachandran, T: Molecular Quantum Electrodynamics
  - A systematic introduction to radiation molecule interactions.
- Byron, Jr., F. W and Fuller, R. W.: Mathematics of Classical and Quantum Physics
  - Chapters 1 – 5 provide a nice review of the basic mathematical concepts
- Christopher Cramer: Computational Chemistry
  - An introduction to electronic structure theory.
- Leach, Andrew: Molecular Modeling: Principles and Applications
  - An introduction to electronic structure theory and other molecular modeling methods.
- Atkins, Peter: Physical Chemistry 7th edition
  - A review of basic physical chemistry.

Topics

- Basic Quantum Mechanics
- Electronic Structure
- Introduction to Matter and Radiation
- Computational Molecular Spectroscopy

Problem Sets Several take-home problem sets will be given out during the semester. These problem sets are to exercise the material we have been discussing and challenge you further in your understanding and basic knowledge. Do not wait until the day before the assignment is due to start the problems. A good practice is to read through the entire problem set once you receive it, jot a few notes down about the problem, the start to work the problem as soon as possible.

Exams: Two exams will be given, a midterm and a final (50%). The midterm exam date will be announced in class while the Final is scheduled for **Friday Dec. 9, 2005; 1:15 – 3:15 p.m.** Quizzes and homework assignments will be given throughout the semester (40%). Class participation will be 10% of the grade.

Class Days We will meet every T Th **except** the following days: Aug. 30, Sep. 1, 8, Oct. 6 and Dec. 1. These days will be made up during the semester

Disability: Any student with a qualified disability that requires special accommodations should inform the instructor as soon as possible so that arrangements can be made.

Part I. Introduction to Quantum Mechanics **(14 lectures)**

- Background
- Postulates
- Particle in free space
- Particle in a box
- Particle in periodic systems
- Rigid rotor
- Harmonic oscillator
- Hydrogen Atom
- Helium Atom
- Electron Spin
- Many Electron Atoms
- Diatomics
- Ab initio Methods
    - Hartree-Fock
    - Post Hartree-Fock, Moller-Plesset Theory, and Coupled Cluster Theory
    - Density Functional Theory
- Semi-empirical Methods (ZNDO, MNDO, AM1 and PM3)
- Group Theory
- Applications of Electronic Structure Theory
    - Potential energy surfaces
    - Vibrational
    - Excited States
    - Solvation
    - Nuclear magnetic

Part II. Electromagnetic Radiation **(14 lectures)**

- Time Dependent Quantum Mechanics
- Interaction of Radiation with Matter
- Occupation Number
- Theories of Reaction Rates
- Time Dependent Approach to Spectroscopy
- Time-correlation functions
- Fluctuation-Dissipation Theorem
- Vibrational-Rotational Spectroscopy
- Spectroscopy of Liquids