SYLLABUS CHM 6470: '**INTRODUCTION TO QUANTUM CHEMISTRY**

Recommended Text; I. Levine, Quantum Chemistry, sixth edition.

Lectures will be 90 mins, Tuesday and Thursday, 10:40 to noon, in the QTP Reading Room. Office hours are noon to 2pm Tuesday and Thursday. My door is open to students anytime I am in my office, but appointments can also be made via email. My email is **bartlett@qtp.ufl.edu.**

Grades will be determined by two exams plus homework. The breakdown is 67% for exams, 33% for homework. Depending upon interest, in some years we also encourage each student to make a quantum chemical application using the QTP software and computers for extra credit.

Prerequisite: Two semesters of undergraduate Pchem, math through Calculus,. and adequate performance on the placement exam.. The syllabus should be viewed as a guide, rather than a strict plan. We emphasize the required foundation, but also try to bring future users up to the point that they can make intelligent applications, time permitting.

SYLLABUS

I. Essential Preliminaries

- Newton's equations of particle motion
- Concept of a differential equation and its solution
- The Lagrangian and Hamiltonian and Hamilton's equations

II. Concept of particle waves and the Schrödinger Eqn.
III. Exactly soluble examples

- Free particle
- Particle in a 1-dim box
- Particle in a 3-dim box
- Harmonic Oscillator
- Harmonic Oscillator in 2-dim

IV. Hydrogen Atom and Atomic Structure
V. Angular Momentum
VI. Electron spin.
VII. He atom and two-particle operators
    - Antisymmetry of Fermions
    - Pauli Principle

VIII. Hartree-Fock Self-Consistent Field Theory (Handouts plus text by Szabo and Ostlund)
    - Properties of the Antisymmetrizer

- Energy expressions for one and two-particle terms
- Use of variational principle to find best MO's.
- Fock operator and HF equations
- Invariance of Fock operator to unitary transformations
- Canonical and non-canonical HF forms
- Basis Set Expansions and Matrix HF equations
- Density Matrices
- Koopmans' Theorem
- Brillouin Theorem

IX. Transition to Molecules

- Born-Oppemheimer Approximation
- Naïve MO theory
- Symmetry Properties of HF Theory
- Restricted and Unrestricted Hartree-Fock

- Numerical performance

X. Electron Correlation Error

- Configuration Interaction
- Perturbation Theory
- Moeller-Plesset Theorem

XI. Density Functional Theory (hiding electron correlation into a one-particle theory)

- Hohenberg-Kohn Theorem
- Kohn-Sham Procedure
- Performance