

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

**Rodney J. Bartlett, Ajith Perera**

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

Lectures will be 90 minutes, Tuesday 10:40 to 11:45, Periods 4 and 5 and Thursday, periods 5 and 6 (noon to 1:30), in the QTP Reading Room. Office hours are 1:30 to 3pm, Thursday. But 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](mailto:bartlett@qtp.ufl.edu). Also, Dr. Perera can be consulted.

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 students up to the point that they can make intelligent applications, time permitting. We will also emphasize current work beyond text book accounts, to illustrate the concepts being learned.

All students are expected to become proficient in applications of calculus, differential equations, linear algebra, and matrix theory which will be taught as those concepts are needed.

### 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-Oppenheimer Approximation
- Naïve MO theory
- Symmetry Properties of HF Theory
- Restricted and Unrestricted Hartree-Fock
- Numerical performance

#### X. Electron Correlation Corrections

- Configuration Interaction
- Perturbation Theory
- Moeller-Plesset Theorem
- Infinite-order PT, Coupled-cluster Theory

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

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

