

## **CH 837 Quantum Chemistry**

### **Syllabus**

- I. Brief introduction to some concepts and principles of quantum mechanics
  - a) Overview of Newton , Lagrangian and Hamiltonian mechanics
  - b) Bohr quantization principle
  - c) Dirac quantization principle
  - d) Schrodinger equation and its shortcomings
  - e) The uncertainty principle
  - f) Time-dependent phenomena and tunneling
  
- II. Exactly solvable problems in quantum mechanics
  - a) particle in the box (degeneracy)
  - b) harmonic oscillator
  - c) rigid rotator
  - d) hydrogen atom
  
- III. Atomic structure
  - a) Pauli principle
  - b) Hartree and Hartree-Fock equations
  - c) classification of atomic spectra
  - d) Zeeman and Stark effects
  
- IV. Molecular structure
  - a) Born-Oppenheimer approximation
  - b) role of symmetry
  - c) linear combination of atomic orbitals (tight band methods)
  - d) valence bond methods
  - e) Huckel methods
  - f) molecular rotations and vibrations
  
- V. Scattering theory and spectroscopy

Recommended textbooks: 1. P.W. Atkins and R.S. Friedman: Molecular Quantum Mechanics (3<sup>rd</sup> Edition) Oxford U.Press. 1997 ; 2. I. Levine , Quantum Chemistry, (5<sup>th</sup> edition) Prentice Hall, N.J. , 2000.