

SYLLABUS CHM 6480: 'INDEPENDENT' PARTICLE THEORY.

Hartree-Fock self-consistent field (SCF) theory and Density Functional Theory

Recommended Texts: Szabo and Ostlund and Parr and Yang.

Lectures will be 90 mins, Tuesday and Thursday, 10:40 to noon, in 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.

Grades will be determined by an exam or two, plus computer programming assignments and homework. The breakdown is 50% for exams, 30% for computer problems, and 20% for homework. All students will be given access to the QTP computers for their work.

Prerequisite: CHM 6470 or permission of instructor.

Essential Preliminaries: Hydrogen Atom, Coordinate Systems, Born-Oppenheimer Approximation.

1. Generic Molecular Orbital Theory
 - Concept of one and two particle operators
 - Effective one-particle operator
 - Antisymmetry
2. Hartree-Fock Self-Consistent Field Theory
 - 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
3. Basis Set Expansions and Matrix HF equations
 - Density Matrices
4. Theorems of HF Theory
 - Koopmans' Theorem
 - Brillouin Theorem
5. Electron Correlation Error
 - Configuration Interaction
 - Perturbation Theory
 - Moeller-Plesset Theorem
6. Symmetry Properties of HF Theory
7. Restricted Hartree-Fock
8. Treatment of Second and Higher-order Properties in HF
9. Time-dependent Hartree-Fock (RPA).
10. Density Functional Theory (Detailed syllabus to come later).
11. Seamless connection with wavefunction theory. Optimized Effective Potential.
12. Ab initio dft

13. Density Matrix Functional Theory