SYLLABUS CHM 6480: '**MEAN FIELD' 'INDEPENDENT' PARTICLE THEORY**.

Hartree-Fock self-consistent field (SCF) theory and Density Functional Theory
Recommended Texts to consult: Szabo and Ostlund and Parr and Yang.

Lectures will be 90 mins, Tuesday and Thursday, 10:15 to 11:45, Tuesday and 10:45 to noon, Thursday in the QTP Reading Room. Times can be adjusted to accommodate student's schedule.
Room. Official office hours are noon to 2pm Thursday, but 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 computer programming assignments and 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, and Generic Molecular Orbital Theory

- 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

  Basis Set Expansions and Matrix HF equations
    - Density Matrices

  Theorems of HF Theory
    - Koopmans' Theorem
    - Brillouin Theorem
    - Symmetry Properties of HF Theory

  Accuracy of HF results

WRITE HF PROGRAM WITH INTEGRALS AND LINEAR ALGEBRA ROUTINES PROVIDED (This should be begun as the HF eqns are derived).

- Electron Correlation Error
    - Configuration Interaction
    - Perturbation Theory
    - Moeller-Plesset Theorem

ADD CIS TO HF PROGRAM
ADD MBPT2 TO HF PROGRAM

- Density Functional Theory

- Hohenberg-Kohn Theorem
- Kohn-Sham Construction

MODIFY HF PROGRAM TO DO DFT CALCULATIONS

- Treatment of Second and Higher-order Properties in HF (CPHF Eqns.)

MODIFY HF PROGRAM TO DO CPHF CALCS.
DO SAME WITH DFT PROGRAM

- Time-dependent Hartree-Fock (RPA).

MODIFY HF PROGRAM TO DO TDHF
ADD TDDFT TO PROGRAM

- Address detailed interconnections of DFT with WFT
- Optimized Effective Potential.
- Ab initio dft
- IP theorem

QTP(0,0) FUNCTIONAL AND ITS FUTURE