The Chem 126/226 midterm on November 10th will cover the following topics

1) **Optimization Methods**
   a. Basic math: functions, derivatives, Hessian matrix
   b. Mathematical conditions for minima and maxima
   c. Examples of situation in which optimization is important
   d. Classification of optimization methods
   e. Steepest Descent: the principles and the algorithm
   f. Newton-Rhapson: the principle and algorithms, its limitations
   g. Hessian update schemes, BFGS: the principle and advantages
   h. Know which optimizer is best suited for a given task

2) **Molecular Mechanics of Isolated Molecules**
   a. The concept of the force field: energy as a sum of many classical terms
   b. Description of bond stretching: quadratic, cubic, quartic terms
   c. Description of bond dissociation: Kratzer and Morse potentials
   d. Description of bond bending: quadratic function
   e. Description of torsional modes: cosine series
   f. Description of Coulombic interaction via multipole expansion
   g. Description of Coulombic interactions via the distributed point charges
   h. Description of van der Waals interactions: the Lennard-Jones potential
   i. Physical meaning of Lennard-Jones parameters sigma and epsilon.
   j. Comparison and applicability of common force fields: MM3, AMBER, OPLS-AA.
   k. Common applications of molecular mechanics: minimization and conformational analysis
   l. Limitations of molecular mechanics

3) **Molecular Mechanics of Molecular Ensembles**
   a. Differences between isolated molecules and condensed media
   b. Role of statistical mechanics in computational chemistry
   c. What is an ensemble?
   d. The Boltzamnn distribution
   e. Calculation of conformational partition function from conformer energies
   f. Relationships between partition function and thermodynamic quantities
   g. Monte Carlo: principles and applications
   h. Calculation of probability distributions from Monte Carlo simulations
   i. Monte Carlo conformational search
   j. Molecular simulations: applications and advantages over minimization

4) **Principles of quantum mechanics**
   a. Description of matter in the quantum theory
   c. Observables as eigenvalues of operator equations
   d. Hamiltonian operator as the quantum mechanical energy operator
e. Time-independent Schröedinger equation
f. The physical meaning of eigenvalues of the Schröedinger equation
g. The physical interpretation of eigenfunction of the Schröedinger equation
h. Analytically solvable problems: the hydrogen atom
i. Molecular Hamiltonian operator in the general case
j. Non-relativistic molecular Hamiltonian in zero-external-field case: complete mathematical expression
k. Born-Oppenheimer approximation: its essence and consequences
l. Difficulties in solving the electronic Schröedinger equation for fixed nuclei: dynamic electron-electron interaction
m. Hartree approximation: one electron in the field of all other electrons
n. Slater determinant as a mathematical way to count for electron’s spin
o. Variational principle as a guide to obtain molecular energy
p. Overlap integral, resonance integral
q. LCAO approach to molecular orbitals
r. The Hartree-Fock method: principles

5) Semiempirical Quantum Chemistry
a. Simplifications to the Hartree-Fock method
b. Characteristics and parameterization of AM1, and PM3 method
c. Applicability and accuracy of semiempirical methods for description of chemical reaction energetics
d. Advantages and limitations of semiempirical methods

6) Ab Initio Quantum Chemistry at the Hartree-Fock Level
a. The need for initial guess for solving the Schrödinger equation
b. Atomic (Slater) orbitals as a natural choice for atomic orbitals
c. Mathematical difficulties with Slater Orbitals; Gaussian primitives as a computationally convenient solution
d. The cusp-related limitations of Gaussian primitives
e. Mathematical form of Gaussian primitives: s, p, and d angular momentum
h. Comparison of STO-3G basis and STO-5G basis
i. The zeta-nomenclature: single-ζ, double-ζ, triple-ζ basis
j. The Pople family of basis sets, polarization and diffuse functions
k. The structure of correlation-consistent basis sets
l. Exponential extrapolation to estimate the HF limit
m. Electron correlation; Møller-Plesset Perturbation theory

7) Practical Aspects of Computation
a. Principles of writing good programs
b. Program input and output considerations
d. The concept of the Z-matrix for molecular structure
e. The concept of atom types and its relation to force field parameters
f. The precision vs. cost dilemma in Monte Carlo simulations
g. How to recognize insufficient sampling in a Monte Carlo simulation
h. Performance considerations for quantum chemistry programs
i. Understanding the output of energy calculations and optimizations
Required Reading

1) All tutorials, homework assignments, and answer keys for assignments 1-3
2) All literature marked “Required” on the course website
3) Many-Electron systems: Ch 3 up to 3.6 or Ch 4.5 in Cramer
4) Basis sets: Ch 5 in Jensen up to 5.5 or Ch 6.2 in Cramer up to