The Chem 126/226 Final will be held on Friday, Dec 12 at 12 – 3 PM in Phelps 1420. The following topics will be covered in addition to topics that were covered in the Midterm.

1) **Electron Correlation: Wavefunction-Based Methods**
   a. What was ignored in the Hartree-Fock theory?
   b. Static and dynamic electron correlation
   c. Multi-configuration SCF for treatment of static electron correlation
   d. Truncated configuration interaction (CISD): principle and limitations
   e. Møller-Plesset perturbation theory: principles
   f. Advantages and limitations of MP2 approach
   g. MP2, MP3, MP4: applicability and cost issues
   h. Coupled cluster theory: principles, advantages, and cost issues
   i. Understanding the output of MP2 and MP3 calculations (Gaussian and PC GAMESS)

2) **Electron Correlation: Density Functional Theory**
   a. Density Functional Theory: principles
   b. Hohenberg-Kohn existence theorem
   c. Hohenberg-Kohn variational theorem
   d. Representation of molecular energy in DFT
   e. Exchange-correlation functionals: B3LYP
   f. Advantages and limitations of DFT

3) **Molecular Structure Optimization: Concepts**
   a. The concept of the potential energy surface (PES)
   b. Mathematical definition of a minimum on a one-dimensional PES
   c. Mathematical definition of a maximum on a one-dimensional PES
   d. Mathematical definition of a minimum on a multi-dimensional PES
   e. Mathematical definition of a saddle point on a multi-dimensional PES
   f. Optimization of minima: advantages and disadvantages of calculating second derivatives. Use of CalcAll, CalcFC, and ReadFC options in Gaussian
   g. Optimization of transition states: Identity reactions and symmetry
   h. Optimization of transition state structures: From a single guess structure
   i. Optimization of transition state structures: QST2 and QST3 methods
   j. Optimization of transition state structures: Scanning the PES
   k. Verification of transition states

4) **Molecular Structure Optimization: Ab initio Methods**
   a. Know which methods and basis sets are giving reasonable structures for
      (i) van der Waals complexes (e.g. neon dimer)
      (ii) dipolar complexes (e.g. water dimer)
      (iii) stable closed-shell molecules (e.g. water monomer, CO, F₂)
(iv) transition states (e.g. in S_n2 reactions)
b. Advantages of using molecular symmetry during optimization
c. Capabilities and limitations of the HF method
d. Capabilities and limitations of the MP2 method

5) Vibrational Spectroscopy and Thermodynamics
   a. Separation of molecular wave function to electronic and nuclear wave functions
   b. Schrödinger equation for one dimensional harmonic oscillator
   c. Vibrational wave functions for the one-dimensional harmonic oscillator
   d. Vibrational energy levels for one-dimensional harmonic oscillator
   e. Relationship between force constant and harmonic frequencies
   f. Reduced mass and the Wilson G-matrix
   g. Analytical and numerical calculation of second derivatives
   h. How to calculate harmonic vibrational frequencies in water: general approach
   i. Accuracy of HF frequencies; scaling
   j. Accuracy of frequencies at correlated (MP3, CCSD, CCSD(T)) ab initio levels
   k. Limitations of the harmonic approximation
   l. Zero-point vibrational energy: how to calculate from frequencies
   m. Gas phase thermodynamics: the principles
   n. Translational contributions to enthalpy and entropy
   o. Rotational contributions to enthalpy and entropy depend on the shape
   p. Vibrational contributions to enthalpy and entropy depend on vibrational frequencies.
   q. How to compare results from calculations with experimental equilibrium constants.
   r. How to compare results from calculations with experimental rate constants
   s. Kinetic isotope effect: origin and computational prediction
   t. Understanding the output of Frequency calculation (Gaussian or PC GAMESS)

6) Electronic spectroscopy
   a. Molecular orbital description of molecules
   b. Ground and excited electronic states
   c. Vertical excitation energies
   d. Valence and Rydberg transitions
   e. Franck-Condon principle and the intensity of vibrational bands in UV spectrum
   f. Conical intersections and photochemistry
   g. Optimization of excited states and adiabatic excitation/emission energies
   h. Calculation of excitation energies: CIS and TDDFT approaches
   i. Understanding the output of CIS calculations (Gaussian or PC GAMESS)

7) Environment effects: description of solvation
   a. Need for the description of solvent effects
   b. Solvent effects by chemical intuition (polarity effects)
   c. Implicit solvent models: the principle
   d. The Onsager, PCM, and SCI-PCM models
   e. Optimization and energy evaluation in the presence of implicit solvent
f. Hybrid QM/MM approach to solvation and biological reactions  
g. Partitioning of total energy to QM, MM, and interaction energy  
h. Calculation of QM/MM interaction energy if the two systems are not covalently connected  
i. Solvent effect in identity $S_N^2$ reactions  
j. Solvent effect in Menschutkin reaction  
k. Solvent effect in aromatic substitution reactions  
l. Free energy perturbation as a practical approach to determine free energy changes in solutions

8) Basic physical and organic chemistry  
   a. The concept of atomic orbitals  
   b. Exo- and endothermic reactions, fast and slow reactions  
   c. $S_N^1$ and $S_N^2$ reactions  
   d. Hammond postulate

**Required reading.** You should be familiar with the tutorials/assignments posted on the website. You should know the material in the “Required reading category”. Additional required reading: “An introduction to the state of the art in quantum chemistry” by Frank Jensen that was given out in the class. In addition to obvious topic coverage in the textbook, please read carefully Chapters 11 to 14 in Jensen book. If you have Cramer’s book, please review pages 203-207, 211-216, 224-237, 249-254, 271-280, 355-370, 385-393, 457-467. However, both textbooks are more detailed and mathematical than what I expect you to know. For the most part, you could take it as a supplementary material to clarify concepts and supplement your lecture notes with information you find interesting.