Course: CHM220 (Winter09)
Title: Introduction to Computational Chemistry
Instructor: M.M. Bryant (Szczesniak), Rm 250, SEB; Phone: 248-370-2087; e-mail: bryant@oakland.edu
Time: MWF: 12 noon-1 pm; Rooms: 378 SEB-lecture; 335 HHS-lab

The objectives of this course are as follows:
i. To learn basic principles of quantum chemistry and to understand the potential, as well as the limitations, of computational techniques;
ii. Exposure to modern computational chemistry software;
iii. Gain a better understanding of chemical principles via computational modeling:
The concepts of chemical bonding, electronic structure, electronic structure-reactivity relationship, etc., will be illustrated by applying the computational chemistry tools.

Attendance: mandatory
Text: There is no textbook; you must take notes
Materials: Small capacity pen-drive

Course Structure:
   Tutorial: Molecule building tutorial (Spartan04)
2. Molecular Orbital theory. Basis set
   Tutorial: Building molecules; Interpreting MOs
3. Interpreting molecular stability via electron density distribution
   Exercise 1: Electrons take-up space
   Experiment 1: Is benzene the most stable form of C₆H₆?
4. Electron distribution vs molecular properties (density, atomic charges, electrostatic potentials, dipole moments).
   Experiment 2: Carboxylic acids and their acidities
5. Treatment of chemical properties and reactivity
   Exercise 2: Protonation sites in 4-amino pyridine
   Experiment 3: Basicities and proton-transfer reactions
   Exercise 3: Molecular vibrations
   Exercise 4: Zero-point corrected proton affinities
   Experiment 4: Conformational energy profile
7. Solvent effect
   Experiment 5: Solution-phase basicities
8. Intermolecular forces: Hydrogen bonding and van der Waals interactions
   Experiment 6: Hydrogen-bonded complexes
9. Reaction coordinate
   Experiment 7: SN2 reaction
10. Reactivity and its predictions using Frontier Molecular Orbitals (FMO)
    Exercise 7: Nucleophiles and electrophiles
    Exercise 8: Dienophiles
    Experiment 8: Biologically relevant molecules: Vitamin E
11.  Density Functional Theory; Using and interpreting DFT results  
    Exercise 9: Dissociation of F2  
12.  Special Projects

    **Grading:** There are 8 graded experiments - 50%; exams - 40%, quizzes - 5%; Final  
    project - 10%; Exams: One mid-term 1-hour exam (15%); 2-hour comprehensive final  
    exam (25%); ca. five 5-min. quizzes (5%).

**Exam Schedule**
- Wednesday, February 20: Mid-term exam  
- Monday, April 20: Last class  
- Monday, April 27: Final Exam (noon -3:00 pm)

**Office hours:**
- Mondays: 107pm - 200pm or by appointment

**Rules of behavior in the computer lab:**

1.  **No eating/drinking is permitted in the computer lab – do not bring bottled water with you to the lab.**
2.  **No cell phones/no text messaging in class and during exams**
3.  **Do not** change any settings for computers and/or any programs
4.  Use Computational Chemistry accounts: Name: CompChem (or IntroCompChem), password: CHM220. **Log-out** after class.
5.  Do not surf the internet unless it is needed for your class assignment
6.  Do not install any software.
7.  Do not leave any unneeded files.
8.  You are responsible for backing up your files.
9.  Report equipment problems/malfunction to your instructor or Pat Colling (Room 249 SEB). **Do not attempt to fix problems with computers/printers!**

**LAB REPORTS**

1.  Each computer experiment will be concluded by a lab report.
2.  Lab reports are essential tools of your learning (keep them for your records, will be included in tests).
3.  Lab reports should be (i) typed; (ii) include all the data collected in the computer experiments and their analysis; (iii) include the discussion of your results and the answers to the questions given in the lab description in full sentences.
4.  Lab reports should be done **at home not in class.**
5.  Your grade will be based on both the intellectual merit and the overall appearance of your report.