CHM4800 Computational Chemistry

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Office Hours: see schedule at http://ux1.eiu.edu/~sapeebles/SP06Schedule.pdf
Class meeting time: MWF at 1300-1350 in Room 4180
Course web page: Material and announcements will be posted frequently on the course web site at http://ux1.eiu.edu/~sapeebles/chm4800.htm  
Check this site often.

Prerequisites: CHM3910 (Thermodynamics & Kinetics) is the only prerequisite for this course. Although CHM3920 (Quantum Chemistry & Spectroscopy) is not officially required, it is highly recommended since the material we will be covering involves the application of concepts that would have been introduced in CHM3920. We will be covering some of the background theory briefly to put things into context but if you find you need additional background detail you will find it informative to consult a quantum mechanics text book such as Quantum Chemistry by D.A McQuarrie.

Textbooks:

Aims: To introduce the basic concepts of computational chemistry so that you feel more confident in applying programs such as Spartan or Gaussian to help solve chemical problems. Emphasis will be placed on how to select and implement appropriate models for particular problems and how to interpret results; numerous examples will be examined to illustrate concepts/applications and to allow you to develop a better appreciation of the increasing number of computational studies found in the literature.

Structure and grading: The course will consist of three 50 minute lectures per week. Several (5 or 6) projects (plus an individual final project of your own choosing – see below) will be assigned throughout the semester – you should start work on these projects as soon as possible to spread the load in the computer lab and to avoid last minute rushes. These projects will be selected to reinforce the concepts encountered in lecture and to allow you hands-on experience with the application of what we have learnt. The final project will be chosen by yourself, with input and assistance from the instructor. This must be an original problem, which can be something related to your research or a project based on a problem you have found by reading the literature; the final project must be approved by the instructor (details will be given later in the semester). The results of your project will be disseminated to the rest of the class via a short PowerPoint or poster presentation (depending on the class size). A portion of your final project grade will come from other students’ critical assessment of your work. The results of each project will be written up and submitted in the form of a short report, along with a discussion of the important conclusions; a hard copy (as well as an electronic copy (via email)) must be submitted for each report. Your input and output files from each project must also be emailed to the instructor at the address above.

Quizzes: Several quizzes (for a total of 120 points) will be given that will test your understanding of the concepts we have introduced (these may be given as take-home quizzes)

Homework projects/assignments: Each project will be worth 50 points, the final project is worth 100 points, with another 50 points from your final project presentation.
The final grade in this course will be assigned as an overall percentage of the available points:
A 88-100%; B 78-88%; C 65-78%; D 55-65%; F <55%

Plagiarism:
All students are expected to abide by the University’s standards of academic integrity. The submission of all (or part) of another student’s work is unacceptable and will be dealt with in accordance with the usual University policies on cheating. Copying of text from books or the internet, or submitting someone else’s computational calculations as your own are considered plagiarism; assigned projects are to be carried out individually – group work is not acceptable. The plagiarism prevention software Turnitin will be used on all submitted papers; further details on Turnitin are available at http://www.eiu.edu/~turnitin/ Cheating of any form in this course will result in a failing grade and will be reported to the Office of Judicial Affairs.

Tentative schedule:
Introduction and fundamental principles
What is computational chemistry?; Overview of methods; Potential Energy Surfaces; Quantum Mechanics, the Schrödinger Equation and the Hamiltonian, Born-Oppenheimer Approximation; Introduction to Gaussian 98, Spartan 04 and the Tru64 Unix workstation;
Ab initio methods
Molecular orbitals, Basis sets & basis set customization (BSSE etc.), Hartree-Fock method, variation principle, SCF theory; Inclusion of electron correlation: Møller-Plesset perturbation theory, Configuration Interaction (CI), Coupled Cluster (CC), Density Functional Theory (DFT)
Semi empirical methods; Molecular mechanics methods
AM1, PM3
Force fields (AMBER, CHARMM)
Single point energy calculations and calculation of molecular properties
Setting up input and interpreting output from Gaussian 98; population analysis, multipole moments, hyperfine constants, optical activity, NMR shifts etc.
Geometry optimizations
Identification of minima and transition states
Calculation of vibrational frequencies
Prediction of vibrational spectra, characterization of stationary points, thermochemistry, zero-point energy
Advanced applications
High accuracy energy models: G3, G2, G2(MP2), Complete basis set (CBS) methods; Study of chemical reactions and reactivity; Conformational searching; Excited states; Solvation Models; Structure-property relationships; Modeling biomolecules

Spring 2006 important dates:
January 9th: First day of classes
January 16th: King’s birthday – no classes
February 17th: Lincoln’s birthday – no classes
March 13th – 17th: Spring Break – no classes
April 27th: Last day of classes