**Course Outline**

Office: MWF (~9:00 - ~noon)

Textbook and Website References


http://www.computationalscience.org/ccce

http://cccbdb.nist.gov/

2 @ ~1 Gb USB Memory Stick

Meeting Schedule

F 1:00 - 1:50 pm SSMB 300

Class Schedule (tentative)

F 1/10 Introduction to Modeling
F 1/17 Background (FF pp xlix-li, App A, FF App B)
F 1/24 Basis Sets (FF 5)
F 1/31 Theoretical Methods (FF 1, FF 6)
F 2/7 Single Point Energy and Geometry Optimizations (FF 2, FF 3)
F 2/14 Accuracy (FF 7)
F 2/21 Electron Density, Electron Potential and Reactivity (FF 8)
F 2/28 IR/Raman Spectroscopy and Thermodynamics (FF 4)
F 3/14 UV/Vis and NMR Spectroscopy
F 3/21 Systems in Solution (FF 10)
F 3/28 Transition States (FF 9)
F 4/4 Chemical Kinetics (GIDES)
F 4/11 QSAR
F 4/18 Project Presentations

[W 3/21 Last Day for Withdrawal W Grade]

Class Preparation

Each class has one or more reading assignments as indicated by parentheses in the above Class Schedule. Please complete the assigned reading before class—this material will not be covered verbatim in class.

Homework assignments will be made each class period. The assignments are due at the beginning of the next class period. Late assignments will be penalized 5 points per school day late. Depending on the assignment, submission of homework in PC compatible format will be by hard copy (printout of results), evaluation of on-line files stored in your WebMO account, and/or USB memory stick (which will undergo a virus screening each time). Please keep a copy of all submitted work. Please use the envelope provided.

Each student is responsible for their own individual work—although group discussion and/or helping each other is encouraged. Most homework items will be worth 30 points each and the kinetics homework assignment will be worth 120 points. If the quality of the submitted material is such that it requires re-submission, 5 points will be deducted for each re-submission. All previous submissions should accompany the re-submission.

The final project will be to develop and write a complete first-draft handout for a molecular modeling “experiment/exercise” suitable for use in one of our classes. Stay alert for ideas. More later...

Point Distribution

The course grade will be based on homework (750 points possible—see above) and the final project (250 possible points) for a total of 1000 possible points. Anyone earning at least 90% of the total possible points will earn a guaranteed A (likewise, 80% for a B, 70% for a C, and 60% for a D) although these standards may be relaxed slightly at the end of the semester resulting in slightly higher grades. A total under 50% will be considered failing. The assignment of + or - to the letter grade will be at the discretion of the instructor.

Please consult with the instructor concerning any absence as soon as possible. Excessive class absences will not be tolerated and will be reflected in the final grade.
Software

We will be using Gaussian and MOPAC as our main molecular modeling software engines with WebMO as the user interface to these computational engines. WebMO is web-based and may be accessed from most computers provided JAVA (jre) is installed. The computers in the labs on the third floor of SSMB will have the jre installed. You may access WebMO at http://webmo.ncsa.uiuc.edu/~webmo/cgi-bin/webmo_sDB/login.cgi using cofc_xx where xx = for your login and ratsrats as your password for your account. Please do not change these codes—I need access to your files for grading homework.

Our molecular modeling calculations will be carried out on a supercomputer located at the University of Illinois at Urbana-Champaign. We acknowledge the educational program at the National Center for Supercomputing Applications for their making this possible.

Later this semester we will be using Vensim PLE as our icon-based system dynamics modeling package (graphical interfaced differential equation solver, GIDES). Vensim PLE is available for free at http://www.Vensim.com/venple.html for academic use and is installed on the computers in the labs on the third floor of SSMB.

Disabilities

If there is a student in this class who has a documented disability and has been approved to receive accommodations through SNAP services, please feel free to come and discuss this with me during my office hours.

Catalog Description

CHEM 343 Introduction to Modeling in Chemistry (1)

An introduction to computer modeling of various properties and structures of molecules, thermodynamic properties and structures of simple crystals, and the kinetics of chemical reactions. Prerequisite: CHEM 231.

Learning Outcomes

This course is not designed to prepare the student as a “quantum” chemist. It is designed to introduce modeling and, in particular, molecular modeling as another tool that chemists can use along with tools such as IR, Raman, UV-Vis, and NMR spectroscopy in their everyday work.

Upon satisfactory completion of this course, the student would be expected to

1) recognize and understand various types of modeling that are used commonly by chemists
2) evaluate some specific models using VVA
3) gain experience in remote access (cloud) computing on a super computer
4) gain experience with a typical molecular modeling user interface for constructing molecular models and for interpreting molecular modeling calculation results
5) understand and choose the appropriate theoretical method(s) and basis set(s) for a given calculation based on desired accuracy and computational “expense”
6) calculate and interpret single point, optimized, and transition structure energies for a molecule
7) calculate and interpret simple molecular properties such as geometry and dipole moment
8) calculate and interpret electron density, electron potential, and reactivity diagrams for molecules
9) calculate and interpret theoretical values of IR, Raman, UV-Vis and NMR spectra and associated thermochemical properties
10) perform and interpret molecular modeling calculations for molecules in solution
11) model simple and complex first order kinetics reaction using GIDES
12) formulate, design, perform the calculations, and interpret the results of a molecular modeling “experiment/exercise” suitable for use in an undergraduate chemistry class