CH 410/510
Chemical Modeling
Spring 2009

Instructor: Dr. Gwen Shusterman; 350 SB2, 725-3897; shustermang@pdx.edu

Office hours: Will be held in SB1 221 (Chemistry Commons), Thursday 9-12.

Recommended Texts: Molecular Modeling Principles and Applications, Leach, A.R. Prentice Hall, 2nd Edition, *good reference for graduate students and future calculations.* Computational Biochemistry, Tsai, C. S., Wiley-Liss; *on reserve in library.* These texts provide the theoretical background for the modeling techniques and general approaches to chemical problems.

Course Objective: This course is intended to provide the theoretical background for the basic understanding of *ab initio* and semi-empirical methods used in modeling small/medium molecules. An introduction to choice of models for application to chemical problems and extracting chemical information from calculations will be the major portion of the course. The approach of the course will be **'nuts & bolts'**, with an emphasis on learning to use software for modeling.
There will be an introduction to some techniques for modeling larger systems. The particular choice of topics is to be determined partly by student interest and modeling program availability.
One year of Calculus and completion of an introductory course in Quantum Mechanics is highly recommended. Organic chemistry required.

Course Structure: One class period each week will be lecture based, providing the theoretical background for calculations. The other class period will be discussion and problem based, with an emphasis on interpretation of and details of calculations for modeling. The Thursday lab time is designed for hands on assistance with calculations. There will be regular assignments, focused on use of the software to solve chemical problems. The majority of work for the course will be computer based, with additional reading assignments; primarily papers from the literature. The end of term assessment will be based on completion of a modeling project and interpretation of results of calculations.

Grades: Based on assigned homework, in-class participation, and a final project. The final exam period will most likely be used for presentations, either of literature or projects. Evaluation of computer competency will be made through informal oral questioning during lab periods. CH 510 credit will require additional literature work and in class presentations beyond that required for 410 credit.

Literature Discussions: There will be periodic literature reading assignments posted on Blackboard. These will be discussed in class with an emphasis on becoming familiar with the type of chemical questions that can be asked and answered, and the appropriate software to use.

Brief Summary of Topics to be Covered: (flexible and developing list)

Potential Energy Surfaces	Molecular Structure Determination
Electron Density Surfaces	Graphical Models
Molecular Orbital Theory	Basis Sets
Vibrational Frequencies	Symmetry
Transition States	Kinetics
Correlated Methods	DFT
Molecular Mechanics Methods	Conformational Analysis
Protein Structure Determination	

Regular reading and computer assignments will be made in class and through Blackboard.