Chemistry (CHM) 6586
Computational Chemistry
Syllabus
Spring 2013

TTh Period 4-5 (10:40-12:35)
2228 NPB

Final Exam
TBD

Professor Ken Merz
2328NPB
merz@qtp.ufl.edu

Overview: This is a team and project oriented class, which will require significant work outside of class for you and your team. This class structure might not be for you. Think carefully about whether you will be able to tackle a course structured in this non-traditional way. Because of the course structure auditing is not permitted.

Requirements: Basic quantum mechanics and statistical mechanics. Access to a laptop or computer is required. Basic understanding of UNIX is also expected. For a quick UNIX tutorial see http://www.ee.surrey.ac.uk/Teaching/Unix/.

Computer accounts: Obtain a **research** account at www.hpc.ufl.edu. This account will allow you to run mostly Gaussian and AMBER jobs during the course of the semester. You will need to have access to the HPC center through a laptop or desktop machine connected to the internet via WiFi or a landline. It is recommended that you obtain a copy of Molden for molecular structure building and graphics at http://www.cmbi.ru.nl/molden/molden.html. For proteins PyMol or VMD are suitable programs to use for visualization purposes.

Required Textbook:
"Essentials of Computational Chemistry" C. J. Cramer.

Suggested Textbooks (not exhaustive):
Computational Chemistry
"Introduction to Computational Chemistry" F. Jensen.
"Molecular Modelling: Principles and Applications" A. Leach
"Molecular Modelling for Beginners" A. Hinchliffe
Quantum Mechanics
"Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory" A. Szabo and N. S. Ostlund.
"Ab Initio Molecular Orbital Theory" W. J. Hehre; L. Radom; P. Schleyer and J. A. Pople.

"Approximate Molecular orbital Theory" J. A. Pople and D. Beveridge

Simulations

"Computer Simulation of Liquids" M.P. Allen and D. J. Tildesley
"Molecular Modeling and Simulation" T. Schlick
"The Art of Molecular Dynamics Simulation" D. Rapaport
"Advances in Chemical Physics, Proteins: A Theoretical Perspective of Dynamics, Structure, and Thermodynamics (Advances in Chemical Physics)" C. L. Brooks; M. Karplus, and B. M. Pettitt.
"Dynamics of Proteins and Nucleic Acids" J. A. McCammon and S. C. Harvey

Course goals: To provide a basic theoretical understanding of computational chemistry and biology methodologies. This class is a project based class and it is expected that students will familiarize themselves with basic theoretical concepts via reading the course textbook. You will be tested on the outside reading via a take home exam for the course. The project portion of the course will involve the identification of a computational problem and its execution utilizing appropriate software. Focus of the project portion of the class will be on the correct and effective use of two basic computational chemistry programs: Gaussian (for quantum mechanical calculations) and AMBER (for classical molecular simulations).

Project Plan:

1) Obtain appropriate HPC accounts
2) Set up project teams
3) Select a computational project
4) Execute the project
5) Analyze the results
6) Present and write-up the project

Grading: There will be one take home exam. The exam will be circulated early in the semester and will be due one week before the end of the class. The results from the project will be graded via your team presentation and by the write-up your team provides. Grading will also include a class participation component. Office hours will be by appointment.