SYLLABUS for CHEM 408/508 Computational Chemistry
Spring 2018, MWF, 11:00 ISC 0248

Instructor: J.C. Poutsma
Office: ISC 1054 Phone 1-2548 e-mail: jcpout@wm.edu
Office Hours. M, W, F (9:30 – 10:45)

Course Goals: I plan to teach this course as a survey of computational methods that are currently being used to solve problems in chemistry. As all of the computational methods involve solving mathematical equations, there will necessarily be some math in this course, but I am planning to de-emphasize theory and concentrate more on applications of the various theoretical methods.

Text: *Essentials of Computational Chemistry: Theories and Models.* , 2nd edition Christopher J. Cramer. We will cover approximately 2/3 of the book. Additional material will be presented in the form of handouts and will include papers to be discussed in class.

Programs: We will be using three different programs in the course. *Gaussian 09W* is an all-purpose computational package that will be used for semi-empirical, ab initio and density functional theory calculations. *GaussView5* is a graphical interface for *Gaussian 09W* that will be used to draw structures and visualize results. *PCMODEL 8.0* is a molecular mechanics/molecular dynamics program with a somewhat cumbersome interface that will be used for MM/MD calculations during the first 1/3 of the course.

Grading: Problem sets: (100 points) There will be approximately six (6) problem sets given out over the course of the semester. These will necessarily involve you performing calculations outside of class.

Paper summaries: (100 points) There will be approximately six (6) paper summary assignments given out over the course of the semester.

Class participation/discussion: (100 points) will be available for students who come to class and participate in the discussion of papers and ask questions during lectures.

Midterm: A take-home mid-term exam will be given worth 100 points total.

Final Group Project: There will be a 100 point project that will cover some aspect of computational chemistry. The groups will be assigned at the beginning of the semester and the project will be developed over the course of the semester. A final group presentation will take place during the last week of class.

Final Exam: The final will be a 100 point paper (6 pages) that will cover the full course. It will be due 5:00 on Wednesday May 3rd.

508 extra assignment: A second 20 minute individual presentation on some aspect of computational chemistry will be required

Tentative!! outline for the course:

I. Introduction (Chapter 1) expectations and goal; theory vs. models; units and conventions; potential energy surfaces

II. Force Fields and Molecular Mechanics (Chapter 2, 3)

- A. Theory of classical mechanics; strain; force fields; parameterization; modern force fields; conformational analysis.
- B. Introduction to PCMODEL
- C. Literature examples
- D. Brief discussion of Monte Carlo/Molecular dynamics
- E. Literature examples

III. Molecular Orbital Theory (Chapter 4)

- A. MO theory; Huckel theory; LCAO
- B. Intro to Gaussian 09W and GaussView 5

IV. Ab Initio Hartree-Fock Theory (Chapter 6, 7, 9, 10)

- A. Review of HF theory; variational principle; electron correlation
- B. Practical issues: basis sets; correlation techniques
- C. Applications: spectroscopy; thermochemistry
- D. Literature examples

VI. Density Functional Theory (Chapter 8)

- A. Theory: Kohn Sham; X-α, modern functionals.
- B. Literature examples

VII. Semi Empirical Methods (Chapter 5)

- A. CNDO, INDO, MNDO;
- B. modern Hamiltonians
- C. molecular geometries; symmetry

VIII. Advanced Topics (Chapters 14, 15) time permitting