SYLLABUS

Chemistry 711 - Computational Chemistry II

Professor D.W. Bennett **Spring, 2015**
Office: Chemistry 845
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Lecture: MWF 2:00 P.M. - 2:50 P.M. Chem 197

Content: Computation Chemistry II is intended as a continuation of Chemistry 630 – Computational Chemistry. The material will be presented with the assumption that the student has taken this course, or has a solid background in quantum mechanics and has covered the fundamentals of electronic structure theory through Hartree Fock single determinant calculations. The course will emphasize what can be extracted from both classical and quantum calculations, but will refer to and expand the theory developed in Chemistry 630.

Grading: About every two weeks I'll assign a calculation along with some specific tasks (having you analyze the output). You will turn in a brief report with your analysis for each assignment. As was the case for Chem 630, your grade will be based primarily on a paper due at the end of the semester. The main point of this paper will be to convince me that you have learned something in the course, and should include as much of the course material as possible. The grade will be assigned based on the amount of course material incorporated and explained in the text. It must be in standard, grammatically correct English. *It must not be sloppily done.*

Text:

Modern Quantum Chemistry: *Introduction to Advanced Electronic Structure Theory* (Paperback) by Attila Szabo and Neil S. Ostlund . Dover Publications. ISBN 0486691861 Purchase from Amazon.com or Dover Publications. This book is relatively cheap and will be used for the major portion of the course. I will also provide some supplemental material by e-mailing you pdf files.

In addition, if you are planning to use density functional theory in your research I recommend that you obtain *A Chemist's Guide to Density Functional Theory* by Wolfram Koch and Max C. Holthausen. Wiley VCH. ISBN 978-3-527-30372-4.

If you are planning to do calculations on surfaces or extended solids, I recommend *Electronic Structure: Basic Theory and Practical Methods* by Richard M. Martin. Cambridge University Press. ISBN 978-0-521-53440-6..

I will refer to these recommended texts as we proceed throughout the semester.

The following are a list of tentative topics, which we can modify, depending on your interests:

Topics

1. A brief review of the last few Chem 630 lectures – the nuts and bolts of HF single determinant calculations. I'll walk you through the simple examples in the book –which will let you see how the Fock, overlap, and density matrices are generated and used (all 2X2). There is a simple Fortran program in the back of the book using simple Gaussian basis functions which I might make use of as well (to show you how the actual code works).
2. Atomic and Molecular properties from the HF wavefunction (expected values) and the charge density.
3. Basis sets.
4. Geometry optimization (I) – Molecular Mechanics and Dynamics (classical).
5. Geometry optimization (II) – Hartree Fock (quantum mechanical).
6. Beyond single determinant HF – Multiple configurations (CI, etc.).
7. Beyond single determinant HF – Density Functional Theory.
8. Excited State Calculations.
9. Transition State Calculations.
10. If I have time -- transition dipoles and time dependent perturbation theory (spectroscopy).