SYLLABUS

Chemistry 630 - Computational Chemistry

Professor D.W. Bennett **Fall, 2014**
Office: Chemistry 845
E-mail: dwbent@uwm.edu

Lecture: MWF 2:00 P.M. - 2:50 P.M. Chem 169

Content: *Computational chemistry* implies a broad spectrum of methods in chemistry for which a computer must be used. Similar courses are often taught with an emphasis on results, in which the use of specific programs to generate molecular properties is the focus – with little regard to the underlying approximations that go into the determination of those properties. The problem in taking such an approach is that it is difficult to know when numbers produced by a "black box" quantum chemistry program actually represent physical reality. We will take a different approach – one in which the underlying principles are the main focus.

In spite of this emphasis, students from previous courses have expressed the need for more "hands on" experience. Not only was a one-semester course inadequate to meet this need, I found it impossible to cover more advanced topics, such as density functional theory, configuration interaction, etc. In order to remedy this, the material will be covered in a two-semester sequence. Ths first semester will cover the basics (as far as I can get). The material in the second semester, which will begin where I end in the first, will be covered in a topics course – Chemistry 711 – Computational Chemistry II. The additional time will allow for the following lecture format:

Monday – lecture
Wednesday – practicum
Friday – lecture.

The Wednesday practicum will begin once I have covered enough material for you to understand what you are doing when you perform a calculation. Until then I will cover background material and reviews that will help you understand the lectures during that time slot.

Since each student in the course comes from a different background, I have found it necessary to review some basic quantum mechanics before venturing into the electronic structure of atoms, molecules, extended systems, etc. I'll try to keep this as brief as possible.

Since it is a computational course, we will be looking at actual computations as examples of the conceptual material. This will work best if you have access to a program such as Gaussian, Gamess, or one of the commercial packages such as Spartan. The PC version of Gamess can be downloaded from the Gamess web site at Iowa State for free. If you are unable to do this I'll have you generate input and I'll run it on my computer.

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. In addition, on or before (preferably before) October 1 you will e-mail (to me) the description of a computational/ theoretical project that you want to do for a "final paper" in the course. I will respond to you, telling you whether or not it is reasonable, and perhaps will make suggestions. If you don't have something in your own research to work with then you will have to tackle something in the literature – or something that interests you. 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.

You can consult any good quantum chemistry book for something to read if you are having trouble grasping the early lectures. E-mail me and I'll recommend something if you need it. A very readable — and straightforward book is *Quantum Chemistry* by Ira. N. Levine.

Topics (Semester I)

Fundamental Concepts.

Schrödinger Equation

Hydrogenlike Atoms

Multielectron Atoms (I) – Hartree Theory

Multielectron Atoms(II) – Hartree-Fock Theory.

Polyatomic Electronic Structure – Molecular Orbital Theory.

Topics (Semester II)

Configuration interaction

Excited State Calculations

Density Functional Theory

Extended Systems, Surfaces and Solids

Molecular Mechanics

Molecular Dynamics

Other