

# CHEM-355: Computational Methods of Modeling Molecules:

A course in applied quantum mechanics

## **Attention graduate students:**

Meets at same time and place as CHEM-555

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Since molecular modeling software is becoming increasingly available, and since employers are starting to have the expectation that “bench” scientists will be able to use this software, it is desirable to try to instruct a wider range of chemists in its proper use. In this class, you will be presented with; an introduction to quantum theory, an overview of the implementation of various common methods of molecular modeling, and hands-on experience in the use of molecular modeling software. The goals of this course are: 1) to develop an understanding of the role quantum mechanics plays in chemistry, and 2) to develop a sufficient understanding of the fundamental theories and their implementations that you are able to use molecular modeling software intelligently for routine calculations, and communicate intelligently with experts about its application to complex problems. Generally speaking, we will first discuss the theory behind a method. I will then assign a problem or problems to help make the concepts more concrete. Next I will demonstrate the use of one of the various programs for this type of modeling, after which you will perform real calculations. Finally, we will get together and discuss the results. In short, you will do quantum real chemistry, both analytically, and with software.

The required text for this course is “Computational Methods of Modeling Molecules,” by Karl Sohlberg. It is a detailed printed version of the lecture notes. You should augment this text with a standard physical chemistry text. One that you have used for P-CHEM (I, II and/or III) is suitable. This is a course for senior chemistry majors. Expected background is:

You have successfully taken a year of calculus.  
You know about partial derivatives and can evaluate multiple integrals.

You have some passing familiarity with linear algebra. For example:  
You can solve a system of N linear equations and N unknowns.  
You know what the determinant of a matrix is.

You have successfully taken general physics.  
You know about potential and kinetic energy.  
You know that  $F = ma$ .  
You know that  $F = (Q_1Q_2)/(4\pi\epsilon_0r^2)$ .

You are not scared of computers. (A healthy respect is OK.)  
You can use a standard word processor.  
You know what a disk file is.  
You can use a mouse.

In addition, use of a spreadsheet program like Excel<sup>TM</sup> and a symbolic algebra program like Maple<sup>TM</sup> will be required. Further details of the required background can be found in the lecture notes/text.

## Approximate outline: (Spring 2007)

(week 1)

4/2 Wait! STOP. Don't use that computer yet!  
Literature searching  
Simple models. (Lewis structures, VSEPR)  
Boltzmann statistics and molecular conformations.

4/4 What is this "molecular mechanics" business?  
Empirical potentials  
PES minimization

(week 2)

4/9 Computer lab (molecular mechanics)  
Chair and skew-boat cyclohexane  
Anti and gauche butane

4/11 What is quantum mechanics good for anyway?  
The ultraviolet catastrophe  
The photoelectric effect  
The Bohr model of the hydrogen atom.

(week 3)

4/16 What is it about waves that gives rise to quantization?  
Vibrations of a string.  
Boundary conditions

4/18 What is the Schrödinger equation and where did it come from?  
Hamiltonian  
Motivation of momentum as a derivative operator

(week 4)

4/23 The classic QM problem: PIB  
4/25 Computer lab (Some quantum mechanics without scary equations)  
Applications of PIB (conjugated polyenes)  
Applications of the particle on a ring (benzene)

(week 5)

4/30 Computer lab (catch up)

5/2 Mid-term exam

(week 6)

5/7 So where do molecular orbitals come from anyway?  
The variational principle  
Linear variation functions

5/9 Computer lab (linear variation functions)

(week 7)

5/14 MO theory

MO theory from series expansions (LCAO-MO)

5/16 Computer lab (Why  $H_2$  exists and  $H_4$  doesn't)

$H_2$

(week 8)

5/21 Computer lab (Why  $H_2$  exists and  $H_4$  doesn't)

$H_4$

5/23 Computer lab (Hückel theory)

benzene

cyclooctatetraene

(week 9)

5/28 Holiday

5/30 Comprehensive 9<sup>th</sup> week examination

(week 10)

6/4 Computer lab (Semiempirical methods)

enol & keto forms

6/6 Computer lab (catch up)

## Grading

Each topic has associated homework. Typically this will consist of a few quite challenging problems that illustrate the basic methodology covered in the lecture. These will be graded and weighted heavily into the final grade. (1/3) I expect each problem to be worked out in extensive detail. The number of problems assigned will be relatively small but the grading standard will be very high. Unsatisfactory work will be rejected for reworking until it is judged satisfactory. Homework will not be accepted by e-mail. The goal is to give you the opportunity to thoroughly understand each problem and its solution. (CHEM555 students will sometimes be given longer and more challenging assignments.)

Each computation section will have an associated assignment, a real computation. These will be graded satisfactory/unsatisfactory. A computational assignment returned in satisfactory form on time receives full credit. Unsatisfactory work will be rejected for reworking until it is judged satisfactory. These late results will receive partial credit; 10% will be subtracted for each week late. These computations will account for (1/3) of the final grade. I expect that these calculations will be done carefully and completely. While I will demonstrate some aspects of the use of the software, it is not at all unlikely that you will run into unforeseen complications while performing the computations for the assignments. It is expected that you will dig through the help menus and users' manuals to sort out the trouble. A very important part of learning how to use modeling software is learning how to understand and use the manuals.

One mid-term examination and one “comprehensive 9<sup>th</sup> week examination” (C9WE) will be summed with weights 0.4 & 0.6 respectively to form the final (1/3) of the course grade. If the mid-term is missed for any reason, the grade on the C9WE will also serve as the grade on the mid-term exam. (CHEM555 exams will be longer and more challenging.)

(Overall course grade) = (1/3)\*(HW average) + (1/3)\*(Comp. average) + (1/3)\*(0.4\*MT + 0.6\*C9WE)

Conversion to a letter grade will be according to the Provost's suggested scale. The instructor reserves the right to lower, but not increase, the letter grade thresholds.

Attendance is expected and may influence the final letter grade in borderline cases.

Adherence to university computer usage policy is expected. Violations of this policy will be dealt with the greatest severity allowed under university policy.