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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Class meeting: Tu 19:30-20:50 & Th 18:00-19:20: Korman 111F
Bring a USB drive with all of your files to every class.

In this class, you will be presented with; an introduction to quantum theory that culminates in molecular orbital 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 overall goals of this course are: 1) to develop a basic understanding of quantum mechanics and the role it 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 simple routine calculations, and are able to communicate in an informed way 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. Finally, you will perform real calculations, some "by hand" and some using modeling software. In short, you will do real quantum 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 version of the lecture notes. Don't buy a copy. Do not use one from a past year. The instructor will provide it piecemeal by PDF. 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 chemistry majors. In addition to the chemistry prerequisites, 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 $F = (Q_1Q_2)/(4\pi\varepsilon_0 r^2)$.

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™ and a symbolic algebra program like Maple™ will be required. Further details of the required background can be found in the lecture notes/text.

Course objectives:

It is a specific objective of this course that the student will;

- develop the ability to express physical and chemical phenomena in mathematical language, specifically quantum-chemical phenomena.
- develop an understanding of the concept of a molecular potential energy surface.
- become more familiar with the language of quantum mechanics; including written jargon, as well as mathematical and graphical tools.
- be introduced to the physical and mathematical foundations of the Schrödinger equation.
- become familiar with the "particle-in-a-box" model and its application to several physical systems.
- develop an improved understanding of the mathematical origins of molecular orbitals.
- develop the ability to carry out basic molecular-mechanics and semi-empirical calculations with commercial software, (specifically Hyperchem).
- understand the quantum-mechanical origins of aromaticity.

Academic policies:

For academic policies please use this link:
http://drexel.edu/studentaffairs/community_standards/studentHandbook/

Approximate schedule: (Fall 2013**)**

(week 1)
9/24 Wait! STOP. Don’t use that computer yet!
- Comments on literature searching
- Brief review of simple models. (Lewis structures, VSEPR)
- Boltzmann statistics and molecular conformations.
- comments on chair/skew-boat cyclohexane & anti/gauche dichloroethane

9/26 What is this “molecular mechanics” business?
- Empirical potentials
- PES minimization

(week 2)
10/1 Molecular mechanics calculations with Hyperchem
- Chair and skew-boat cyclohexane
- Anti and gauche butane

10/3 Catch-up

(week 3)
10/8 Exam 1

10/10 What is quantum mechanics good for anyway?
- The ultraviolet catastrophe
- The photoelectric effect
- The Bohr model of the hydrogen atom.

(week 4)
10/15 What is it about waves that gives rise to quantization?
- Vibrations of a string.
- Boundary conditions

10/17 What is the Schrödinger equation and where did it come from?
- Converting the classical Hamiltonian to a quantum one
- Motivation of momentum as a derivative operator
- The free particle

(week 5)
10/22 The classic QM problem: PIB

10/24 Some quantum mechanics without scary equations
- Applications of PIB (conjugated polyenes)
- Applications of the particle on a ring (benzene)

(week 6)
10/29 Catch-up

10/31 Exam 2.

(week 7)
11/5 So where do molecular orbitals come from anyway?
The variational principle
Linear variation functions

11/7 MO theory
MO theory from series expansions (LCAO-MO)

(week 8)
11/12 Why H_2 exists and H_4 doesn't
H_2

11/14 Why H_2 exists and H_4 doesn't
H_4
H_4 with Hyperchem

(week 9)
11/19 Hückel theory
benzene
cyclooctatetraene

11/21 Exam 3

(week 9.5)
11/26 Semiempirical methods, enol & keto forms, ion exchange reactions

(week 10)
12/3 Semiempirical calculations with Hyperchem

12/5 Catch-up

Grading

There will be four components of the overall course grade:

1) Throughout the text there are problems labeled "**Assignment**". These assignments illustrate the basic methodology covered in lecture. You are expected to work **all** of these assignment problems, (unless explicitly told otherwise) on or before a specific date to be announced in class. (A few of the Assignment problems will be required only of CHEM555 students.) Each problem should be worked out in extensive detail. After the due date, the instructor will call upon students to volunteer to present the solutions to these assignment problems in class. Each presentation, if properly done, will earn 2% added to the final course grade. A student may present multiple times, but students who have presented fewer times will have precedence in presenting.

2) There are several special Assignments that require the use of the modeling software Hyperchem. These assignments must be turned in on or before a specific date to be announced in class. Taken together these computations will count for 18% of the course grade. I expect these computations to be done carefully, correctly and completely. While some aspects of the use of the software will be covered in class, 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 software is learning how to understand and use the manuals.

3) Three mid-term examinations will each count for 16% of the course grade.

4) The final exam will count for 34% of the course grade. (Scheduled as per the official university final exam schedule)

The final letter grade for the course will be determined according to the following scale:
90.00-92.99, 93.00-97.99, 98.00-100 are A-, A, A+, respectively.
80.00-82.99, 83.00-86.99, 87.00-89.99 are B-, B, B+, respectively.
70.00-72.99, 73.00-76.99, 77.00-79.99 are C-, C, C+, respectively.
0.00-59.99, 60.00-66.99, 67.00-69.99 are F, D, D+, respectively.
The instructor reserves the right to lower, but not raise, the letter grade thresholds, but in no case will a score of less than 50% result in a passing grade for the class.

Notes:

- CHEM555 exams will be longer and more challenging but allotted the same time.
- In the event of a missed mid-term exam, the final exam will count for 50% of the course grade. A second mid-term missed, for any reason, will receive a zero.
- Late work less than one week overdue will be graded as normal but awarded only 75% of the points earned. Work more than one week late will not be accepted except in cases of a documented emergency life-threatening to the student.
- 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 at the greatest severity allowed under university policy.