CHEM*4880 Winter 2014

This course is all about molecules; the building blocks of much of the world around us (including our own bodies!). The emphasis of this course is on molecular properties – mostly the structure (geometric and electronic) and dynamics of molecules.

Chemistry courses seem to place more and more emphasis on bulk properties of matter and reactivity. This makes sense since these are the properties we can directly observe and which make materials useful. However, less emphasis is being placed on the molecules themselves and how molecular properties, in turn, can influence (or directly determine) these bulk properties.

The best chemists are those who are not just “pot boiler” synthetic chemists or simply those who make routine measurements to characterize a substance, but those who understand molecular structure and how it relates to what they are making or measuring in the lab.

In this course we will look at the 3 main methodologies for the determination of molecular (and electronic) structures and properties: 1) diffraction, 2) quantum chemical calculations and 3) spectroscopy.

An integral part of this course is the use of the Gaussian software to calculate and predict molecular properties.

Tentative evaluation (this will be determined in the 1st class):

Problem Set #1	15%
Test #1	25%
Problem Set #2	15%
Project	20%
Test #2	25%

Tentative Course Outline:

A. Introduction

1. Introduction to molecular structure
2. Introduction to molecular dynamics

B. Computational Chemistry

1. Background (and short review of CHEM*3860)
    a) Variational theory
    b) Perturbation theory
    c) The Hartree-Fock method
2. Basis sets
3. Methods
    a) HF
    b) MP2
    c) CI
    d) DFT
4. Calculations using Gaussian software
    a) Tutorial/Review
    b) Comparison of different basis sets & methods for calculating molecular structure and dynamics
    c) Solvent effects

C. Spectroscopic Methods

1. Rotational spectroscopy and rotational fine-structure
    a) The rigid rotor Hamiltonian
    b) Solving simple structures from rotational spectra
    c) Comparison to computational methods

2. Vibrational Spectroscopy

   a) relationship between molecular structure (symmetry) and vibrational spectroscopy

   b) Rotational fine-structure in vibrational spectra

3. NMR Spectroscopy

   a) The dependence of chemical shifts on molecular and electronic structure.

   b) The dependence of coupling constants on molecular and electronic structure.

   c) The dependence of dipolar and quadrupolar coupling constants on molecular and electronic structure.

   c) Molecular dynamics in liquids and solids.

D. Diffraction Methods

1. Diffraction in Solids

   a) Crystal symmetry and space groups

   b) The x-ray diffraction experiment

   c) Neutron diffraction

   d) Results and comparison with spectroscopic and computational results

2. Gas Phase Diffraction

   a) Electron diffraction in gasses

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(celebrating 10 years without a criminal conviction)