

The University of Ottawa

## CHEMISTRY 3140 Fall 2017

### Introduction to Quantum Chemistry and Molecular Modeling

- Instructor:** Professor Tom Woo  
**Office:** D'Iorio Hall 303 (please knock if the door is shut)  
**Lab:** King Edward 558 2<sup>nd</sup> floor  
**Phone:** (613) 562-5800 ext. 6145  
**E-mail:** [twoo@uottawa.ca](mailto:twoo@uottawa.ca)  
**Office Hours:** email for appointment
- Course Web:** <http://titan.chem.uottawa.ca>  
Go to the teaching section of the website. The 3140 site is password protected.
- Lectures:** Tuesdays 10:00 – 11:30 MNT 103  
Thursday 08:30 – 10:00 LMX 339
- Textbook:** lecture notes will be provided in-class and on-line
- Prerequisites:** Chemistry 2330/2730 or equivalent course with an introduction to quantum mechanics. Please contact Professor Woo as soon as possible if you do not have the prerequisites.
- Exams:**
- one midterm exam, tentatively set for Thur. Nov. 2 (in-class)
  - final exam 3 hours (to be scheduled by the registrar)
- Assignments:** Problem sets will be assigned as the material is covered in lectures. There will be approximately 5 of these. Each is weighted equally unless otherwise stated.
- Grading Scheme:**
- |     |               |
|-----|---------------|
| 30% | assignments   |
| 25% | mid-term exam |
| 45% | final exam    |

The University of Ottawa will not tolerate any act of sexual violence. This includes acts such as rape and sexual harassment, as well as misconduct that take place without consent, which includes cyberbullying. The University, as well as various employee and student groups, offers a variety of services and resources to ensure that all uOttawa community members have access to confidential support and information, and to procedures for reporting an incident or filing a complaint. For more information, please visit <http://www.uOttawa.ca/sexual-violence-support-and-prevention/>.

## TENTATIVE COURSE OUTLINE

Quantum chemistry has made many fundamental contributions to our understanding of chemistry and in particular our concepts of bonding. With the advent of powerful, low cost computers, quantum chemistry has also emerged as a widely used tool in modern chemical research. This course builds upon basic quantum mechanics introduced in earlier courses with the goal of introducing students to modern quantum chemical methods for investigating molecular properties, reaction thermodynamics and reaction mechanisms. Practical, working knowledge of quantum chemical calculations that are typically reported in the current chemical literature will be provided. Assignments in the latter portion of the course will involve performing actual calculations and analysis commonly encountered using a commercial software package.

### 1. Review of Introductory of Quantum Mechanics

The postulates of quantum mechanics are reviewed with an emphasis on how to use them to study specific physical systems of interest. Basic quantum mechanical systems and phenomena will be reviewed such as the harmonic oscillator, zero-point energies, and rotational motion.

### 2. The Hydrogen Atom

The quantum mechanical treatment of a one-electron atom or ion is presented. Energies, quantum numbers, atomic properties, electron densities, spectra and selection rules are discussed.

### 3. Many electron systems

Introduction to approximate methods. The Variational principle. Introduction to electron spin. The Hartree-Fock approximation.

### 4. Practical Introduction to Computational Chemistry

Introduction to modern quantum chemistry methods for calculating molecular properties.

- introduction to the potential energy surface
- ab initio methods
- basis sets
- density functional theory
- molecular properties and analysis of electron distributions