Chemistry 3360

Elementary Quantum Chemistry

Fall 2019

In Chemistry 3360, we will learn the mathematical formalism of quantum mechanics and apply it to chemical problems. In order to master these principles, a good command of mathematics is important.

By its very nature, quantum chemistry implies the use of calculus, complex numbers, operators, vectors, determinants, matrices and differential equations. At the same time most chemistry students do not have this necessary mathematical background. To remedy this, these tools will be introduced in lectures throughout the course. In the lab, students will be introduced to Maple and its use as a tool for mathematics and problem solving. Labs are designed to encourage students to put the mathematical tools to work in solving quantum mechanical problems.

Instructor: Dr. Jennifer van Wijngaarden (she/her)
vanwijng@cc.umanitoba.ca

Office hours: Please set up appointment via email

Website: Go to the UMLearn site for class announcements, lecture slides, assignments.

Texts: ***Quantum Chemistry*** by Ira N. Levine (5th, 6th or 7th edition)
-I put two copies on 7-day reserve in the library, a third can be checked out
- I have other copies available for personal loan

Grading:

Laboratory	**10%**
Midterm	**20%**
Assignments	**30%**
Final Exam	**40%**

The conversion to final letter grades will be as follows:

A+ ≥86%	B+ 72-77%	C+ 60-65%	D 48-55%
A 78-85%	B 66-71%	C 55-59%	F <48%

Schedule of Important Dates:

Lab starts	Sept. 16
Midterm exam	October 21 in lab
Final exam	Scheduled by Registrar

Academic Integrity:
There is zero tolerance for academic offences such as cheating and plagiarism in all aspects of this course! All academic misconduct (including lab offences) will be reported to the Department of Chemistry and the Faculty of Science. For more information, read the Faculty of Science penalties and policies on academic misconduct including the section on **improper collaboration**.
http://umanitoba.ca/faculties/science/undergrad/resources/webdisciplinedocuments.html

Labs:
The lab begins Sept 16 in **350 Parker** with **Dr. Carl Bartels** (bartels@cc.umanitoba.ca).

Please note that the Department is undergoing curriculum changes. Any lab exemptions earned in this course or others in the 2019-2020 academic year will only be honoured for one year and must be used in 2020-2021.

Assignments:
Problem sets will be given every 1-2 weeks during the term to give you a chance to practice material learned in class and to encourage you to keep on top of the material. While you may discuss problems with classmates or with me, the work you hand in must be your own.

The best way to avoid inappropriate collaboration (i.e. a charge of academic misconduct) is to not share written work with classmates. You can ask each other questions, point to examples or equations in textbooks or class notes, etc. but once you show a written solution, you run the risk of your classmate copying your work to closely.

Final Exam:
The final exam will be cumulative and will be based on material presented in the lectures and practiced in the assignments and labs. This is scheduled by the Registrar's office during the final exam period in December.

Course Description:
The first part of the course (September, most of October) will be devoted to solving the Schrödinger equation for 4 model systems: the particle in the box, the harmonic oscillator, the rigid rotor and the hydrogen atom. In the process, we will learn how to solve elementary differential equations, introduce the postulates and operators of quantum mechanics and learn how to use symmetry to simplify quantum mechanical systems.

The latter part of the course will focus on the electronic structure of atoms and molecules which, in contrast to the beginning sections of course, have Schrödinger equations which are not exactly solvable. We will make use of the variational principle, as for example used in the Hartree Fock method, to find approximate solutions in these cases. We will also introduce spin and the resulting antisymmetry nature of electronic wave functions and briefly look at their effects on atoms, as for example the singlet and triplet states of helium. Moving on to molecules, we will separate nuclear motion from electronic motion in the molecular Hamiltonian using the Born Oppenheimer approximation and examine the molecular orbital and valence bond methods for the case of the hydrogen molecule. At the end of the course, time permitting, we will focus on polyatomic molecules applying the semi-empirical Hückel method and molecular symmetry to predict chemical reactivity, via the Woodward-Hoffman rules.

Course Goals:
1. Students will attain a sound understanding of the postulates of quantum mechanics, probability, operators, wave functions and orbitals.
2. Students will gain mathematical tools that will enable them to solve simple eigenvalue problems
3. Students will learn how approximate methods are used to model properties of atoms and molecules