

**CHEM 4010 — Fall 2014**  
**Quantum and Computational Chemistry**

Course Director: René Fournier

Lectures: Friday 14:30 to 17:30 in Ross South 501

Required Text: John P. Lowe and Kirk A. Peterson, *Quantum Chemistry*, 3rd Edition  
(Elsevier Academic Press, New York)

ISBN-13: 978-0-12-457551-6

ISBN-10: 0-12-457551-X

Outline

This course will cover roughly chapters 1 to 11 of Lowe and Peterson (LP). The approach taken is to “learn by doing”. There will be 5 assignments and a fair amount of time will be spent solving or discussing problems in LP. Answers to all the problems are already given in LP, and hints or sketchy solutions are given for some of the problems: your assignments will be to generate *detailed* solutions that show logically, step by step, how to get to the answer. There will also be a mini-project in computational chemistry where you will run electronic structure calculations on a UNIX computer in order to obtain energies of reaction and other properties.

Evaluation:      five assignments:  $30\% = 5 \times 6\%$   
                        computational project: 15%  
                        mid-term: 15%  
                        final exam: 40%

*Assignments will be due* on Fridays: September 26; October 10 and 24; November 7 and 21. The *final exam* will be divided into 3 parts. The *first* part will test basic knowledge with “fill in the blanks” type of questions or simple calculations. The *second* part will have a few problems identical to, or very similar to, problems that were given in assignments throughout the term. The *third* part will have two or three essay-type questions.

Topics we will try to cover:

The time-independent Schrödinger equation. The particle in a box, polyenes. The harmonic oscillator, vibrations of diatomic molecules. The hydrogen atom. Many-electron atoms. Postulates of Quantum Mechanics. The variation method. The Hückel method and  $\pi$  electron systems. Linear algebra and molecular orbital theory. The SCF-MO method. The Kohn-Sham method.

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