CHEM 4010 — Fall 2014
Quantum and Computational Chemistry
Revised course outline, September 25 2014

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). Unfortunately only a few copies of the book are available at the bookstore and additional copies may not arrive until end of October. This forces us to change the way we will do things, in particular, the evaluation. There will be only two assignments, the one I already sent and one more. 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:
two assignments: 20% = 2 × 10%
computational project: 15%
mid-term: 20%
final exam: 45%

Assignments due dates are tentatively: assignment 1: November 7; and assignment 2: November 28. A *short report* on your mini-project will be due Friday December 5. The mid-term will be 50-minutes long and will take place on Friday October 24. Note that Friday October 31 is a co-curricular day, we can not have a test on that day; and Friday November 7 is the deadline for dropping a course without receiving a grade. 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 π electron systems.

Linear algebra and molecular orbital theory. The SCF-MO method. The Kohn-Sham method.

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