Chemistry 462/565
Introduction to Quantum Chemistry/Quantum Chemistry I
Fall Semester 2007 (updated 8/13/07)

Time: Monday, Wednesday, Friday 12:20-1:10 pm
Location: 209 Willard

Professor: John Asbury                        Lasse Jensen
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          (Required for all students)
                        Modern Quantum Chemistry, by Szabo and Ostlund

Course website: http://courses.chem.psu.edu/chem565/

General remarks:
This course is an introduction to quantum mechanics and its applications to the study of
chemical bonding and the structure of simple molecules. Topics to be covered are: (1) an
introduction to the principles of quantum mechanics; (2) approximation methods,
including perturbation theory and the variation method; and (3) applications of these
principles and techniques to chemical bonding. The prerequisite for the course is an
introductory level physical chemistry course for chemistry majors (such as Chemistry
452 at Penn State or the equivalent).

Grading:
  Problem sets 25%
  Paper 10%
  Midterm (evening exam) 25%
  Final (during finals week) 40%

Problem sets:
There will be several problem sets for this course. The only way to learn quantum
mechanics is to do the problems on your own. After you have spent significant time
working on all of the problems independently, you may confer with your classmates or
with Drs Asbury or Jensen. However, you must write up the solutions to the problems on
your own. You may not look at any solutions from previous year’s problem sets. Please
staple your problem sets. There will be both required and optional problems. Solutions
to all problems will be posted on the course website.

In-Class Problems:
There will be in-class problems at the end of each lecture series. The problems will be
written on the board and you as a class will be asked to work on them. Every 5-10
minutes I will ask for advice as to how to proceed with the problem, and I will write a
few steps on the board. This is not meant to be a pressured situation, but rather is meant
to give you practice in problem solving in an interactive environment.
Paper:
You will be required to write a 2-page paper (double-spaced text, including figures and references) on an application of quantum mechanics in the literature. The goal will be to choose a recent paper from the literature and point out the role of quantum mechanics in the research. This is meant to illustrate the usefulness and importance of quantum mechanics in modern research.

Exams:
The midterm and final must be done completely independently.

All Penn State policies (http://www.psu.edu/ufs/policies/) regarding ethics and honorable behavior apply to this course.
Tentative Schedule:

Monday, August 27: First day of class

Friday, August 31: Problem Set 1 due (Lowe, Chapter 1)

Friday, September 7: Problem Set 2 due (Lowe, Chapter 2)

Monday, September 17: Problem Set 3 due (Levine, Chapter 4; Lowe Chapter 3)

Wednesday, September 26: Problem Set 4 due (Lowe, Chapter 4)

Monday, October 8: Problem Set 5 due (Lowe, Chapter 6)

Wednesday, October 10: Midterm (evening), covers Chp 1-4, 6 of Lowe

Monday, October 22: Problem Set 6 due (Lowe, Chapter 5)

Friday, November 2: Paper due

Monday, November 5: Problem Set 7 due (Lowe, Chapter 12, Perturbation Theory)

November 19-23: No Classes (Thanksgiving Break)

Monday, November 26: Problem Set 8 due (Lowe, Chapter 7, Variation Method)

Monday, December 10: Problem Set 9 due (Lowe, Chapter 11, SCF (HF) Method)

Friday, December 15: Last day of class -- review for final

Final exam: TBA