Quantum Chemistry

Chem 3060 - Fall 2010

Lectures: MWF 9:40 – 10:30 am, room 2004 HEB

Instructor: Professor Valeria Molinero, 324 INSCC (Enter through INSCC 305).

Office hours: Monday 2:30 – 4 pm or by appointment (phone 801-585-9618).

If you need to send an email, please do it through the course site in blackboard. If you cannot use blackboard, send it to my account Valeria.Molinero@utah.edu but please write "3060" in the title of any email regarding the course to ensure they will be read and responded.

Discussion TA: Robert DeMille (office hours Thursday 2 – 3 pm; place to be indicated)

Grading TAs: Wan Rang and Peng Zhao (office hours and location to be indicated later)

Secretary: Nodira Kholbaeva Codell, 308 INSCC.

Textbook: *Quantum Chemistry & Spectroscopy* by Thomas Engel (1st edition or 2nd edition by Engel and Reid). Alternatively, you can use *Physical Chemistry* of Engel and Reid, as it includes the contents of the QC&E book plus Thermodynamics.

The course will be organized around Engel's book. You are, however, encouraged to read other books that may help you better understand the topics and provide additional problems for you to practice. *Physical Chemistry: A Molecular Approach* is a very good text that you may find appealing.

Course Organization: Quantum Chemistry is the foundation of modern Chemistry. The course will focus on the fundamental principles of quantum mechanics and their application to models that represent the translational, vibrational, rotational and electronic properties of atoms and molecules. The organization of the course is as follows:

1. Fundamentals of quantum mechanics (Chapters 1 – 8).
2. The quantum mechanics of atoms (Chapters 9-11).
3. Structure and spectroscopic properties of molecules (Chapters 12-15).
4. Computational Chemistry (Chapter 16, if time allows).

The Chapter numbers indicated above refer to the 1st edition of *Quantum Chemistry & Spectroscopy*. The same chapters are found in the *Physical Chemistry* book with different numbers (they will be indicated in class). Equivalent contents are found in other books of Quantum Chemistry.

Discussion sessions: Each student must be registered for a discussion session.

Exams: There will be two mid-term exams and a final exam. Each mid-term is worth 25% of the course grade and the final is comprehensive and worth 35% of the grade. Except in *very* special circumstances, no makeup exams will be given, so you should make every effort to take each exam. If circumstances beyond your control prevent you from attending any of the exams, contact Professor Molinero before the exam period, not after. Bring a calculator (programmable is ok) and several writing implements. You will be given any integrals, or complicated formulae that might be needed, but you will need to remember some of the most important equations (these will be indicated in class). **Use of electronic devices other than calculators are NOT permitted in the exams, and must be turned off and stowed in a backpack or handbag.**

The dates for the midterms will be announced during the course. The exams will be held in class. The final exam will on Friday, December 17, 2010, 8:00 – 10:00 am.

Homework: Homework problems will be assigned every Wednesday, and are due the following Wednesday *in lecture*. Homework will count for 20% of the course grade. No late homework is allowed. A large fraction of the exams will be made up of problems similar to the homework, so if you really understand the homework problems, you will do well on the exams. It is OK to work on assignments in groups; however, each student must turn in an individual copy of the answers with her/his own writing and reasoning.

Computers: P-Chem is a quantitative science and the problems will require computations. Some homework will require using a computer for the calculations and for plotting up the result. We will not require (or teach you how to use) a particular program – you can use a spreadsheet or math program such as Maple/MathCad/MatLab available on computers in HEB 1100 or in the library.

Drops/Withdrawals: Drop deadline: 9/1.Withdraw deadline: 10/22.

Academic dishonesty will result in an automatic failing grade, as well as other sanctions by the University.

From CDS: "The University of Utah seeks to provide equal access to its programs, services and activities for people with disabilities. If you have need of accommodations in the class, reasonable prior notice needs to be given to the Center for Disability Services, 162 Olpin Union Building, 581-5020 (V/TDD). CDS will work with you and the instructor to make arrangements for accommodations. All written information in this course can be made available in alternative formats with the prior notification to the Center for Disability Services."