Chemistry 488: Quantum Chemistry

Spring 2013

MW 11:00-12:15 in Kenan B121

Instructor

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Course Materials

1. “Quantum Chemistry” Levine

2. Time-Dependent Quantum Mechanics and Spectroscopy Lecture Notes
   http://www.mit.edu/~tokmakof/TDQMS/

3. Notes and homework problems will be posted at the CHEM 488 Sakai website

Topics

- Vibrational motions
  - Anharmonic oscillators
  - Coupled harmonic oscillators
- Dynamics of two-level systems
  - Fermi’s Golden Rule
  - Rabi’s formula
- Time correlation functions and linear response theory
- Density matrices and reduced quantum mechanical descriptions
- Applications
  - Light absorption and emission
  - Electron transfer
  - Electronic and/or vibrational energy transfer
  - Internal conversion
  - Scattering of Frenkel excitons
- Additional topics to be decided by interests of students

Preparation and Attendance

Students will be expected to contribute to class discussions and solve problems in groups. Attendance is mandatory.
Software

We will solve problems using numerical methods. Assistance and examples will be given for Matlab. Copies of Matlab are available at the software acquisition office.

http://software.sites.unc.edu/software/

Exams

The dates of two in-class exams will be announced at least one week in advance.

Project

Each student will decide on the topic of a project by February 1. All topics that involve quantum mechanics will be acceptable. The project will involve writing a paper and giving a presentation at the end of the semester. An initial draft of the paper will be due on March 8.

Grade

The distribution of course credit is as follows.

Attendance and homework=30%

Exams=40% (20% each)

Project=30%