Chem 557: Physical Chemistry I

Total Credit: Three

Schedule: Tuesday, 7.30 – 8.50 p.m.; Thursday, 6.00-7.30 p.m.

Location: Disque 307

Lecturer: Reinhard Schweitzer-Stenner; RSchweitzer-Stenner@drexel.edu, Disque Hall 605, phone: 215-895-2268

Textbook: The book is based on multiple textbooks, **e.g. H. Haken and H.C. Wolf.** ***Molecular Physics and Elements of Quantum Chemistry,*** **H. Haken and H.C. Wolf Atom an Quantum Physics (main textbooks).** *McQuarrie, Simon: Physical Chemistry, Demtröder: Laser Spectroscopy,* Engel. *Quantum Chemistry and Spectroscopy. J.A. Shelnutt: Vibronic Spectroscopy.* The books printed in bold will be mostly used for the class. Copies of chapters from the Shelnutt book can be made available by the instructor.

Prior knowledge: I expect that the students have a basic knowledge of what is generally taught in a undergraduate quantum chemistry or spectroscopy class. They should know the Schrödinger equation and its most fundamental applications, including the 'particle in the box' problem and the hydrogen atom. They should know the basic spectroscopy of diatomic molecules. Students lacking this knowledge will have to read extra chapters in traditional physical chemistry textbooks (Atkins, de Paula; Engels). This is a graduate level class.

Course objectives:
Overall objective: Develop an advanced understanding of quantum mechanics and its relevance for the interpretation of spectroscopic data, know and understand its basic concepts.
Acquiring basic knowledge of: Time dependent and independent Schrödinger equation, Heisenberg uncertainty principle, the basic postulates of quantum mechanics, Dirac notation and commutators, time dependent and independent perturbation theory.
Specific skills and application: Student should be able (a) to derive spectroscopic properties of atoms and molecules just based on the knowledge of electron configuration and molecular structure, (b) distinguish spectra of diatomic molecules and interpret them qualitatively and quantitatively; they should have developed a basic understanding of (a) molecular vibrations and the physics behind proton NMR spectra.
General skills: Student should be able (a) to apply the knowledge and understanding acquired in class to research literature and (b) communicate what they learnt orally and in writing, they should have improved their mathematical and abstract thinking

Assignments: Regular home assignments will generally be provided on Wednesday and shall be submitted by 12.00 a.m. on the Friday of the week which follows, if mot indicated otherwise. Additionally, extra homework will be given which might comprise only one or two tasks or problems and which is directly related to the teaching. This will be due within 48 hours. All assignments will be graded and count 50%.

Exams: Besides the final there will be a written midterm, open book exam. The **midterm** is scheduled for **Tuesday, October 27**. It will count for 25% of the grade. Students are allowed to bring along with themselves all types of textbooks and class notes. For the **final exam,** which also counts 25%, students have to give an oral presentation paper on a (research) topic related to class material. A one-page summary of the presentation has to be delivered as well. Students will have ample opportunities in class to obtain extra credit. The final grade will be obtained on the basis of the total score, i.e. 0.5*(assignment points+extra points) + 0.25*mid-term-exam points+0.25*final exam points. I intend to apply the following grading scheme: A+: 98%-100%, A: 85%-97%, A-: 84.%-80%, B+: 77%-79%, B: 65%-76%, B-:60%-64%; C+: 57%-59%, C: 48%-56%, C-: 45%-47%, D+: 42%-54%, D: 35%-41%, D-:30%-34%, F: < 30%. There will be no curving.

Complaints: Complaints about the grading of assignments and exams have to be brought to the attention of the lecturer within 48 hours after their return. All grades are considered final afterwards.

Americans with disabilities act. Students requesting accommodations due to a disability at Drexel University need to present a current Accommodation Verification Letter (AVL) to faculty before accommodations can be made. AVL's are issued by the Office of Disability Resources (ODR). For additional information, visit the ODR website at http://www.drexel.edu/oed/disabilityResources, or contact the Office for more information: 215-895-1401 (V), or disability@drexel.edu.

Academic honesty. Drexel University is committed to a learning environment that embraces academic honesty. In order to protect members of our community from results of dishonest conduct, the University has adopted policies to deal with cases of academic dishonesty. Please read, understand, and follow the academic policies on Academic Dishonesty located at http://www.drexel.edu/provost/policies/academic_dishonesty.asp.).

Add, drop and withdrawl policies

- You can **add** this course until the end of week 2: see http://www.drexel.edu/provost/policies/course_add.asp
- If you add this course after the start of the term, you are responsible for completing ALL work that you may have missed.
- You can **drop** this course until the end of week 2; the course will then be removed from your transcript: see http://www.drexel.edu/provost/policies/course_drop.asp

The course **withdrawal** deadline is November 7. You will have received some graded work prior to this deadline. If you have any questions about your progress at any time of the term, please contact me. If you choose to Withdraw, a "W" will be recorded in your transcript. See http://www.drexel.edu/provost/policies/pdf/course_withdrawal.pdf

Office hour: To comply with Drexel policy I officially offer office hours on Monday from 3.30 through 5.00 p.m. **However, students are urged to see me in my office anytime in the case of any problems and questions**.

Principal philosophy: The course will emphasize conceptual thinking instead of memorizing. Students shall be prepared to employ concepts introduced in class to a variety of problems. Exams will frequently contain question, which check the understanding of the subject. It is assumed that the participating students have a solid working knowledge of pre-calculus, calculus, linear algebra, complex numbers, vector analysis and elementary statistics. The lecturer will be ready to work on mathematical deficiencies, if this is necessary, but there will be no compromise with regard to the level to the teaching. In order to complete this class successfully, students have to work on the class material on a weekly basis**. This includes additional reading as indicated below.**

Behavior in class: Students are asked to appear on time for the class and to switch off their cellular phones. Cheating will lead to an F for the entire course and to serious consequences for the student's standing in the program. I am encouraging discussions, but not chattering while I am lecturing.

Syllabus

References is made to related chapters in textbooks. However, some of the chapters go beyond the respective contents of this book.

1. The fundamentals of quantum mechanics (Haken, Wolf; Atomic Physics: Chapters 9 and 10; Haken, Wolf: Molecular Physics: Chapter 10; McQuarrie: Chapter 4; Shelnutt, chapter1; week 1 and week 2, in part)

- Schrödinger equations as eigenvalue problem
- Operators, expectation values, orthonormality, Dirac notation
- Remembering examples: harmonic oscillator, rigid rotor and hydrogen atom
- Variation method
- Time independent perturbation theory
- Solving the coupled oscillator problem

2. **Interactions between matter and light (Haken, Wolf: Molecular Physics, Chapter 16; Demtröder, chapter3; Shelnutt, chapter 2 and 3, week 2, in part and 3)**
    - Absorption and emission, Einstein coefficients
    - Lorentzian, Gaussian and Voigtian profiles
    - Some basics of classical theoretical physics
    - Time dependent perturbation theory
    - The Hamilton operator for molecules in a radiation field
    - Sketching the evaluation of the interaction operator
    - Fermi's Golden Rule
    - Selection rules

3. **Atomic spectra of multi-electron systems (Haken, Wolf: Atomic Physics, Chapters 11-14, week 4 and in part 5)**
    - Helium atom
    - LS-coupling
    - Normal Zeeman effect
    - Anormal Zeeman effect
    - Stark effect
    - EPR-spectroscopy

4. **Molecular spectra (Haken, Wolf: Molecular Physics; Chapters 9-12, McQuarrie, Shelnutt, chapter 4 and 5, week 5 in part, week 6, week 7, week 8 in part)**
    - Born-Oppenheimer approximation
    - Remembering vibrational-rotational spectra of diatomic molecules
    - Vibrations of polyatomic molecules
    - IR and Raman spectroscopy
    - Selection rules and group theory
    - Electronic and vibronic transitions

- Resonance Raman scattering
- Fluorescence
- Circular dichroism spectroscopy

5. **Modern Spectroscopies (Haken, Wolf: Molecular Physics, Chapters 15 and 17, week 9, part 10)**

   - Two-photon spectroscopy
   - Photoelectron spectroscopy
   - Ultrashort pulse spectroscopy
   - Coherent AntiStokes Raman spectroscopy

6. **Nuclear Magnetic Resonance Spectroscopy (Haken, Wolf, Molecular Physics, Chapter 18, pat 10, week 11)**
   - Fundamentals
   - Proton resonances
   - Relaxation times
   - Non-proton resonance
   - Two-dimensional nuclear resonance