<u>Chem 557: Physical Chemistry I</u>

Total Credit: Three

Schedule: Tuesday 6.00 – 7.20 p.m., Thursday 7.00 – 9.50 p.m.

Lecturer: Reinhard Schweitzer-Stenner; RSchweitzer-Stenner@drexel.edu, Disque Hall 307, phone: 215-895-2268

Textbook: The book is based on multiple textbooks, **e.g.** ***McQuarrie/Simon: Physical Chemistry (main textbook),*** H. Haken and H.C. Wolf. *Molecular Physics and Elements of Quantum Chemistry, W. 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 spectroscopy of diatomic molecules. Students lacking this knowledge will have to read extra chapters in traditional physical chemistry textbooks (Atkins, de Paula). This is a graduate level class.

Course objectives: Develop an advanced understanding of quantum mechanics, know and understand its basic concepts: particle-wave duality, Schrödinger equation, Heisenberg uncertainty principle, the basic postulates of quantum mechanics, Hilbert space, Dirac notation and commutators. With regard to spectroscopy students should understand (a) the physics of multi-electron systems, (b) the behavior of atoms and molecules in electric and magnetic field, (c) the basic formalism describing the interaction between light and matter and (d) the fundamentals of vibrational and electronic spectroscopy of polyatomic molecules.

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. Additionally, extra home work 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 **Monday, February 11**. 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. 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%.

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.

Drop out: According to Drexel University policy, students are allowed to drop courses until the last day of the sixth week.

Office hour: To comply with Drexel policy I officially offer office hours on Monday from 4.30 through 6.00 p.m. **However, students are urged to see me in my office 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. 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 the McQuarrie/Simon textbook. However, some of the chapters go beyond the respective contents of this book.

1. The fundamentals of quantum mechanics (McQuarrie, Chapter 4, Shelnutt, chapter1, students should know the content of chapters 1-3 of McQuarrie, week 1 and 2)

- State system
- Operators, observables, eigenvalues and expectation values
- Time dependent Schrödinger equation
- The Hilbert space
- The Dirac notation

Selfstudy: Chapter 5 and 6 of McQuarrie

2. Approximation methods (McQuarrie, chapter 7, Shelnutt, chapter 3, week 3 and 4)

- The Variation method
- Time independent perturbation theory and its application to an anharmonic oscillator
- Time dependent perturbation theory

3. **Electronic states of many electron systems (McQuarrie/Simon, chapter 8, and additional literature given in class, weeks 5 and 6)**

- The He-atom
- Hartree equation
- Pauli-principle and antisymmetrization of wavefunctions
- Magnetic field effects (Zeeman effect)
- Hund's rule
- Electronic states and transitions in metal complexes

4. Interactions between matter and light (Demtröder, chapter3; Shelnutt, chapter 2 and 3, additional material will be provided, weeks 7 and 8)

- Absorption and emission
- Lorentzian, Gaussian and Voigtian profiles
- Some basics of classical theoretical physics
- The Hamilton operator for molecules in a radiation field
- Sketching the evaluation of the interaction operator
- Fermi's Golden Rule
- The density operator approach

5. **Molecular spectroscopy (McQuarrie, chapter 13; Shelnutt, chapter 4 and 5, Chapter 1, weeks 9 and 10)**
    - The Born-Oppenheimer approximation
    - Vibrations of polyatomic molecules
    - Resonance Raman and fluorescence spectroscopy of chromophores
    - Circular dichroism spectroscopy
    - IR-femtosecond spectroscopy

6. **Laser spectroscopy (McQuarrie, chapter 15, week 11, if time allows)**
    - Transition in two- and three-level systems
    - Laser optics
    - The He-Ne laser
    - Pulsed laser spectroscopy