Chem 557: Physical Chemistry I

Total Credits: 3

Schedule: Aday 6:00 – 7:20 p.m., Bday 7:30 – 8:50 p.m.

Lecturer: Reinhard Schweitzer-Stenner; RSchweitzer-Stenner@drexel.edu, Disqué Hall 218, phone: 215-895-2268

Textbook: *Peter Atkins and Julio de Paula, Physical Chemistry, 7th edition (an earlier edition is also o.k.) Chapter 11-18, or corresponding chapters in similar textbooks.*

Assignments: 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. The assignments will be graded and count 50%.

Exams: Besides the final there will be a written midterm, open book exam. It will count for 25% of the grade. Students are allowed to bring along with themselves all types of textbooks and class notes. The final exam also counts 25%. It will be organized as a mini-symposium with presentations from students, which will be graded. These presentations will mostly be based on research papers. The final grade will be obtained on the basis of the total score, i.e. 0.5*assignment points + 0.25*mid-term-exam points+0.25*final exam points. Students will have ample evidence in class to obtain extra credit.

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 Thursday 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 and elementary statistics. The lecturer will be ready to work on mathematical deficiencies, if this is necessary.

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. I am encouraging discussions, but not chattering while I am lecturing.

Syllabus

1. Elementary quantum mechanics

- Wave-particle duality, theory and experiment
- Heisenberg uncertainty principle
- Time independent and time-dependent Schrödinger equation
- Operators and observables
- Quantum theory of rotation
- Quantum theory of vibration
- Perturbation theory

2. Absorption and emission of light

- Absorption
- Spontaneous and induced emission
- Black body radiation
- Linewidths
- Coherent light
- Lasers

3. Atomic structure and spectra

- A single electron in a Coulomb field
- Electronic states of many electron atoms
- Spectra of many electron atoms
- The Zeeman and Paschen-Back effect
- Hyperfine structure
- EPR spectroscopy

4. Molecular structure

- Born-Oppenheimer approximation
- Valence bond theory
- Molecular orbital theory

5. Elementary group theory

- Symmetry elements
- Point groups
- Irreducible representations and character tables

6. Rotational and vibrational spectra

- Pure rotational spectra
- Harmonic and anharmonic vibrations
- Rotational-vibrational spectra of diatomic molecules
- Techniques of vibrational spectroscopy

7. **Electronic transitions**
    - Franck-Condon principle
    - Coupling of electronic and vibrational transitions
    - absorption, fluorescence and phosphorescence
    - resonance Raman spectroscopy
    - photoelectron spectroscopy
    - ultrafast spctroscopy

8. **Nuclear spectroscopy**
    - NMR I: Basics
    - NMR II: Pulse techniques
    - Mössbauer spectroscopy