Syllabus for Chem 359: Atomic and Molecular Spectroscopy

Instructors: Dr. Reinhard Schweitzer-Stenner and Ms. Siobhan E. Toal
Office: Disque 605/Disque 306
Tel: (215) 895-2268
Email: rschweitzer-stenner@drexel.edu and st478@drexel.edu
Office hours: Monday, 4.00---6.30 p.m. in Disque 605.

Total Credit: 3

Schedule: Monday, Wednesday and Friday, 9.00-9.50 a.m., room: to be determined

Student Learning Information

A. Course Description and Calendar

Since students enrolled in this class have to take Chem 355, it is assumed that they know the basics of quantum mechanics such a particle-wave duality, de Broglie relation and Schrödinger equation. The course emphasizes the basic concepts of atomic and molecular spectroscopy

1. **Principles of Quantum Mechanics (R. Schweitzer-Stenner, week 1).** Teaching in class covers the chapters 2,3 and 6 of Engels, Quantum Chemistry and Spectroscopy. In addition, students have to read chapters 1 and 4, which will not be explicitly covered in class.
   - Schrödinger equation
   - General properties of quantum mechanical wavefunctions
   - Operators, observables, eigenfunctions and eigenvalues
   - Expectation values
   - Time dependent Schrödinger equations
   - The Stern-Gerlach experiment
   - Heisenberg Uncertainty Principle

2. **Particle in the Box in the real world (Siobhan E. Toal, week 2).** The teaching covers chapter 5 of Engels, Quantum Chemistry and Spectroscopy and additional reading assignment provided by the instructor.
   - Particle in the Finite Depth Box
   - π-electrons in conjugated molecules
   - Conductors and insulators
   - Quantum mechanical tunneling
   - Scanning tunneling and atomic force microscopes
   - Quantum wells and dots

3. **Rotation and Vibration of Molecules (Siobhan E. Toal, 2nd and 3rd week).** The teaching covers chapter 7 and 8 of Engel, Quantum Chemistry and Spectroscopy.

- Classical descriptions
- The quantum mechanical oscillator
- Quantum mechanical rotation
- Quantization of angular momentum (operators, eigenfunctions, eigenvalues and commutation rules)
- Vibrational and Rotational Spectroscopy
- Raman spectroscopy

4. **Absorption and Emission of Light (Reinhard Schweitzer-Stenner, 4th week).** The teaching covers part of chapter 3 of Demtröder, Laser Spectroscopy. (The chapter can be provided by the instructor on request).

- Absorption, induced and spontaneous emission
- Lorentzian profiles
- Doppler broadening, Gaussian and Voigtian profiles

5. **The Hydrogen Atom (Siobhan, E. Toal, 4th week).** The teaching covers chapter 9 of Engel, Quantum Mechanics and Spectroscopy.

- Schrödinger equation
- Eigenfunctions and Eigenvalues
- Hydrogen atom orbitals
- Radial probability distribution function
- The shell model of atoms

6. **Many electron atoms (Reinhard Schweitzer-Stenner, 5th week).** The teaching covers chapter 10 of Engel, Quantum Mechanics and Spectroscopy and additional information about He-spectra.

- First approach for helium
- The influence of the spin on the molecular eigenfunctions and eigenstates of He.
- Helium spectra
- A brief description of Hartree-Fock methods

Midterm exam at the beginning of the sixth week

7. **Atoms in magnetic fields (Siobhan E. Toal, 6 th and 7th week).** The teaching covers part of chapter 11 of Engel, Quantum Mechanics and Spectroscopy as well as part of Chapters 11 and 12 of Haken, Wolf: The Physics of Atoms and Quanta.

- The normal Zeeman effect
- Spin-orbit coupling in alkali atoms
- The anomalous Zeeman effect

- Russel-Saunders coupling and jj-coupling in many-electron atoms
- Microstates and eigenstates
- NMR and EPR spectroscopy

8. **Atom and Electronspectroscopy and applications (Reinhard Schweitzer-Stenner, 8th week).** The teaching covers the 2nd part of chapter 11 of Engel, Quantum Chemistry and Spectroscopy.

   - Helium neon laser
   - Laser isotope separation
   - Auger and X-ray photoelectron spectroscopy

9. **Molecular Structure and Electronic States (Siobhan E. Toal, 8th and 9th week).** The teaching covers the chapter 13 of Engel, Quantum Chemistry and Spectroscopy. Students are expected to read chapter 12 in addition.

   - Hybridization and wavefunctions
   - Molecular orbital theory
   - Hückel theory of aromatic molecules
   - Semiconductors

10. **Electronic Spectroscopy (Reinhard Schweitzer-Stenner, 9th and 10th week).** The teaching covers the chapter 14 of Engel, Quantum Chemistry and Spectroscopy.

    - Energy of electronic transitions
    - Electronic states of diatomic molecules
    - Vibrational fine structure and vibronic coupling
    - UV - absorption
    - Fluorescence

11. **Group theory (Siobhan Toal, 10th week)** The teaching covers part of chapter 15 of Quantum Chemistry and Spectroscopy.

    - Symmetry elements, operations and point groups
    - Molecules and point groups
    - Representations
    - Symmetries of molecular orbitals
    - Symmetries of normal modes of molecules
    - Selection rules

B. Purpose of course

The overall goal of this course is to show how basic concepts of quantum mechanics can be utilized to quantitatively explain atomic and molecular spectra. Students should learn that spectroscopic data cannot be understood without quantum mechanics.

C. Statement of expected learning

After completing this course, the students should have learned:

- how atoms and molecules absorb and emit light and how this process can be affected by magnetic and electric fields,
- how to describe the electronic state of atoms in terms of quantum numbers,
- the complexity of atomic spectra due to spin-orbit coupling and the interpretation of term symbols,
- the contributions of transitions between rotational, vibrational and electronic states to the spectra of diatomic molecules, vibrations and electronic structure of polyatomic molecules,
- basic spectroscopic techniques (absorption, fluorescence, Raman, EPR, NMR).

Course Material

Textbook: The course is predominantly based on Engel, Quantum Chemistry & Spectroscopy, Pearson 2013. The chapters of this book can also be found in the Physical Chemistry textbook of Engel and Ried. Students must have one of these textbooks. Additional material: Demtröder, Laser Spectroscopy (Springer) and Haken, Wolf, The Physics of Atoms and Quanta, Springer

Assessment of student performance

Assignments: 3-4 home assignments will be provided. All assignments will be graded and the total grade will count for 35% of the final grade. Homework assignments will access the capability of students to apply learned concepts to a quantum mechanics bases analysis of atoms, molecules and their respective spectra.

Quizes: Students have to prepare for the class by reading the corresponding chapters of Engel, Quantum Chemistry and Spectroscopy as well as additional chapters mentioned in the syllabus. Instructors can assign additional readings. The preparation will be checked will sporadic quizzes

Exams:

A *midterm, open book exam* will be given during the sixth week of the class. The content will cover chapters 1-6 of the class. This exam checks the capability of students to use class material for the solution of relatively simple problems under exam conditions. One or two of the problems will check the students' capabilities to describe learnt course content with their own words (mini-essay). The midterm exam will count for 25% of the final grade.

A *final, oral exam* will be conducted during the finals week by both instructors. Each student will see the instructors jointly for approximately 30 minutes. This exam, which counts for 25% of the final grade, will assess the understanding of basic concepts and the capability of students to describe them orally.

Extra points;

Students can earn extra points in class by solving short problems given by the instructor. This strategy helps the instructors to check the understanding of students right after a subject has been taught.

Grade scale

The final grade will be obtained on the basis of the total score, i.e. 0.35*(assignment points +extra points) + 0.25*mid-term-exam points + 0.25*final exam points + 0.15*(points on quizzes). We intend to apply the following grading scheme: A+: 98%-100%, A: 88%-97%, A-:85.%-87%, B+:
82%-84%, B: 73%-81%, B-:70%-72%; C+: 67%-69%, C: 58%-66%, C-:55%-57%, D+: 52%-54%, D: 43%-51%, D-:40%-32%, F: < 40%.

Academic policies

Complaints: Complaints about the grading of assignments and exams have to be brought to the attention of the lecturers 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. Students will be informed about their midterm grades on the wednesday after the exam.

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. It is assumed that the participating students have a solid working knowledge of pre-calculus, calculus, linear algebra, vector analysis and basic quantum mechanics.

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. The student will be reported to the office of student conduct. I am encouraging discussions, but not chattering while I am lecturing. Students are expected to show up on time and leave at the end of the lecture. Class attendance will not be checked, but everybody should be assured that it is practically impossible to obtain an above average grade (A or B) or even finish the class with a passing grade, if one does not attend class.