CHEM 348
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2017

# CHEM 348 – Physical Chemistry
# Spring 2017 Syllabus

**Instructor:** Fabien Goulay, CRL 465, Fagoulay@mail.wvu.edu

**Lecture:** CHEM348 Section 001, 3 credit hours

Pre-requisite: CHEM 346 and MATH 251. Continuation of CHEM 346

Lectures will be held on Monday, Wednesday and Friday between 9:30 am –10:20 am in Clark Hall, Room 317.

**Office Hours (CRL 465):**

Monday 10:30 am-11:30 am
Wednesday 10:30 am -11:30 am
Friday 10:30 am -11:30 am
Students unable to meet at these times due to schedule conflicts should make an appointment (via email) if a meeting is desired. Drop-ins may or may not be accommodated.

**Description of the class:** In this class we will describe the basic principles of physical chemistry, quantum mechanics, and molecular collision to understand, analyze, and predict the spectra and reactivity of molecules.

**Learning objectives:** The objectives of the course are to:

- Understand the limitations of classical mechanics that led to the development of quantum mechanics.
- Apply the postulates of quantum mechanics to 1D, 2D, and 3D motions of particles. Use the result to predict the absorption wavelength of simple unsaturated molecules.
- Write the Schrodinger equation for a particle travelling through a potential barrier and use the boundary conditions to infer the wavefunction. Calculate the transmission probability.
- Calculate the standard deviation of a measurement. Apply the Heisenberg uncertainty principle to simple translational motions.
- Have a basic knowledge of the technics of approximation used in quantum chemistry.
- Write the Schrodinger equation for the hydrogen atom, separate the variables and solve the angular part of the wavefunction.
- Draw the orbitals and probability densities of the hydrogen atoms.
- Write the Schrodinger equation for a multi electron atom.
- Understand the orbital approximation and give the Slater determinant for small atoms.
- Calculate the first ionization energy of atoms.
- Give all the atomic term symbols associated with an atomic configuration (non-equivalent electrons).
- Draw the energy diagram and emission/absorption spectrum of atomic transitions.
- Write the Schrodinger equation for rotational and vibrational motions of molecules.
- Analyze the rotational and vibrational spectra and infer molecular properties.
- Draw the molecular energy diagram of diatomic molecules.
- Give the ground electronic state configuration and bond order.
- Have basic knowledge of the kinetic theory of gases.

**Learning outcomes:** After completing the course, the student will grasp the fundamental principles of quantum mechanics and be able to apply them to understand and predict the structure of atoms and diatomic molecules. The students will also be able to interpret the rotational and vibrational spectrum of diatomic molecules and infer molecular properties.

**Textbooks**

*Physical Chemistry* by P. W. Atkins et al., tenth Edition (Required)

and

*Solution manual for physical chemistry* by P. W. Atkins, et al. (Recommended)

**Additional resources**

Additional information may be found in the following books (NOT REQUIRED):

-*Quantum Chemistry and Spectroscopy* by T. Engel, 2nd Edition.

-*Quantum chemistry* by D. A. McQuarrie, 2nd edition, University Science Books.

-*Modern Spectroscopy* by J. M. Hollas, 4nd edition (Wiley, 2009).

-*Chemical Kinetics and Reaction Dynamics* by P. L. Houston, Dover Publication.

**Pre-requisite:** You are expected to review the most relevant topics from mathematics before proceeding to quantum chemistry and its applications. Refer to the textbook for important Mathematical background.

Differentiation and integration..... *Mathematical background 1 p 59*

Multivariable calculus..... *Mathematical background 2 p 109*

Complex numbers ..... *Mathematical background 3 p 314*

Differential equations ..... *Mathematical background 4 p 354*

Matrices ..... *Mathematical background 6 p 443*

Additional information can be found in "*Mathematics for Physical Chemistry*" D. A. McQuarrie, University Science Books.

**Grading**

Grades are based on performance assessments that reflect achievement of learning outcomes outlined for this course.

***Grade Formulation:***

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|---|---|
| Homework (7) | 350 points |
| Exams (2) | 400 points |
| Final Exam (1) | 250 points |

The exams account for 40.0%, the final accounts for 25.0%, the homework assignments for 35.0% of the total grade. 100 (10%) extra credit points will be distributed among the homework assignments and exams.

**Important dates:**

| | | | |
|---|---|---|---|
| **01/9** | **First day of class** | 03/31 | Due date Homework 6 |
| 01/16 | *MLK day-no class* | 04/07 | Exam 2 |
| 01/17 | Due date Homework 1 | 04/14 | *Easter Friday no class* |
| 01/27 | Due date Homework 2 | 04/21 | Due date Homework 7 |
| 02/10 | Due date Homework 3 | 04/28 | Last day of class |
| 02/17 | Exam1 | 05/01-05/05 | Final Exam Week |
| 03/03 | Due date Homework 4 | **05/02** | **Final Exam 2:00pm to 4:00pm** |
| *03/4-03/12* | *Spring break* | | |
| 03/17 | Due date Homework 5 | | |

| **Tentative Course Outline** | ***Chapters in book*** |
|---|---|
| **Part A Fundamentals of Quantum Chemistry** | |
| Chapter 0 Science at the end of the 19th century | Reviews |
| Chapter 1 From classical to quantum | 7A |
| 1.1 The black body radiation | |
| 1.2 The photoelectric effect | |
| 1.3 Atomic spectra and the Bohr model of the atom | |
| 1.4 Particle wave | |
| 1.5 Classical vs. quantum mechanics | |
| Chapter 2 Quantum mechanical postulates | 7B, 7C.1(a), (b), 7C.2, 7C.4 |
| 2.0 Definition of a postulate | |
| 2.1 The physical meaning of the wave function | |
| 2.2 Every observable has a corresponding operator | |
| 2.3 The result of an individual measurement | |
| 2.4 The expectation value | |
| 2.5 The time evolution of a quantum mechanical system | |
| Chapter 3 The Schrodinger equation and its solutions | 7B.1, 8A |
| 3.1 Time dependent and time independent equations | |
| 3.2 Solving the Schrodinger equation | |
| 3.3 Properties of quantum mechanical eigenfunctions | |
| 3.4 The particle in a box | |
| 3.5 Tunnelling | |
| Chapter 4 Operators in quantum chemistry | 7C.1(c), (d), 7C.3 |
| 4.1 Some properties of quantum operators | |
| 4.2 Commuting operators | |
| 4.3 The uncertainty principle | |
| Chapter 5 Techniques of approximation | 10D.2 |
| 5.1 Variation theory | |
| 5.2 Perturbation theory | |
| **Part B Atomic and Molecular Structures** | |
| Chapter 1 The hydrogen atom | 9A, 8.C |
| 1.0 Spherical coordinates | |
| 1.1 The Schrodinger equation for the one-electron atom | |
| 1.2 Eigenvalues and eigenfunctions of the H atom | |
| 1.3 The hydrogen atom orbitals | |
| 1.4 The electron spin | |
| Chapter 2 Many electron atoms | 9B |
| 2.1 The orbital approximation | |
| 2.2 The Pauli principle | |
| 2.3 Trends in the periodic table | |
| 2.4 Atomic term symbols | |
| Chapter 3 Introduction to spectroscopy | |
| 3.1 Time dependent perturbation theory | |
| 3.2 Spectroscopic selection rules | |
| 3.3 Application to atomic spectroscopy | |
| Chapter 4 Vibration and rotation of molecules | 8B, 8C, 12B, 12C, 12D |
| 4.2 Pure rotational spectroscopy of linear molecules | |
| 4.3 The harmonic oscillator | |
| 4.4 Rovibrational spectroscopy of diatomic molecules | |
| Chapter 5 Molecular orbital theory | 10B, 10C, 10D |
| 5.1 Variation theory and orbital overlap | |
| 5.2 Molecular energy diagram of diatomic molecules | |
| 5.3 Rovibronic spectroscopy of diatomic molecules | |
| **Part C Molecular Dynamics** | |
| Chapter 1 Kinetic theory of gasses | 1B |
| 1.1 Pressure and energy of an ideal gas | |
| 1.2 The Maxwell distribution of speeds | |
| 1.3 Mean free path and collision number | |
| Chapter 2 Reactive collisions | 21A |
| 2.1 The thermal reaction rate | |
| 2.2 Reaction with an activation energy | |

**Lecture:** It is important that you take notes during lecture, which are legible and organized. Your notes will become your most important study material for the examinations. **You must review your notes before the next class**, this will prevent you from being "lost" during the lecture period. Read the textbook assignments after the class period for which they are assigned.

**Homework assignments:** Students will be given several homework assignments during the semester. They will be assigned at least one week before the due date. In order to receive credit, students must provide full detail, including unit analysis, mathematical derivation, and insightful justification unless otherwise noted. Carry units through your work and clearly indicate your result in a box. Illegible work will be given a score of 0 %. Material covered on these assignments may differ from the lecture in order to encourage critical thinking and problem solving skills. Turn in your assignments stapled and clearly labeled with your name and problem numbers. On due dates, the problem sets can be turned in during class or placed in my mailbox (Clark 217 or CRL 465) by the end of the day (5 PM). Late homework assignments will not be accepted.

**Exams:** Two 50-min exams will be given during the term. A variety of problems will be included on each exam. Material covered on the exams will be taken mainly from the lecture and assigned problems.

**Final Examination:** The final examination will be comprehensive and cumulative, covering the entire course. Your study during the semester should be designed for comprehensive and long-term retention of the factual material, principles, and their application.

**Make-up Policy:** Absences/makeups will be dealt with on an individual basis. Please contact the instructor as soon as possible. No make-up exams will be given after the test has been discussed in class. Homework assignments are due on the specified date. Extensions will be given for appropriately excused absences as outlined above.

**Attendance:** Attendance is mandatory for CHEM 348.

**Syllabus Statements**

***Social Justice Syllabus Statement:*** West Virginia University is committed to social justice. I concur with that commitment and expect to foster a nurturing learning environment based upon open communication, mutual respect, and non-discrimination. Our University does not discriminate on the basis of race, sex, age, disability, veteran status, religion, sexual orientation, color or national origin. Any suggestions as to how to further such a positive and open environment in this class will be appreciated and given serious consideration. If you are a person with a disability and anticipate needing any type of accommodation in order to participate in this class, please advise me and make appropriate arrangements with Disability Services (293-6700).

***Syllabus Statement on Days of Special Concern:*** WVU recognizes the diversity of its students and the needs of those who wish to be absent from class to participate in Days of Special Concern, which are listed in the Schedule of Courses. Students should notify their instructors by the end of the second week of classes or prior to the first Day of Special Concern, whichever is earlier, regarding Day of Special Concern observances that will affect their attendance. Further, students must abide by the attendance policy of their instructors as stated on their syllabi. Faculty will make reasonable accommodation for tests or field trips that a student misses as a result of observing a Day of Special Concern.

***Students withdrawing from courses:*** Students may withdraw from courses without a W being placed on their record through the end of the first week of the semester. They may withdraw with a W from the end of the first week through the end of the 10th week of the semester. Students must withdraw from courses themselves through the STAR system.