

Physical Chemistry II (CHEM 302)

Spring 2018

Lecture: Tue, Th 10:00 - 11:15 AM, Cuneo Hall 203

Discussion: We 8:15 – 9:05 AM, Flanner Hall 105

Instructor: Jan Florián

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Office Hours: Tue 11:15 – 11:45 AM, 1:00 – 2:30 PM

Course Objectives

Part 1: Introduction to Applied Quantum Mechanics

1. Understand the basic concepts of quantum mechanics and underlying mathematics
2. Apply quantum mechanics to the study of model systems and electronic structure of atoms

Part 2: The Chemical Bond

3. Apply quantum mechanics to the study of molecular structure

Part 3: Foundations of Chemical Spectroscopy

4. Understand how light interacts with matter on the molecular level
5. Understand the relationship between quantum mechanics and spectroscopy.

Required Materials:

Physical Chemistry, Atkins & De Paula, W.H. Freeman, 10th Edition

A simple calculator (i.e. calculator not capable of being programmed or drawing graphs)

Grade components	Maximum number of grading points
Homework&quiz	20
Exam 1	20
Exam 2	20
Final exam	40
Total	100 grading points

Homeworks: Homework assignments, each worth two or three grading points will be assigned on Thursdays. To receive full credit, a student's homework has to be submitted in person at the beginning of the next lecture. Each homework must present meaningful steps to solving assigned problems. Incorrect, late, or less than 1/2 completed homework assignments will receive zero points. Students may compare and discuss their homework solutions, but each solution has to be arrived at independently.

Quiz: A short in-class exam (worth four grading points) will be assigned early in the semester to test the knowledge of introductory quantum mechanics covered in Physical Chemistry I.

Exams: Two 70 minute mid-semester exams and one 120 minute final exam will be cumulative. No make-up exams will be administered for mid-semester exams. Students who miss a mid-semester exam for a valid reason will have the grading-point value of the final exam increased by 20 points. For the absence to be classified as having valid reason, students must notify the instructor about their absence before the exam and provide valid excuse (e.g. a doctor's note) that covers the exam day. The doctor's note must be signed and contain legible name, hospital/office address and phone number and the reason for the absence. If the student disagrees with her/his score for the exam, she/he must request re-grading within one week from the day he/she received the graded exam. The exam questions may originate from end-of-chapter problems, homeworks, solved exercises from the textbook, problems solved during lecture&discussion (and their variations). Exams may also contain derivations or essays on topics presented during the lecture. Grading of all exams will include partial positive or negative credit for all significant steps taken to arrive to the final answer. Answers containing only the correct final answer without solution leading to this answer will receive a 70% grading penalty. Only non-programmable scientific calculators (e.g. TI-30XA) will be allowed during exams. Students must follow the seating assignments.

Class preparation: In order to understand the material presented during lectures and discussions, it is important to come to the class with good background knowledge. This can be achieved by reading (and thinking about) material in the textbook, reviewing appropriate material from calculus, physics and general chemistry classes, and solving end-of-chapter problems.

Work together with your classmates; if you don't understand something, someone else may. You will also find that explaining a solution to your classmate will improve your understanding and long-term retention of the material. It is recommended that students devote to the preparation for this class a minimum of two hours every day.

Letter grades for the class will be calculated using both a fixed scale and a Gaussian scale. The scale that yields a better letter grade will determine your final letter grade.

Fixed scale

A = 100 – 80 grading points; A⁻ = 80 - 75; B⁺ = 75 - 70; B = 70 - 65; B⁻ = 65 - 60; C⁺ = 60 - 55; C = 55 - 50; C⁻ = 50 - 45; D⁺ = 45 - 40; D = 40 - 35; F = Less than 35 grading points.

Gaussian scale (M denotes a class average, and σ denotes standard deviation):

Earned Grading Points	Letter Grade	Earned Grading Points	Letter Grade
M – 0.2 σ to M + 0.2 σ	C+	M – 0.5 σ to M – 0.2 σ	C+
M + 0.2 σ to M + 0.5 σ	B-	M – 0.8 σ to M – 0.5 σ	C-
M + 0.5 σ to M + 0.8 σ	B	M – 1.1 σ to M – 0.8 σ	D+
M + 0.8 σ to M + 1.1 σ	B+	M – 1.4 σ to M – 1.1 σ	D
M + 1.1 σ to M + 1.4 σ	A-	less than (M – 1.4 σ)	F
More than (M + 1.4 σ)	A		

Midterm grade: Your midterm grading points will be based on midterm exam(s) (0.75 weight) and homeworks&quiz (0.25 weight).

Ethical Considerations: *Students will not collaborate on any exams or quizzes. Only those materials and devices permitted by the instructor may be used to assist in examinations. Students will not represent the work of others as their own. Any student caught cheating during an exam will be reported to the Deans office and will receive zero points for the given exam.*

Tentative Schedule

Date	Lecture topics	Reading
16,18-Jan	Energy versus free-energy differences, Coulomb law, Golden rule of spectroscopy, Boltzmann law, QM formalism	Chapter 7
23, 25-Jan	Particle in a 1-D box (Quiz), Tunneling, Particle in a 2-D and 3-D box,	Chapter 8A
30-Jan,1-Feb	Electronic spectroscopy with applications to the π -electron model, Beer-Lambert law	Chapter 8A&12A
6,8-Feb	Vibrational motion, Harmonic oscillator, Vibrations of diatomic molecules, Vibrational Spectroscopy	Ch. 8B&12D,E
13,15-Feb	Rotational motion, Angular momentum, spin, molecular rotations	Chapter 8C&12B
20,22-Feb	Hydrogenic atoms, Ionization energies and spectroscopic transitions	Chapter 9A
27-Feb,1Mar	Many-electron atoms, Exam 1 Spring break (March 4 – 9)	Ch. 9B, review
13,15-Mar	Molecular orbital theory, Diatomic molecules, Polyatomic molecules	Chapter 10
20,22-Mar	Hückel approximation	Chapter 10E
27,29-Mar	Molecular Symmetry	Chapter 11
3,5-Apr	Exam 2 , Electronic spectra	Review, Ch. 13A
10,12-Apr	Fluorescence and phosphorescence, Magnetic resonance – general principles	Chapter 13B,14A
17,19-Apr	The chemical shift, NMR fine structure	Chapter 14A,B
24,26-Apr	Pulse techniques in NMR, EPR spectra	Chapter 14C, D
1-May	Final Exam , Cuneo Hall-203, 1-3 pm	

Notes: The instructor reserves the right to make changes to the schedule. Any changes to exam dates will be announced in class and on Sakai.