Physical Chemistry II (CHEM 302)
Spring 2019

Lecture: Tue, Th 10:00 - 11:15 AM, Flanner Hall 105
Discussion: We 8:15 – 9:05 AM, Flanner Hall 105
Instructor: Jan Florián

Office: Flanner Hall 314B, Phone: (773) 508-3785, Email: jfloria@luc.edu
Office Hours: Tue 11:15 – 11:45 AM, 1:00 – 2:30 PM
Prerequisites: Chem 222 or 224; Phys 112 or 112K; Math 263 or the equivalent

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 properties

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
Homeworks	18
Exam 1	20
Exam 2	20
Final exam	42
Total	100 grading points

Homeworks: Homework assignments, each worth two to four 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.

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 doctors 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 mid-semester 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 knowledge 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 – 0.2σ to M + 0.2σ	C+	M – 0.5σ to M – 0.2σ	C+
M + 0.2σ to M + 0.5σ	B-	M – 0.8σ to M – 0.5σ	C-
M + 0.5σ to M + 0.8σ	B	M – 1.1σ to M – 0.8σ	D+
M+ 0.8σ to M + 1.1σ	B+	M – 1.4σ to M – 1.1σ	D
M + 1.1σ to M + 1.4σ	A-	less than (M – 1.4σ)	F
More than (M + 1.4σ)	A		

Midterm grade: Your midterm grading points will be based on midterm exam(s) (75% weighting) and homeworks (25%).

Student Accommodations: The university provides services for students with disabilities. Any student who would like to use any of these university services should contact the Student Accessibility Center (SAC), Sullivan Center, (773) 508-3700 and let me know in the first week of classes.

Ethical Considerations: *Students will not collaborate on any exams. 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. Materials from the course cannot be shared outside the course without the instructor's written permission.*

Tentative Schedule[%]

Date	Lecture topics	Reading
15,17-Jan	Key physical principles and tools for chemists: Energy versus free-energy, Coulomb law, Golden rule of spectroscopy, Boltzmann law, QM formalism	Chapter 7
22, 24-Jan	Key physical models for chemists 1: Particle in a 1-D box, Tunneling, Particle in a 2-D and 3-D box.	Chapter 8A
29,31-Jan	Electronic spectroscopy with applications to the π-electron model. Vibrational motion, Harmonic oscillator.	Chapter 8A&12A
5,7-Feb	Vibrations of diatomic molecules, Vibrational Spectroscopy	Ch. 8B&12D,E
12,14-Feb	Rotational motion, Angular momentum, spin, molecular rotations	Chapter 8C&12B
19,21-Feb	Hydrogenic atoms, Ionization energies and spectroscopic transitions	Chapter 9A
26,28-Feb	**Exam 1,** Many-electron atoms	Chapter 9B
	Spring break (March 4 – 9)	
12,14-Mar	Molecular orbital theory, Diatomic molecules, Polyatomic molecules	Chapter 10
19,21-Mar	Hückel approximation	Chapter 10E
26,28-Mar	Molecular Symmetry	Chapter 11
2,4-Apr	**Exam 2,** Electronic spectra	Chapter 13A
9,11-Apr	Fluorescence and phosphorescence, Magnetic resonance – general principles	Chapter 13B,14A
16,18-Apr	The chemical shift, NMR fine structure	Chapter 14A,B
23,25-Apr	Pulse techniques in NMR, EPR spectra	Chapter 14C, D
30-Apr	**Final Exam**, Flanner Hall-105, 1-3 pm	

[%] The instructor reserves the right to make changes to the schedule, except the date and time of the final exam. Any changes to other exam dates will be announced in class and on Sakai. There will be no make-up final exams given under any circumstance, and the exam will not be given early, either.