CHEM 431: Physical Chemistry
Spring 2018

Instructor	Prof. Vadim Cherezov Office: TRF 119 (213) 821-1464 cherezov@usc.edu
Office Hours	Fri 3 – 4 pm (or by appointments)
Lectures	Mon, Wed, Fri 11:00-11:50 am, SOS B2
Discussion	Problem solving practice led by TAs Fri 1:00 – 2:50 pm, GFS 207 Fri 1:00 – 2:50 pm, SGM 226
TAs	TBD TBD
Text	Required: *Physical Chemistry*, by R. J. Silbey, R. A. Alberty, and M. G. Bawendi, 4th Edition (John Wiley & Sons, 2005). Recommended: *Physical Chemistry, a Molecular Approach* by D. A. McQuarrie and J. D. Simon
Course coverage	This course focuses on quantum mechanics as the foundation of atomic and molecular physics, chemical structure and reactivity, and spectroscopy. The emphasis will be made on the *fundamental physical principles* that form a unified base for understanding chemical and physical properties of matter. Selected topics from Part Two and Part Four of Silbey, Alberty, Bawendi: Quantum Mechanics (Ch. 9); Atomic Structure (Ch. 10); Molecular Structure (Ch. 11); Symmetry (Ch. 12); Rotational and Vibrational Spectroscopy (Ch. 13); Electronic Spectroscopy (Ch. 14); Electric and Magnetic Properties of Molecules (Ch. 22), and Solid State (Ch. 23).
Exams and Quizzes	♦ There will be 15 min. quizzes during the lectures (a total of ~10 throughout the semester) that will count toward the final grade. At the end, two lowest quiz scores may be dropped. ♦ There will be **2 midterm exams** (1 hr each) given during regular class hours. Each of the midterm exams will include the material covered up to that point from the previous midterm exam. ♦ At the end of the semester, there will be a **comprehensive final exam** (2 hrs) covering the whole course. ♦ *All exams and quizzes will be closed-book.* ♦ All exam dates are ***final***, there will be no make-up exams

Homework

♦ Homework assignments will be handed out and posted on Blackboard.
♦ In addition to regular problems, homeworks will contain more challenging bonus problems for extra credit.
♦ All homework assignments must be turned in on time
♦ All homeworks will be graded and count toward the final grade.

Course Policies

♦ Full attendance and active participation in all lectures and discussion is expected.
♦ The reading assignments from textbook must be completed ***before*** each lecture.
♦ You must study BOTH lecture notes and the textbook – they do not duplicate one another.
♦ Zero score will be assigned if an exam/quiz is missed without a legitimate excuse or a homework assignment is not turned in on time.
♦ Individuals with excused absences will be given special consideration at the end of the semester. Absences will be excused on the basis of official university policy. To secure an excused absence, bring verification to Prof. Cherezov prior to the absence, or in case of illness, immediately upon your return. All excuses will be verified.
♦ Incomplete grade (IN) will be assigned when work is not completed because of documented illness or other "emergency" occurring after the twelfth week of the semester.

Academic Integrity

Rules regarding academic integrity and general student conducts will be strictly enforced. For details of the University Student Conduct Code and possible sanctions for academic integrity violations, see http://www.usc.edu/dept/publications/SCAMPUS/gov

Grading

There will be no curve grading. The final grade will be determined based on the cumulative weighed average score using the grading scale below.

Homework: 15%
Quizzes: 15%
Midterm exams: 40%
Final exam: 30%

Grading Scale:

94-100%	A	
88-93%	A-	
82-87%	B+	
75-81%	B	
69-74%	B-	
63-68%	C+	
56-62%	C	
50-55%	C-	
44-49%	D+	Failing grade
37-43%	D	Failing grade
31-36%	D-	Failing grade
<30%	F	Failing grade

CHEM 430b: Physical Chemistry

Tentative schedule of lectures/exams

Week	Date	Topics	Reading assignment (SAB)
1	1/08	Introduction to the course. Math review.	
	1/10	Classical mechanics: a deterministic theory. Failures of classical mechanics.	9.1
	1/12	The wave-particle duality. The de Broglie wavelength. The Heisenberg Uncertainty Principle. The wavefunction.	9.1 - 9.3
2	1/15	MLK Day – no class	
	1/17	The time-dependent Schrödinger equation. Separation of time dependence. Time-independent S.E.	9.14, 9.3
	1/19	Particle in a 1D box: quantization of energy, nodes of wavefunction.	9.6
3	1/22	Operators. Physical observables. Eigenfunctions and eigenvalues.	9.4, 9.5, 9.13
	1/24	Commutators. Generalized uncertainty principle. Hermitian operators.	9.8, 9.4
	1/26	The superposition principle.	9.5
4	1/29	Particle in a 2-D and 3-D box. Degeneracy. Quantum dots.	9.7
	1/31	Tunneling. STM.	9.15
	2/2	Classical harmonic oscillator. Vibrations of molecules. Quantum mechanical harmonic oscillator.	9.9, 9.10
5	2/5	Operator algebra for harmonic oscillator. Lowering and raising operators.	handout
	2/7	Rotational motion in 2D: particle on a ring. Rigid rotor.	9.11
	2/9	Rotational motion in 3D: angular momentum.	9.12
6	2/12	Generalized angular momentum: operator algebra.	handout
	2/14	Hydrogen atom: the Schrödinger equation, separation of variables.	10.1
	2/16	Hydrogen atom: Atomic units, energy levels, spectra.	10.1, 10.2, 10.15
7	2/19	President's Day – no class	
	2/21	Hydrogen atom: wavefunctions and atomic orbitals, expectation values of physical observables.	10.3, 10.4
	2/23	***Midterm Exam I***	
8	2/26	Variational Method. Helium atom.	10.6, 10.7
	2/28	Electron spin. Pauli Exclusion Principle.	10.5, 10.8
	3/2	Multi-electron atoms: the Aufbau principle and the periodic table.	10.10, 10.11
9	3/5	Angular momentum of multi-electron atoms.	10.12
	3/7	Atomic term symbols.	10.13
	3/9	Atomic spectroscopy: symmetry and selection rules.	10.14
	3/11-3/18	Spring Recess	
10	3/19	Quantum Chemistry. The mean field approximation and SCF Hartree-Fock Method. Modern applications.	10.9
	3/21	Diatomic molecules: the Born-Oppenheimer Approximation.	11.1
	3/23	The hydrogen molecular ion H_2^+. Multielectron diatomics.	11.2, 11.3, 11.4

11	3/26	Electron configuration of homonuclear diatomics. Molecular terms symbols.	11.5
	3/28	Polyatomic molecules: Valence bond method.	11.6
	3/30	***Midterm Exam II***	
12	4/2	Polyatomic molecules: Huckel MO theory.	11.7, 11.10
	4/4	The band theory of solids: metals, semiconductors, insulators.	handout
	4/6	Symmetry operations, symmetry elements, point groups.	12.1-12.5
13	4/9	Group theory, polarity, chirality.	12.6, 12.7
	4/11	Time-independent perturbation theory.	handout
	4/13	Time-independent perturbation theory: examples.	handout
14	4/16	Spectroscopy: an introduction. Einstein coefficients. Lasers.	13.1, 13.2, 14.9
	4/18	Molecular spectroscopy. Rotational spectra of diatomics and polyatomic molecules.	13.3, 13.4
	4/20	Vibration and vibration-rotation spectra of diatomics.	13.6, 13.7
15	4/23	Vibrations of polyatomic molecules. Normal modes. Raman spectroscopy	13.8, 13.9
	4/25	Electronic Spectroscopy.	14.1-14.8
	4/27	Course Review, Q&A session.	
	5/2	***Final Exam 11:00 am – 1:00 pm***	