Spring 2019

CHEM 235-002: Physical Chemistry II

Lev Krasnoperov

NJIT New Jersey Institute of Technology

THE COLLEGE OF SCIENCE AND LIBERAL ARTS

THE DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

Chemistry:
Spring 2019 Course Syllabus

NJIT Academic Integrity Code: All Students should be aware that the Department of Chemistry & Environmental Science (CES) takes the University Code on Academic Integrity at NJIT very seriously and enforces it strictly. This means that there must not be any forms of plagiarism, i.e., copying of homework, class projects, or lab assignments, or any form of cheating in quizzes and exams. Under the University Code on Academic Integrity, students are obligated to report any such activities to the Instructor.

COURSE INFORMATION

Course Description:

CHEM 235 Physical Chemistry II

Phase equilibrium, Multi-component phase equilibrium, Electrochemical Equilibrium, Thermochemistry of Ions in Solutions, Kinetic Theory of Gases, Transport Phenomena, Chemical Kinetics, Gas Phase Reactions, Chemical Dynamics, Photochemistry.
Prerequisites: Basic chemical principles, Basic principles of Thermodynamics, Functions of two and several variables, Partial derivatives, Integrals, Ordinary differential equations

Number of Credits:
3

Prerequisites:
Chem 231, Math 211 or 213, Phys 111

Co requisite:
N/A

Course-Section and Instructors

Course-Section	Instructor
CHEM 235-001	Lev Krasnoperov

Office Hours for All Chemistry & Environmental Science Instructors: Fall 2018 Office Hours and Emails

Required Textbook:

Title	Physical Chemistry
Author(s)	Peter Atkins and Julio De Paula
Edition	10th Edition
Publisher	Freeman & Co.

ISBN #	2014, ISBN-13:978-1-4292-9019-7
Chapters to be covered	5, 6, 19, 20, 21A, 21C

University-wide Withdrawal Date: The last day to withdraw with a **W** is Friday, February 1, ??? 2019. It will be strictly enforced.

Learning Outcomes:

By the end of the course, students should be able to do the following:

1. **Sketch and interpret the phase diagrams for liquid-gas, liquid-liquid, and liquid-solid equilibria for mixtures.**
2. **Calculate chemical equilibria in simple reactions and predict impact of temperature and pressure.**
3. **Calculate activities of ions in solutions.**
4. **Calculate the transfer parameters (diffusion coefficient, viscosity, thermal and electrical conductivity).**
5. **Determine the Arrhenius parameters of a chemical reaction from the rate vs. temperature data.**
6. **Process data for reactions of simple orders.**
7. **Build up mechanisms of complex chemical reactions, construct corresponding systems of ODE, and use the steady-state approximation.**
8. **Estimate rate constants of elementary chemical reactions using the Simple Collision Theory and the Transition State Theory.**

POLICIES

All CES students must familiarize themselves with, and adhere to, all official university-wide student policies. CES takes these policies very seriously and enforces them strictly.

Grading Policy: The final grade in this course will be determined as follows:

Homework	220[a)]
Quizzes	[a)]
Midterm Exam I	200
Midterm Exam II	200
Final Exam	300
Attendance	80

[a)]**Homework grades will be given based on THREE quizes 110 pts each, 35 min, two problems similar to those from the homework assignments, with different numerical data, TWO BEST quizes will be taken into account (homework grades will be assigned contingent submission of all homework assignments). The quizes are POP UP (i.e., are NOT announced in advance). No requests whether a quiz would appear on a specific date must be made. NO make-up quizes will be offered.**

Your final letter grade in this course will be based on the following **tentative** curve:[b)]

A	>850	C	500 - 600
B+	750 - 850	D	450 - 500
B	650 - 750	F	<450
C+	600-650		

[b]**Scores less than 45% of the total normally result in F. Scores larger than 85% of total always result in A. The distribution of the grades between these benchmarks as well as the F and A boundaries depend on the overall performance of the class.**

Attendance Policy: Attendance at classes will be recorded and is **mandatory**. Each class is a learning experience that cannot be replicated through simply "getting the notes."

Homework Policy: Homework is an expectation of the course. The homework problems set by the instructor are to be handed in for grading and will be used in the determination of the final letter grade as described above.

Exams: There will be two midterm exams held in class during the semester and one comprehensive final exam. The following exam periods are *tentative and therefore possibly subject to change*:

Midterm Exam I	February 25 – March 8 (after the material from lectures 1 -9 is completely covered)
Midterm Exam II	April 8 -12 (after the material from lectures 10-17 is completely covered)
Final Exam Period	May 10 - 16, 2019

The final exam will test your knowledge of all the course material taught in the entire course.

Makeup Exam Policy: There will normally be **NO MAKE-UP QUIZZES OR EXAMS** during the semester. In the event that a student has a legitimate reason for missing a quiz or exam, the student should contact the Dean of Students office and present written verifiable proof of the reason for missing the exam, e.g., a doctor's note, police report, court notice, etc. clearly stating the date AND time of the mitigating problem. The student must also notify the CES Department Office/Instructor that the exam will be missed so that appropriate steps can be taken to make up the grade.

Cellular Phones: All cellular phones and other electronic devices must be switched off during all class times. Such devices must be stowed in bags during exams or quizzes.

ADDITIONAL RESOURCES

Chemistry Tutoring Center: Located in the Central King Building, Lower Level, Rm. G12. Hours of operation are Monday – Friday 10:00 am - 6:00 pm. For further information please click here.

Accommodation of Disabilities: Office of Accessibility Resources and Services (***formerly known as Disability Support Services***) offers long term and temporary accommodations for undergraduate, graduate and visiting students at NJIT.

If you are in need of accommodations due to a disability please contact Chantonette Lyles, Associate Director at the Office of Accessibility Resources and Services at 973-596-5417 or via email at lyles@njit.edu. The office is located in Fenster Hall Room 260. A Letter of Accommodation Eligibility from the Office of Accessibility Resources Services office authorizing your accommodations will be required.

For further information regarding self-identification, the submission of medical documentation and additional support services provided please visit the Accessibility Resources and Services (OARS) website at:

- http://www5.njit.edu/studentsuccess/disability-support-services/

Important Dates (See: Fall 2018 Academic Calendar, Registrar)

Date	Day	Event
January 22, 2019	T	First Day of Classes
February 1, 2019	F	Last Day to Add/Drop Classes
April 8 2019	M	Last Day to Withdraw

March 17 – 24, 2019	S – S	Spring Recess – No Classes Scheduled
May 7, 2019	T	Friday Classes Meet
April 19, 2019	F	Good Friday - University Closed
May 7, 2019	T	Last Day of Classes
May 8, 9, 2019	W, R	Reading Days
May 10-16, 2019	F - R	Final Exam Period

Course Outline

Lecture	Section	Topic	Assignment[c)]
1	001	**Phase equilibria in multi-component systems. Phases. Phase diagrams. Components. Degrees of freedom. The Gibbs phase rule.**	
2	001	**Liquid-vapor equilibria in binary systems. Completely miscible liquids. Ideal solutions. Pressure -composition diagrams. Temperature-composition diagrams. Real solutions. The lever rule. Fractional distillation.**	**Homework #1 Exercises: 5B.10(a), 5B.11(a), 5B.12(a), 5B.13(a Problems: 5C.1**
3	001	**Liquid-liquid phase equilibria. Partially miscible liquids. Upper and lower critical temperature.**	
4	001	**Liquid-solid phase equilibria. Partially miscible solids. Simple eutectic systems. Cooling curves. Solid compound formation. Congruently and incongruently melting compounds. Fractional crystallization**	**Homework #2 Exercises: 5C.2(a), 5C.5(a), 5C.10(a) Problems: 5C.4, 5C.6, I.A. 5.4**
5	001	**Chemical equilibrium. The stoichiometric equation. The extent of reaction. The reaction Gibbs energy and the Standard Gibbs Energy of the reaction. The Gibbs energy minimum. The reaction quotient. The equilibrium constant. The equilibrium constant expressed via the Standard Gibbs Energy of the reaction.**	
6	001	**Constructing the reaction quotient. Activities. Activities in the gas phase, in solution, and of pure solids and liquids. Equilibrium constant in terms of partial pressures, Kp. Equilibrium constant in terms of mole fractions, K_x. Sample equilibrium calculations.**	**Homework#3 Exercises: 6A.4(a), 6A.5(a), 6A.6(a), 6A.8(a), 6B.1(a), 6A.9(a) Problems: 6A.1, 6B.2**
7	001	**The response of equilibria to temperature and pressure. The Le Chatelier Principle. The van't Hoff equation. Sample equilibrium calculations using the equilibrium constant in terms of mole fractions and partial pressures.**	
8	001	**Thermodynamics of ions in solutions. Thermodynamic functions of formation of ions in solutions. The convention for H_3O^+. Activities of ions in solution. Activities of electrolytes. The mean ionic activity and the activity coefficient.**	**Homework #4 Exercises: 6A.10(a), 6A.11(a), 6B.6(a) Problems: 6B.3, 6A.3, 6B.4**

9	001	**The Debye-Huckel limiting law. The ionic strength.**	
		FIRST MIDTERM EXAM	
10	001	**Equilibrium electrochemistry. Reduction and oxidation. Redox reactions. Electrochemical cell. Half-reactions and electrodes. The variety of cells. The variety of electrodes. Electrochemical cell at equilibrium. The cell potential. The Nernst equation.**	
11	001	**The standard potentials. The reference electrode. The electrochemical series. Solubility constants. Thermodynamic functions from the cell potential measurements.**	
12	001	**Molecules in motion. Mean free path. Collisions with walls and surfaces. Effusion.**	
13	001	**Migration down gradients. Transport properties of gas. Diffusion, thermal conductivity and viscosity.**	**Homework #5 Exercises: 5F.1(a), 5F.3(a), 6C.1(a), 6C.2(a), 6D.1(a), 6D.2(a)**
14	001	**Molecular motion in liquids. The conductivity of electrolyte solutions. The molbilities of ions.**	
15	001	**Mobility and diffusion. Conductivity of weak and strong electrolytes. The Ostwald dilution law. The Kohlrausch law**	**Homework #6 Exercises: 19A.1(a), 19A.2(a), 19A4(a), 19A.7(a), 19A10(a)**
16	001	**The rates of chemical reactions. Elementary and complex chemical reactions. The rate law. Reactions of simple orders. The rate constant.**	
17	001	**The formal chemical kinetics. First, second and third order chemical reactions. The integrated rate laws.**	**Homework #7 Exercises: 19B.2(a), 19B.4(a), 19B.5(a), 19B.6(a) , 19B.7(a)**
		SECOND MIDTERM EXAM	
18	001	**The temperature dependence of reaction rates. The Arrhenius expression. The A-factor and the activation energy. The apparent activation energy of chemical reaction.**	

19	001	**Simple complex reactions. Reversible first order reaction. Approaching the equilibrium. The relationship between the forward and reverse rate constant and the equilibrium constant. Parallel first order reactions. Consecutive first order reactions. Pre-equilibrium. The steady-state approximation.**	**Homework #8** **Exercises: 20A.2(a), 20A.4(a), 20B.2(a), 20B.3(a)** **Problems: 20A.2, 20B.13, 20B,17**
20	001	**Application of the steady-state approximation. Unimolecular reactions. The Lindemann-Hinshelwood mechanism. Enzimatic kinetics (Chapter 23.2). The Michaelis-Menten mechanism.**	
21	001	**The kinetics of complex reactions. The system of ordinary differential equations. The structure of chain reactions. Application of the steady-state approximation. The chain length. Chain initiation, propagation and termination. The rate controlling step.**	**Homework #9** **Exercises: 20D.1(a), 20E.1(a), 20E.2(a), 20F.1(a), 20H.1(a)** **Problems: 20D.4, 20H.2(a)**
22	001	**Chain branching reactions. Chain branching explosions. The criterion of the explosion limits.**	
23	001	**Molecular reaction dynamics. The collision theory. The steric factor.**	**Homework #10** **Exercises: 21A.4(a), 21C.2(a)** **Problems: 21A.1, 21C.5**
24	001	**The reaction coordinate and the transition state. The Transition State Theory. The Standard Entropy and Standard Gibbs Energy of Activation.**	
25	001	**(*Chapter 21.10).* Photochemical reactions. The quantum yield.**	**Homework #11** **Exercises: 21A.5(a), 21C.15(a), 21F.4(a)** **Problems: 21A.3, 21C.1, 21A.5, 20G.1**

[c)] Eleven weekly homeworks. The position in the table is tentative.