CHEM 235
Physical Chemistry II
NJIT
Spring Semester, 2016

Prerequisites:	**Chem 231 or equivalent,** **Math 211 or 213, Phys 111**
Textbook:	**P. W. Atkins and J. de Paula** **Physical Chemistry** **10th Edition, Freeman and Co.** **2014, ISBN-13:978-1-4292-9019-7** **ISBN-10: 1-4292-9019-6**
Chapters to be covered:	**5, 6, 19, 20, 21A, 21C**
Instructor:	**Dr. Lev Krasnoperov** **Tiernan Hall** **Room 358, phone x3592** **krasnoperov@adm.njit.edu** **Office Hour: Friday 10:00-11:00**
Topics:	**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, Reactions in Liquid Phase, Photochemistry.**
Prerequisites:	**Basic chemical principles,** **Basic principles of Thermodynamics,** **Functions of two and several variables,** **Partial derivatives** **Integrals** **Ordinary differential equations**

Course outline:

Two lectures per week. Three pop-up quizes. Two mid-term exams. Final exam.

Chapter 5. Phase Equilibria in Multi-component Systems.

Lecture 1. Phase equilibria in multi-component systems. Phases. Phase diagrams. Components. Degrees of freedom. The Gibbs phase rule.
Lecture 2. Liquid-vapor equilibria in binary systems. Completely miscible liquids. Ideal solutions. Pressure -composition diagrams. Temperature-composition diagrams. Real solutions. The lever rule. Fractional distillation. Azeotropes.
Lecture 3. Liquid-liquid phase equilibria. Partially miscible liquids. Upper and lower critical temperature.
Lecture 4. Liquid-solid phase equilibria. Partially miscible solids. Simple eutectic systems. Cooling curves. Solid compound formation. Congruently and incongruently melting compounds. Fractional crystallization.

Chapter 6A,B. Chemical Equilibrium.

Lecture 5. 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.
Lecture 6. 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.
Lecture 7. 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.

Chapter 5F.

Lecture 8. 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.
Lecture 9. The Debye-Huckel limiting law. The ionic strength.

Midterm exam I.

Chapter 6C,D. Equilibrium Electrochemistry.

Lecture 10. 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.
Lecture 11. The standard potentials. The reference electrode. The electrochemical series. Solubility constants. Thermodynamic functions from the cell potential measurements.

Chapter 19. Transport Phenomena.

Lecture 12. Molecules in motion. Mean free path. Collisions with walls and surfaces. Effusion.
Lecture 13. Migration down gradients. Transport properties of gas. Diffusion, thermal conductivity and viscosity.
Lecture 14. Molecular motion in liquids. The conductivity of electrolyte solutions. The molbilities of ions.
Lecture 15. Mobility and diffusion. Conductivity of weak and strong electrolytes. The Ostwald dilution law. The Kohlrausch law.

Chapter 20. Chemical Kinetics

Lecture 16. The rates of chemical reactions. Elementary and complex chemical reactions. The rate law. Reactions of simple orders. The rate constant.
Lecture 17. The formal chemical kinetics. First, second and third order chemical reactions. The integrated rate laws.

Midterm exam II.

Lecture 18. The temperature dependence of reaction rates. The Arrhenius expression. The A-factor and the activation energy. The apparent activation energy of chemical reaction.
Lecture 19. 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.
Lecture 20. Application of the steady-state approximation. Unimolecular reactions. The Lindemann-Hinshelwood mechanism. Enzimatic kinetics (Chapter 23.2). The Michaelis-Menten mechanism.

The Kinetics of Complex Reactions

Lecture 21. 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.
Lecture 22. Chain branching reactions. Chain branching explosions. The criterion of the explosion limits.

Chapter 21. Molecular reaction dynamics.

Lecture 23. Molecular reaction dynamics. The collision theory. The steric factor.
Lecture 24. The reaction coordinate and the transition state. The Transition State Theory. The Standard Entropy and Standard Gibbs Energy of Activation.
Lecture 25. (*Chapter 21.10)*. Photochemical reactions. The quantum yield.

Learning outcomes:
By the end of the course, you 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.**

Grade determination.

Grading:

Midterm Exam 1 (after approx. 4 - 5 weeks)	**200**
Midterm Exam 2 (after approx. 8 - 9 weeks)	**200**
Final Exam	**300**
Homeworks[a)] (via Quizes)	**220**
Attendance	**80**
Total:	**1000**

Scores less than 45% of the total <u>normally</u> result in F. Scores larger than 85% of total <u>always</u> 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.

[a)]Homework grades will be given based on THREE pop-up* quizes 110 pts each, 30 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 NJIT honor code will be upheld and any violations will be brought to the immediate attention of the Dean of Students.

Students will be consulted with by the instructor and must agree to any modifications or deviations from the syllabus throughout of the semester.

***)** Quizes are <u>unannounced.</u> Personnel teaching the class (TAs, etc.) is instructed not to reveal any information about the quizes scheduling. Students should not make attempts to acquire this information.

<u>Exams.</u> Mid-term exams are 1.5 hours long and are closed book, closed notes exams. One double-sided formula sheet per exam (only formulas, no text) is allowed. No smartphones, ipads, laptops, etc. are allowed. Final exam (2.5 hours) will be given during the final exam period and will follow the same rules. The final exam will be comprehensive with the emphases on the final part of the course.

<u>The NJIT HONOR CODE will be upheld. Any violations will be brought to the attention of the Dean of Students.</u>

<u>Exams make-up policy.</u>—Make-up exams are only given in the case of well-documented, serious conditions. Documentation should be provided to the Dean of Students, who will decide if a make-up should be given.

Prepared: **Dr. Lev Krasnoperov**
Date: **January 15, 2016**

CHEM 235, Physical Chemistry 2
Atkins, 10th edition

Homeworks are due one week after the assignment. The date of the assignment of the first homework is the first lecture. Adjustment due to the delay caused by the class cancellations or other reasons that can not be foreseen are possible.

Homework assignments:

Homework #	Exercises	Problems
#4	5B.10(a), 5B.11(a), 5B.12(a), 5B.13(a)	5C.1
#5	5C.2(a), 5C.5(a), 5C.10(a)	5C.4, 5C.6, I.A. 5.4
#3	6A.4(a), 6A.5(a), 6A.6(a), 6A.8(a), 6B.1(a), 6A.9(a)	6A.1, 6B.2
#4	6A.10(a), 6A.11(a), 6B.6(a)	6B.3, 6A.3, 6B.4
#5	5F.1(a), 5F.3(a), 6C.1(a), 6C.2(a), 6D.1(a), 6D.2(a)	5F.1, 6D.1
#6	19A.1(a), 19A.2(a), 19A4(a), 19A.7(a), 19A10(a)	
#7	19B.2(a), 19B.4(a), 19B.5(a), 19B.6(a) , 19B.7(a)	19B.4, 19B.6
#8	20A.2(a), 20A.4(a), 20B.2(a), 20B.3(a)	20A.2, 20B.13, 20B,17
#9	20D.1(a), 20E.1(a), 20E.2(a), 20F.1(a), 20H.1(a) 20H.2(a)	20D.4,
#10	21A.4(a), 21C.2(a)	21A.1, 21C.5
#11	21A.5(a), 21C.15(a), 21F.4(a)	21A.3, 21C.1, 21A.5, 20G.1