

# SYLLABUS

## Physical Chemistry II

### ChBE 212

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#### Course Goals:

This course serves as an introduction to chemical kinetics, statistical thermodynamics, quantum chemistry, spectroscopy and molecular modeling. It offers a detailed understanding of chemical phenomena in terms of the structure and dynamics of the molecules involved.

You will first learn the basic principles of chemical equilibrium and chemical kinetics, thus you will gain the ability to approach chemical reactions from a molecular point of view. Then, you will learn the underlying principles of quantum mechanics, how they can be applied to a number of model systems and how the spectra of the molecules are governed by the quantum mechanical properties of molecules. And, finally you will develop the ability to model molecules and chemical reactions, to formulate all the thermodynamic and kinetic parameters in terms of the properties of the atoms and molecules that make up macroscopic chemical systems.

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#### Course Outline:

##### 1. Chemical Equilibrium (*Week 1-3*)

- The properties of chemical potential, thermodynamic properties of mixtures, chemical equilibrium in a mixture of ideal gases, the equilibrium constants, the temperature dependence of the equilibrium constant-van't Hoff equation, the LeChatelier principle.

##### 2. Chemical Kinetics (*Week 4-6*)

- Reaction rate, effect of temperature, Arrhenius equation, effect of concentration, rate laws, order of a reaction, first-order and second-order reactions, steady state approximation, complex reactions, opposing, parallel and consecutive reactions.

##### 3. Kinetic Theories (*Week 7*)

- The activation energy, unimolecular reactions – Lindemann mechanism, the collision theory, the transition state theory.

##### 4. Quantum Chemistry (*Week 8-12*)

- The structure of matter, electromagnetic radiation, blackbody radiation, the photoelectric effect, atomic spectra, Bohr's model of the atom, DeBroglie's principle, classical wave equation, Schrodinger equation, the postulates of quantum mechanics, the quantum mechanics of some model systems-the free

particle, particle in a box, the harmonic oscillator, the rigid rotator, the Hydrogen atom, approximation methods and multielectron atoms, molecular structure and covalent bond, Huckel molecular orbital theory,  $\pi$ -approximation, reaction indices, molecular spectroscopy.

#### 5. Structure and Thermodynamic Properties (Week 13-14)

- The energy of a system, the entropy of a system, partition functions, molecular motions-translational, rotational and vibrational motions, calculation of molecular properties, calculation of kinetic parameters.

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#### Course Materials :

- Lecture Notes**

ÇINAR Zekiye, <http://www.zdo.com/cinarz>

- Textbooks**

- P.W. ATKINS , "Physical Chemistry", Oxford University Press, 7<sup>th</sup> Ed., N.Y., 2002.
- ÇINAR Zekiye, "Kuantum Kimyasi", 2. Baski, Caglayan Yayınevi, 1992.

- Additional References**

- McQuarrie D.A., Simon J.D., "Physical Chemistry-A Molecular Approach", University Science Books, U.S.A., 1997.
- LAIDLER K.J., MEISER J.H., "Physical Chemistry", Addison-Wesley Pub.Com.,U.S.A., 1982.
- ALBERTY R.A., SILBEY R.J., "Physical Chemistry", John Wiley and Sons Inc.,U.S.A., 1992.

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#### Grading Scheme:

<b>Midterm Exams :</b>	There will be 2 midterm exams.
<b>Quizzes :</b>	There will be 5 10-15 minute quizzes.
<b>Homework :</b>	Homework to be handed in will be assigned in order to encourage collaboration with the classmates, to give the students the practice that they need to feel confident with the material
<b>Questions :</b>	Questions will be directed during the lectures in order to give the students the opportunity to explain ideas and listen to each other. The best answer will be awarded by an extra quiz grade.

	Number	Effective Proportion %
<b>Midterm Exams</b>	2	42
<b>Quizzes</b>	5	12
<b>Homework</b>	5	6
<b>Final Exam</b>	1	40

#### Letter Grades

90-100	AA	60-69	CC
85-89	BA	55-59	DC
80-84	BB	50-54	DD
70-79	CB	...-50	F