PREDLAGANE SPREMEMBE	
Predmet:	FIZIKALNA KEMIJA
Course Title:	PHYSICAL CHEMISTRY

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
UŠP Kemija, 1. stopnja	**/**	**2.**	**3. in 4.**
USP Chemistry, 1st Cycle	**/**	**2nd**	**3rd and 4th**

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code:

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
100	**50**	**/**	**/**	**/**	**150**	**10**

Nosilec predmeta / Lecturer: prof. dr. Andrej Jamnik / Dr. Andrej Jamnik, Full Professor

Jeziki / Languages:

Predavanja / Lectures:	**slovenski / Slovenian**
Vaje / Tutorial:	**/**

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisites:**
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	The course has to be assigned to the student.

Vsebina:	**Content (Syllabus outline):**
Osnovni pojmi in enačbe stanja Sistem, stanje, funkcije stanja in funkcije poti. Plinski zakoni, idealni plin. Realni plini, van der Waalsova enačba, virialna enačba, kritični pojavi. **Kinetična teorija plinov** Tlak plina. Maxwellova porazdelitvena funkcija hitrosti molekul in translacijskih kinetičnih energij. Kinetična energija in temperatura. Pogostost trkov med molekulami in trkov molekul s steno. **Prvi zakon termodinamike** Energija, toplota, delo. Prvi termodinamski zakon. Obrnljivi in neobrnljivi procesi. Entalpija. Toplotna kapaciteta. Termokemija. **Entropija in drugi zakon termodinamike**	**Basic concepts and equations of state** System, state, state functions and path functions. Gas laws, ideal gas. Real gases, van der Waals equation, virial equation, critical phenomena. **Kinetic theory of gases** Pressure of a gas. Maxwell distribution of molecular speeds and translational kinetic energies. Kinetic energy and temperature. Frequency of intermolecular collisions and collisions of molecules with the walls and surfaces. **First law of thermodynamics** Energy, heat, work. First law of thermodynamics. Reversible and irreversible processes. Enthalpy. Heat capacity.

UL FKKT

Spontane in nespontane spremembe. Termodinamska definicija entropije. Sprememba entropije v izoliranem in v zaprtem sistemu, Clausiusova neenenakost. Molekularna interpretacija entropije. Računanje entropijskih sprememb pri različnih spremembah stanja.

Entropija in tretji zakon termodinamike

Praktične absolutne entropije. Standardne entropije. Sprememba entropije pri kemijskih reakcijah.

Prosta energija in prosta entalpija

Termodinamski potenciali, splošni pogoji za ravnotežje in za spontane procese. Sprememba proste entalpije pri kemijskih reakcijah. Odvisnost proste entalpije od temperature in tlaka. Maxwellove enačbe.

Fazna ravnotežja

Faza in komponenta. Kemijski potencial. Prostostne stopnje, fazno pravilo. Clapeyronova in Clausius-Clapeyronova enačba. Fazni diagrami čistih snovi.

Raztopine

1) *Raztopine dveh hlapnih tekočin*

Parcialne molske količine. Idealne in neidealne raztopine. Raoultov zakon in Henryjev zakon. Fazni diagrami parni tlak-sestava in vrelni diagrami. Kemijski potencial, aktivnost in aktivnostni koeficient posameznih komponent raztopine. Standardna stanja na osnovi Raoultovega in Henryjevega zakona. Termodinamika mešanja. Ravnotežje trdno-tekoče: enostavni eutektični fazni diagrami.

2) *Raztopine trdnega topljenca v tekočem topilu* Standardno stanje, kemijski potencial, aktivnost in aktivnostni koeficient topila in topljenca. Kemijski potencial močnih elektrolitov, aktivnost ionov in srednja aktivnost elektrolita, aktivnostni koeficient in srednji aktivnostni koeficient. Koligativne lastnosti.

Fazni diagrami trokomponentnih sistemov.

Kemijsko ravnotežje

Izpeljava splošnega izraza za kemijsko ravnotežje. Konstanta ravnotežja. Homogena in heterogena ravnotežja. Odvisnost konstant ravnotežja od temperature in tlaka, Le

Thermochemistry.

Entropy and the second law of thermodynamics

Spontaneous and nonspontaneous changes. Thermodynamic definition of entropy. Entropy changes in isolated and in closed systems, Clausius inequality. Molecular interpretation of entropy. Calculation of entropy changes for various changes of state.

Entropy and the third law of thermodynamics

Practical absolute entropies. Standard entropies. Entropy changes in chemical reactions.

Free energy and free enthalpy

Thermodynamic potentials, general conditions for equilibrium and for spontaneous changes. Free enthalpy changes in chemical reactions. Temperature and pressure dependence of the free enthalpy. Maxwell relations.

Phase equilibria

Phase and component. Chemical potential. Degrees of freedom. Phase rule. Clapeyron and Clausius - Clapeyron equation. Phase diagrams of pure substances.

Solutions

1) *Liquid – liquid solutions*

Partial molar quantities. Ideal and non-ideal solutions. Raoult's law and Henry's law. Vapour pressure - composition and temperature - composition phase diagrams. Chemical potential, activity, and activity coefficient of individual components of the solution. Raoult's law and Henry's law standard states. Thermodynamics of mixing. Solid-liquid equilibrium: simple eutectic phase diagrams.

2) *Solid – liquid solutions*

Standard state, chemical potential, activity and activity coefficient of the solvent and the solute. Chemical potential of strong electrolytes, activity of ions and mean activity of electrolyte, activity coefficient and mean activity coefficient. Colligative properties.

Phase diagrams of ternary systems.

Chemical equilibrium

Derivation of a general expression for the chemical equilibrium. Equilibrium constant. Homogeneous and heterogeneous equilibria.

UL FKKT

Chatelierov princip. **Raztopine elektrolitov** Močni in šibki elektroliti. Specifična in molska prevodnost. Električni tok skozi raztopino, transportno število, gibljivost ionov. Koligativne lastnosti raztopin elektrolitov. Debye - Hückelova teorija, Debye - Hückelov limitni zakon. **Elektrokemijski členi** Elektroliza. Galvanski členi: delovanje, spontana reakcija v členu. Reverzibilna napetost člena. Termodinamika galvanskega člena. Nernstova enačba. Standardni redukcijski potenciali. Različni tipi členov. Uporaba galvanskih členov. **Kemijska kinetika** Hitrost reakcije. Elementarne reakcije: red reakcije, hitrostni zakon in konstanta reakcijske hitrosti. Empirični hitrostni zakoni. Zaporedne, vzporedne in obojesmerne reakcije. Vpliv temperature na hitrost reakcije, Arrheniusova enačba. Mehanizem reakcije. Verižne reakcije in eksplozije. Trkovna teorija in teorija prehodnega stanja. Homogena in heterogena kataliza. Encimska kataliza. **Površinska kemija** Površinska napetost in kapilarni pojavi, Laplaceova enačba in Kelvinova enačba. Površinsko aktivne snovi, micelizacija. Kemisorpcija in fizisorpcija. Termodinamika adsorpcije. Langmuirjeva in Freundlichova adsorpcijska izoterma.	Temperature and pressure dependence of equilibrium constants, Le Chatelier principle. **Solutions of electrolytes** Strong and weak electrolytes. Specific and molar conductivity. Electric current through the solution, transport number, mobility of ions. Colligative properties of electrolyte solutions. Debye - Hückel theory, Debye - Hückel limiting law. **Electrochemical cells** Electrolysis. Galvanic cells: operation, spontaneous reaction in the cell. EMF of galvanic cell. Thermodynamics of galvanic cells. Nernst equation. Standard reduction potentials. Various types of cells. Application of galvanic cells. **Chemical kinetics** Rate of reaction. Elementary reactions: order of reaction, rate law and rate constant. Empirical rate equations. Consecutive and parallel reactions, reactions approaching equilibrium. Effect of temperature on reaction rate, Arrhenius equation. Reaction mechanism. Chain reactions and explosions. Collision and transition state theories. Homogeneous and heterogeneous catalysis. Enzyme catalysis. **Surface chemistry** Surface tension and capillarity, Laplace and Kelvin equations. Surfactants, micellization. Chemisorption and physisorption. Thermodynamics of adsorption. Langmuir and Freundlich adsorption isotherms.

Temeljna literatura in viri / Readings:

- A. Jamnik, Fizikalna kemija (1. izdaja), založba FKKT (2013), ISBN: 978-961-6756-39-6 (1. zvezek) in ISBN: 978-961-6756-40-2 (2. zvezek).

Dopolnilna literatura

- P. Atkins and J. de Paula, Atkins' Physical Chemistry (9. izdaja), Oxford University Press (2010), ISBN: 978-0-19-954337-3.
- R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Physical Chemistry (4. Izdaja), John Wiley, New York (2005), ISBN: 978-0-471-21504-2.

Cilji in kompetence:	**Objectives and Competences:**
Pri fizikalni kemiji, ki sodi med osnovne kemijske predmete, študenti spoznajo povezavo med fizikalnimi in kemijskimi pojavi	Physical chemistry is one of the basic chemistry courses. The objective of this subject is to study connections between physical and chemical

UL FKKT

ter med fizikalnimi in kemijskimi lastnostmi snovi. Njegov cilj je študentu posredovati temeljno znanje fizikalne kemije, ki kasneje zadošča na običajnem delovnem mestu kemika, omogoča pa tudi samostojno nadaljnje izobraževanje. Pri tem se ne omejuje samo na podajanje posameznih enačb in zakonov, ampak daje poseben poudarek interpretaciji metod in razvoju modelov, ki do njih vodijo. Pri študiju fizikalne kemije študent nedvomno razvija sposobnost kritičnega razmišljanja in logičnega sklepanja.	phenomena and between physical and chemical properties of the matter. Its main goal is to convey the principal laws of physical chemistry. A great deal of attention is paid to training the students in the application of theoretical expressions to problems that are commonly encountered by chemists at ordinary working places. It provides the understanding of a group of principles and methods helpful in solving many different types of problems encountered in natural sciences. In the study of physical chemistry students undoubtedly develop the ability of critical thinking and logical reasoning.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Poznavanje osnovnih fizikalno-kemijskih količin kot so notranja energija, delo, toplota, entalpija, prosta energija in entropija. Poznavanje osnovnih zakonov termodinamike. Razumevanje pojmov obrnljivosti (reverzibilnosti) in neobrnljivosti (ireverzibilnosti) procesov. Uporaba tabeliranih fizikalno-kemijskih podatkov (standardne tvorbene entalpije, standardne entropije, toplote faznih prehodov, toplotne kapacitete) pri določanju termodinamike kemijskih reakcij pri različnih pogojih. Poznavanje kriterijev za spontanost poteka kemijskih reakcij ter za kemijsko ravnotežje. Razumevanje razlike med termodinamiko (spontanostjo poteka) ter kinetiko (hitrostjo poteka) kemijske reakcije.	<u>Knowledge and Comprehension</u> Knowledge of the basic physicochemical properties like internal energy, work, heat, enthalpy, free energy, and entropy. Knowledge of the basic thermodynamic laws. Understanding the concept of reversibility and irreversibility of processes. Use of tabulated thermodynamic data (standard enthalpies of formation, standard entropies, heats of phase changes, heat capacities) for the thermodynamic description of chemical reactions at different conditions. Knowledge of various criteria for chemical equilibrium and for the direction of spontaneous chemical or physical change at different conditions. Understanding basic differences between thermodynamics (spontaneity) and kinetics (rate) of chemical reactions.
<u>Uporaba</u> Zaradi svojega temeljnega pomena je pridobljeno znanje fizikalne kemije zelo široko uporabno. Vse moderne analizne metode so osnovane na fizikalno kemijskih principih. Poleg tega je, tako iz energetskega kot iz kinetičnega vidika, znanje fizikalne kemije nujno potrebno pri vodenju kemijskih in biokemijskih procesov. Podobno velja, da je globlje razumevanje procesov, ki nastopajo v bio-sistemih, brez ustreznega znanja fizikalne kemije nemogoče. Iz vsega tega sledi, da je znanje fizikalne kemije nepogrešljivo pri razvojnem, proizvodnem ter kontrolnem delu	<u>Application</u> Because of the fundamental importance of physical chemistry the acquired knowledge offers very broad applicability. All modern analytical methods are based on physicochemical principles. Moreover, the knowledge of physical chemistry is necessary for a controlled conduct of chemical and biochemical processes, both from energetic as well as from kinetic point of view. Deeper understanding of various biochemical processes is also impossible without adequate knowledge of physical chemistry. Hence it follows that the knowledge of physical chemistry is

UL FKKT

vrste porabnikov kot so npr. kemijska, farmacevtska, živilsko-predelovalna in tekstilna industrija ter mnogi razvojni in kontrolni laboratoriji v drugih dejavnostih.	indispensable for the development, production and control work type of users, such as chemical, pharmaceutical, food-processing, textile industries as well as for many development and control laboratories.
Refleksija Pridobitev občutka za fizikalno-matematični način razmišljanja ter spoznanja o splošnih fizikalno-matematičnih metodah za reševanje različnih praktičnih problemov iz naravoslovja. Globlje razumevanje pomena abstraktnih fizikalno-kemijskih pojmov in količin.	Analysis Students gain a sense for physico-mathematical thinking and a knowledge of the general physico-mathematical methods for solving various practical problems in natural sciences. In addition, they gain a deeper understanding of the significance of abstract physico-chemical principles and properties.
Prenosljive spretnosti Uporaba splošnih naravoslovnih zakonitosti pri študiju naravoslovnih vsebin, ki so zajete pri drugih predmetih. Pri študiju fizikalne kemije se pri večini študentov razvije kritičen in analitičen način razmišljanja, kar jim zelo koristi pri identifikaciji in reševanju različnih teoretičnih in praktičnih problemov, s katerimi se soočijo na svoji poklicni poti. Kritično ovrednotenje rezultatov katerihkoli (ne le fizikalno-kemijskih) meritev. Uporaba domače in tuje znanstvene literature.	Skill-transference Ability Use of the general physico-chemical principles in the study of various topics covered by other subjects. During the study of physical chemistry the students develop critical and analytical way of thinking, which helps them in identifying and solving very different practical and theoretical problems being encountered at any working place during their professional career. They also acquire the ability to critically evaluate whichever (not only physico-chemical) experimental data. Use of scientific literature.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Predavanja - Seminarji	- Lectures - Seminars

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit, ki ga lahko nadomestijo štirje pozitivno ocenjeni kolokviji. Ocenjevanje: 6-10 (pozitivno); 1-5 (negativno).		Written examination, which can be accomplished by achieving positive grades of four written tests. Marks: 6-10 (positive); 1-5 (negative).

Reference nosilca / Lecturer's references:

- A. Jamnik, Effective interaction between large colloidal particles immersed in a bidisperse suspension of short-ranged attractive colloids, J. Chem. Phys. 131, 2009, art. no. 164111-1-1644111-8.
- A. Jamnik, Simulating asymmetric colloidal mixture with adhesive hard sphere model, J. Chem. Phys. 128, 2008, art. no. 234504 (10 str.).
- A. Lajovic, M. Tomšič, G. Fritz-Popovski, L. Vlček, A. Jamnik, Exploring the structural properties of simple aldehydes: A Monte Carlo and small-angle x-ray scattering study, J. Phys. Chem. B 113, 2009, 9429-9435.
- M. Tomšič, A. Jamnik, G. Fritz, O. Glatter, L. Vlček, Structural properties of pure simple

UL FKKT

alcohols from ethanol, propanol, butanol, pentanol, to hexanol: Comparing Monte Carlo simulations with experimental SAXS data, J. Phys. Chem. B 111, 2007, 1738-1751.
- S. Zhou, A. Jamnik, E. Wolfe, S. Buldyrev, Local structure and thermodynamics of a core-softened potential fluid: Theory and simulation, ChemPhysChem. 8, 2007, 138-147.

UL FKKT