



Univerza v Mariboru

Fakulteta za naravoslovje
in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet:	Fizikalna kemija 1
Course title:	Physical Chemistry 1

Študijski program in stopnja

Študijska smer

Letnik

Semester

Study field

Academic year

Semester

Study programme and level

Enovit magistrski študijski program druge stopnje Predmetni učitelj	/	3.	5
Five-year master's degree program Subject Teacher	/		

Vrsta predmeta / Course type

Obvezni / Obligatory

Univerzitetna koda predmeta / University course code:

Predavanja

Seminar

Vaje

Lab. vaje

Terenske vaje

Samost. delo

ECTS

Lectures

Seminar

Tutorial

Laboratory
work

Field work

Individ. work

60

90

5

Nosilec predmeta / Lecturer:

Urban Bren

Jeziki /

Predavanja / Lectures:

slovenski / slovene

Languages:

Vaje / Tutorial:

slovenski / slovene

Prerequisites:

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:

Osnovno znanje splošne in anorganske kemije, matematike in fizike.

Basic knowledge of general and inorganic chemistry, mathematics and physics.

Vsebina:

- Plini in sile med molekulami: idealni plin, kinetična teorija plinov, interakcije med molekulami, van der Waalsov plin
- Energija: prvi zakon termodinamike, spremembe notranje energije in entalpije v fizikalno-kemijskih procesih, termokemija
- Entropija: drugi zakon termodinamike, entropija plinov in plinastih mešanic, entropijske spremembe v fizikalno-kemijskih procesih, tretji zakon termodinamike
- Gibbsova prosta energija: posebna formulacija drugega zakona, spremembe proste energije v fizikalno-kemijskih procesih, kemijski potencial, ravnotežje v fizikalno-kemijskih sistemih
- Ravnotežje čistih snovi: fazni diagram, termodinamika ravnotežnih črt, zamrzovanje, tlak tekočin in parni tlak
- Binarne mešanice: fazno pravilo, idealne mešanice, idealne razredčene mešanice, koligativne lastnosti, topnost, realni plini, fugativnost, realne raztopine, aktivnost
- Fazni diagrami: diagram parnih tlakov, vrelni diagrami, ravnotežje tekoče-tekoče, ravnotežje trdno-tekoče
- Kemijsko ravnotežje: homogeno kemijsko ravnotežje, heterogeno ravnotežje

Content (Syllabus outline):

- Gasses and intermolecular forces : the ideal gas, kinetic theory of gases, intermolecular interactions, the van der Waals gas
- Energy: the first law of thermodynamics, changes of internal energy and enthalpy in physicochemical processes, thermochemistry
- Entropy: the second law of thermodynamics, entropy of gasses and gas mixtures, entropy changes in physicochemical processes, the third law of thermodynamics
- Gibbs free energy: specific formulations of the second law, free energy changes in physicochemical processes, the chemical potential, equilibrium in in physicochemical systems
- Equilibrium in pure substances: the phase diagram, thermodynamics of equilibrium lines, refrigeration, liquid pressure and vapour pressure
- Binary mixtures: the phase rule, ideal mixtures, ideally diluted mixtures, colligative properties, solubility, real gases, fugacity, real liquid mixtures, activity
- Phase diagrams: vapour pressure diagrams, temperature-composition diagrams, liquid-liquid phase diagrams, liquid-solid phase diagrams
- Chemical equilibrium: homogeneous chemical equilibrium, heterogeneous equilibrium

Temeljni literatura in viri / Readings:

- P. W. Atkins, J. de Paula: *Physical Chemistry, 8th Ed.*, Oxford University Press, 2006.

Dodatna literatura:

- P. W. Atkins, J. de Paula: *Physical Chemistry, 7th Ed.*, Oxford University Press, 2002.
- P. W. Atkins: *Physical Chemistry, 6th Ed.*, Oxford University Press, 1998.
- Aljana Petek: *Zapiski predavanj* - interno študijsko gradivo (Course notes), 2007

Cilji in kompetence:

Razumeti fizikalni pomen fizikalno-kemijskih zakonov in formul ter povezave med njimi in to znati uporabiti pri plinih, tekočinah, trdnih snoveh in raztopinah.

Objectives and competences:

Have more insight in the physical meaning of the physicochemical principles and formulas and the links between them and applied these to gases, liquids, solids, and solutions.

Predvideni študijski rezultati:

Znanje in razumevanje:

Po zaključku tega predmeta bo študent sposoben:

- razumeti pojme in zakone kemijske termodinamike in njihove uporabe v fizikalnem in kemijskem ravnotežju;
- razumeti osnovne pojme v termodinamiki raztopin elektrolitov in ravnotežni elektrokemiji.

Prenesljive/ključne spretnosti in drugi atributi:

Študenti bodo razvili spretnost pisnega komuniciranja, reševanja problemov, računanja, kot tudi sposobnost samostojnega študija.

Intended learning outcomes:

Knowledge and understanding:

On completion of this course the student will be able to:

- understand the concepts, laws and ways of thinking of chemical thermodynamics and its applications to physical and chemical equilibrium;
- have insight into fundamental concepts of thermodynamics of electrolyte solutions and equilibrium electrochemistry.

Transferable/Key Skills and other attributes:

Students will develop written communication skills, problem solving, computational skills, as will the ability to study independently.

Metode poučevanja in učenja:	Learning and teaching methods:
• Predavanja • Reševanje problemov • Domače naloge	• Classroom lectures • Classroom problem solving sessions, • Homework assignments.

Delež (v %) /

Načini ocenjevanja:

Weight (in %)

Assessment:

• Pisni izpit • Ustni izpit	50	• Written exam • Oral exam
	50	

Opombe:

Pisni in ustni izpit se lahko nadomestita s kolokviji v enakem deležu 50%.

Comments:

Written and oral exam can be replaced by written midterm examination in the weight of 50%.

Reference nosilca / Lecturer's references:

1. UDOMMANEETHANAKIT, Thanyarat, RUNGROTMONGKOL, Thanyada, FRECEER, Vladimir, SENECEI, Pierfausto, STANISLAV, Miertus, BREN, Urban. Drugs against avian influenza A virus : design of novel sulfonate inhibitors of neuraminidase N1. *Current pharmaceutical design*, ISSN 1381-6128, 2014, vol. 20, issue 21, str. 3478-3487. <http://www.eurekaselect.com/114879/article>, doi: 10.2174/13816128113199990629. [COBISS.SI-ID 5396250]
2. GRAF, Michael, BREN, Urban, HALTRICH, Dietmar, OOSTENBRINK, Chris. Molecular dynamics simulations give insight into D-glucose dioxidation at C [sub] 2 and C [sub] 3 by Agaricus meleagris pyranose dehydrogenase. *Journal of computer-aided molecular design*, ISSN 0920-654X, 2013, vol. 27, iss. 4, str. 295-304, ilustr., doi: 10.1007/s10822-013-9645-7. [COBISS.SI-ID 5218330]
3. BREN, Urban, OOSTENBRINK, Chris. Cytochrome P450 3A4 inhibition by ketoconazole : tackling the problem of ligand cooperativity using molecular dynamics simulations and free-energy calculations. *Journal of chemical information and modeling*, ISSN 1549-9596. [Print ed.], 2012, vol. 52, issue 6, str. 1573-1582. <http://pubs.acs.org/doi/abs/10.1021/ci300118x>, doi: 10.1021/ci300118x. [COBISS.SI-ID 4965658]
4. BREN, Urban, JANEŽIČ, Dušanka. Individual degrees of freedom and the solvation properties of water. *The Journal of chemical physics*, ISSN 0021-9606, 2012, vol. 137, iss. 2, str. 024108-1-024108-11. http://jcp.aip.org/resource/1/jcpsa6/v137/i2/p024108_s1?isAuthorized=no. [COBISS.SI-ID 5014554]
5. BREN, Matevž, JANEŽIČ, Dušanka, BREN, Urban. Microwave catalysis revisited : an analytical solution. *The journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory*, ISSN 1089-5639, 2010, vol. 114, iss. 12, str. 4197-4202, ilustr. [COBISS.SI-ID 1851882]