Univerza v Mariboru

Fakulteta za naravoslovje in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	**Fizikalna kemija 1**
Course title:	**Physical Chemistry 1**

	Študijska smer **Study field**	**Letnik** **Academic year**	**Semester** **Semester**
Študijski program in stopnja **Study programme and level**			
Enovit magistrski študijski program druge stopnje Predmetni učitelj	**/**	**3.**	**zimski** **Autumn**
Five-year master's degree program Subject Teacher	**/**		

Vrsta predmeta / Course type	Obvezni / Obligatory
Univerzitetna koda predmeta / University course code:	

Predavanja **Lectures**	**Seminar** **Seminar**	**Vaje** **Tutorial**	**Lab. vaje** **Laboratory work**	**Terenske vaje** **Field work**	**Samost. delo** **Individ. work**	**ECTS**
60					**90**	**5**

Nosilec predmeta / Lecturer:	Urban Bren

Jeziki / **Languages:**	**Predavanja / Lectures:**	slovenski / slovene
	Vaje / Tutorial:	slovenski / slovene

Prerequisits:

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:	**Content (Syllabus outline):**
• 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	• 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 • Equlibrium 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 equlibrium: homogeneous chemical equlibrium, heterogeneous equilibrium

Temeljni literatura in viri / Readings:

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

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
• Pisni izpit, • Ustni izpit.	50 50	• Written examination, • Oral examination.

Reference nosilca / Lecturer's references:

1. UDOMMANEETHANAKIT, Thanyarat, RUNGROTMONGKOL, Thanyada, FRECER, Vladimir, SENECI, 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]