



Univerza v Mariboru

Fakulteta za kemijo
in kemijsko tehnologijo

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet:	Fizikalna kemija II
Course title:	Physical Chemistry II

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Izobraževalna kemija / 1. stopnja UN Educational Chemistry / 1 st level UN		3.	poletni Spring

Vrsta predmeta / Course type:

Univerzitetna koda predmeta / University course code:

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Laboratory work	Teren. vaje Field work	Samost. delo Individ. work	ECTS
30	15		60		195	10

Nosilec predmeta / Lecturer:

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

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

Osnovno znanje matematike, fizike in fizikalne kemije

Prerequisites:

Basic knowledge of mathematics, physics and physical chemistry

Vsebina:

- Molekule v gibanju: Kinetičen model plina, Transportne lastnosti idealnega plina, Prevodnost raztopin elektrolitov, Difuzija
- Kemijska kinetika: Eksperimentalna kinetika, Mehanizem reakcije, Kinetika kompleksnih reakcij, Reakcije v plinih, Reakcije v tekočinah
- Procesi na trdnih površinah: Adsorpcija, Kataliza, Reakcije na površinah
- Laboratorijske vaje: Kalorimetrija, Parni tlak in izparilna entalpija, Viskoznost, Površinska napetost, Parcialna molska prostornina, Krioskopija, Vrelni diagrami, Heterogeno ravnotežje, Galvanski členi, Prevodnost

Content (Syllabus outline):

- Molecules in motion: The kinetic model of gases, Transport properties of a perfect gas, The conductivities of electrolyte solutions, Diffusion
- Chemical kinetics: Experimental kinetics, The reaction mechanism, The kinetics of complex reactions, Gas reactions, Liquid phase reactions
- Processes at solid surfaces: Adsorption, Catalysis, Reaction at surfaces
- Laboratory: Calorimetry, Vapour pressure and Enthalpy of vaporization, Viscosity, Surface tension, Partial molar volume, Cryoscopy, Temperature – composition diagrams,

elektrolitov, Transportno število, Kemijska kinetika, Adsorpcija

Heterogeneous equilibrium, Electrochemical cells, Conductivity of electrolyte solutions, Transport number, Chemical kinetics, Adsorption

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.
- Več avtorjev: *Laboratorijske vaje iz fizikalne kemije*, FKKT – UL Ljubljana, 2000.

Cilji in kompetence:

Razumeti fizikalni pomen fizikalno-kemijskih zakonitosti in formul ter povezave med njimi in to znati uporabiti pri reševanju enostavnih znanstvenih problemov. Pridobiti osnovne spretnosti za izvedbo in ovrednotenje eksperimentalnih meritev.

Objectives and competences:

Have more insight in the physical meaning of the physicochemical principles and formulas and the links between them and apply these when solving simple scientific problems. Acquiring basic skills to conduct and evaluate experimental measurements.

Predvideni študijski rezultati:

Znanje in razumevanje:

Po zaključku tega predmeta bo študent sposoben:

- določiti lastnosti idealnih plinov na osnovi kinetične molekularne teorije;
- razumeti, kako izpeljemo iz eksperimentalnih podatkov hitrostne zakone, v kakšni povezavi so hitrostni zakoni in reakcijski mehanizmi in kako teoretično razložimo reakcijsko hitrost.

Prenesljive/ključne spretnosti in drugi atributi:

Študenti bodo razvili spretnost pisnega komuniciranja, reševanja problemov, kritičnega in logičnega razmišljanja, kot tudi sposobnost samostojnega študija.

Intended learning outcomes:

Knowledge and Understanding:

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

- determine properties of ideal gases using kinetic molecular theory;
- understand how rate equations are deduced from experimental data, how rate equations and reaction mechanisms are related and how the reaction rate is interpreted theoretically.

Transferable/Key Skills and other attributes:

Students will develop written communication skills, problem solving, critical and logical thinking, as will the ability to study independently.

Metode poučevanja in učenja:

Predavanja, reševanje problemov, domače naloge, laboratorijske vaje

Learning and teaching methods:

Classroom lectures, Classroom problem solving sessions, homework assignment, laboratory work

Načini ocenjevanja:

Delež (v %) /

Weight (in %)

Assessment:

Izpit je opravljen, če so pozitivno opravljene naslednje obveznosti:

- računski del izpita
- teoretični del izpita
- laboratorijske vaje

35
35
30

Student has to pass successfully the following obligations:

- the calculus part of the exam
- the theoretical part of the exam
- lab work

Računski in teoretični del tvorita celoto in se

The calculus and the theoretical part of exam

preverjata hkrati. Izpit se lahko nadomesti s sprotnimi testi.		are performed simultaneously. The exam can be replaced with partial exams.
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Reference nosilca / Lecturer's references:

UDOMMANEETHANAKIT, Thanyarat, RUNGROTMONGKOL, Thanyada, FRECER, Vladimir, SENECL, 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](https://doi.org/10.2174/13816128113199990629). [COBISS.SI-ID [5396250](#)], [JCR, SNIP, WoS do 4. 8. 2014: št. citatov (TC): 1, čistih citatov (CI): 1, normirano št. čistih citatov (NC): 0, Scopus do 22. 7. 2014: št. citatov (TC): 1, čistih citatov (CI): 1, normirano št. čistih citatov (NC): 0]

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](https://doi.org/10.1007/s10822-013-9645-7). [COBISS.SI-ID [5218330](#)], [JCR, SNIP, WoS do 4. 6. 2014: št. citatov (TC): 3, čistih citatov (CI): 3, normirano št. čistih citatov (NC): 2, Scopus do 28. 5. 2014: št. citatov (TC): 3, čistih citatov (CI): 3, normirano št. čistih citatov (NC): 2]

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](https://doi.org/10.1021/ci300118x). [COBISS.SI-ID [4965658](#)], [JCR, SNIP, WoS do 3. 9. 2014: št. citatov (TC): 15, čistih citatov (CI): 13, normirano št. čistih citatov (NC): 10, Scopus do 20. 8. 2014: št. citatov (TC): 15, čistih citatov (CI): 13, normirano št. čistih citatov (NC): 42]

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](#)], [JCR, SNIP, WoS do 4. 8. 2014: št. citatov (TC): 10, čistih citatov (CI): 9, normirano št. čistih citatov (NC): 4, Scopus do 13. 8. 2014: št. citatov (TC): 12, čistih citatov (CI): 11, normirano št. čistih citatov (NC): 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](#)], [JCR, SNIP, WoS do 8. 7. 2014: št. citatov (TC): 6, čistih citatov (CI): 5, normirano št. čistih citatov (NC): 3, Scopus do 12. 8. 2014: št. citatov (TC): 6, čistih citatov (CI): 5, normirano št. čistih citatov (NC): 3]