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
MAG Kemija, 2. stopnja	/	1.	2.
USP Chemistry, 2nd Cycle	/	1st	2nd

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE214

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	30	/	/	/	75	5

Nosilec predmeta / Lecturer: prof. dr. Barbara Hribar Lee / Dr. Barbara Hribar Lee, Full Professor
prof. dr. Vojeslav Vlachy / Dr. Vojeslav Vlachy, 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):
Osnove: Merjenje, časovna odvisnost in časovno povprečje. Zakona statistične termodinamike. Opis mikroskopskega stanja. Kanonična porazdelitev. Povprečja in kolebanja okoli povprečne vrednosti, povezava s termodinamiko. Izolirani sistem. Odprt sistem, kolebanja koncentracije, stisljivost in stabilnost sistema. Drugi sistemi. Neodvisni podsistemi: Einsteinov model kristala. Paramagnetna snov. Fermi-Diracova in Bose−Einsteinova statistika. Boltzmannova statistika: razredčeni plini. Izračun konstante kemijskega ravnotežja. Adsorbcija, Langmuirjeva in B.E.T. izoterma, vezanje ligandov na makromolekulo.	Introduction: Time-average of measured quantity. Laws of statistical thermodynamics. Description of microscopic state of a system. Canonical distribution. Averages and fluctuations; the relations with thermodynamics. Isolated system. Open system, concentration fluctuations, compressibility, stability of the system. Other (N,P,T) systems. Independent subsystems: Einstein model of crystal. Paramagnetic materials. Fermi-Dirac and Bose-Einstein statistics. Boltzmann statistics: diluted gasses. Evaluation of the chemical equilibrium constant. Adsorption, Langmuir and B.E.T. isotherms, ligand binding to

Klasična statistična termodinamika: Konfiguracijski integral in povprečja. Parski potencial. Računalniške simulacije, metoda Monte Carlo, molekulska dinamika. Teorije na osnovi parske porazdelitvene funkcije. Računanje termodinamičnih količin (notranja energija, enačbe stanja). Osnove termodinamične perturbacijske teorije.	macromolecules. Classical statistical thermodynamics: Configuration integral and averages. Pair potential. Introduction to computer simulations, Monte Carlo method, molecular dynamics. Evaluation of thermodynamic quantities (internal energy, equation of state). An introduction to thermodynamic perturbation theory.

Temeljna literatura in viri / Readings:

- Friedman, H. L., *A Course in Statistical Mechanics*, New Jersey: Prantice-Hall, 1985, pp 1-109.
- Hill, T. L., *Introduction to Statistical Thermodynamics*, Reading: Addison-Wesley, 1960, pp 124-188.
- V. Vlachy, B. Hribar Lee: Fizikalna kemija II - Uvod v statistično termodinamiko, skripta

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Naloga statistične termodinamike je, da iz podatkov o lastnostih atomov in molekul ter sil med njimi izpelje makroskopske lastnosti snovi. Na ta način omogoča molekularno interpretacijo merskih podatkov. *Kompetence:* V prvem delu obravnavamo osnove statistične termodinamike, le−te omogočajo globje razumevanje pojavov kot so toplota, entropija, termodinamično povprečje, kolebanje okoli povprečne vrednosti in drugi. Drugi del predmeta je namenjen prikazu posameznih primerov uporabe statistične termodinamike v kemiji in sorodnih vedah.	***Objectives:*** The purpose of statistical thermodynamics is to predict macroscopic properties of a given thermodynamic system, using as input the knowledge about constituent atoms (or molecules) and intermolecular forces between them. It makes possible to interpret the experimental data from molecular point of view. ***Competences:*** Profound understanding of thermodynamic quantities, such as heat, entropy, thermodynamic averages, fluctuations, and others. Application to real chemical and physical problems.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Poznavanje osnov statistične termodinamike, ki jih obravnava predmet Fizikalna kemija, omogoča globlje razumevanje pojmov iz fizikalne kemije ter interpretacijo eksperimentalnih podatkov na osnovi lastnosti atomov in molekul.	Knowledge and Comprehension The basic knowledge of statistical thermodynamics that is the subject of this course enables the students a deeper understanding of the physical chemistry concepts, as well as the interpretations of the experimental data in view of the properties of atoms and molecules.

Uporaba Pri tem predmetu se spoznamo z modernimi teoretičnimi metodami za študij lastnosti snovi. Metode se uporabljajo v kemiji, farmaciji in biologiji, pa tudi pri načrtovanju različnih tehnoloških procesov kot so, na primer, separacijske metode. Predmet je osnova raziskovalnemu delu na področju kemije.	Application The students get to know the modern theoretical methods used for studying the properties of different substences. The methods are used in chemistry, pharmacy and biology, as well as in planning different technologocal processes, such as separation methods. The course is prociding the bases for the research work in the chemistry field.
Refleksija Znanja, ki jih študent osvoji pri tem predmetu, pomagajo pri kritičnem vrednotenju merskih podatkov, razumevanju lastnosti fizikalnih sistemov in s tem omogočajo kvalitetno in samostojno delo na drugih področjih kemije.	Analysis The knowledge that the students obtain via this course is meant to be used in the critical assesment of measuring data, as well as the understanding the system properties which is neede in different areas of chemistry.
Prenosljive spretnosti Spretnosti uporabe domače in tuje literature in drugih virov, identifikacija in reševanje problemov, kritična analiza rezultatov, kvantitativno razumevanje drugih (bolj opisnih) predmetov.	Skill-transference Ability The ability of using different literature, as well as other resources, identification and problem solving, critical evaluation of the results, quantitative interpretation of knowledge obtained in other courses.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Predavanja, seminarji.	- Lectures - Seminars

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni (nadomestita ga lahko dva pozitivno ocenjena kolokvija) in ustni izpit.		Written and oral exam.

Reference nosilca / Lecturer's references:

- DILL, Ken A., TRUSKETT, Thomas Michael, VLACHY, Vojko, **HRIBAR-LEE, Barbara**. Modeling water, the hydrophobic effect, and ion solvation. Annu Rev Biophys Biomol Struct, 2005, vol. 34, str. 173-199.
- JARDAT, Marie, HRIBAR, Barbara, VLACHY, Vojko. Self-diffusion of ions in charged nanoporous media. *Soft matter*, 2012, vol. 8, no. 4, str. 954-964.
- HRIBAR, Barbara, LUKŠIČ, Miha, VLACHY, Vojko. Partly-quenched systems containing charges. Structure and dynamics of ions in nanoporous materials. *Annu. rep. prog. chem. Sect C. Phys. chem*, 2011, vol. 107, no. 1, str. 14-46

- B. Jamnik and V. Vlachy, *Ion Partitioning between Charged Micropores and Bulk Electrolyte Solution. Mixtures of Mono- and Divalent Counterions and Monovalent Co-Ions*, J. Am. Chem. Soc. **117**, 8010– 8016 (1995).

- B. Hribar and V. Vlachy, *Evidence of Electrostatic Attraction between Equally Charged Macroions Induced by Divalent Counterions*, J. Phys. Chem. B **101**, 3457– 3459 (1997).
- V. Vlachy, *Ionic Effects Beyond the Poisson-Boltzmann Theory*, Annu. Rev. Phys. Chem. **50**, 145–165 (1999).