UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	METODE SIPANJA ZA DOLOČANJE STRUKTURE IN DINAMIKE V NANOSISTEMIH
Course Title:	METHODS OF SCATTERING FOR DETERMINING STRUCTURE AND DYNAMICS IN NANOSYSTEMS

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

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I20

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
30	**15**	**30 LV**	**/**	**/**	**75**	**5**

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

Jeziki / Languages:

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

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):
Uvod v metode sipanja Svetloba. Interakcija svetlobe s snovjo. Lorentzov model. Lorentzova limita in limita sipanja. Interferenca. **Statično sipanje laserske svetlobe (metoda SLS)** Rayleighovo sipanje, RDG področje. Teorija fluktuacij za razredčene sisteme. Zimmov diagram. Monodisperzni in polidisperzni sistemi. Eksperimentalni sistem. **Ozkokotno rentgensko sipanje (metoda SAXS)** Rayleigh-Debye-Gansova (RDG) teorija. Sipanje in inverzni problem sipanja. Razredčeni monodisperzni sistemi. Radij giracije, molska	**Introduction to scattering methods** Light. Interaction of light with matter. Lorentz model. Lorentz limit and scattering limit. Interference. **Static light scattering (SLS method)** Rayleigh scattering. RDG domain. Fluctuation theory for dilute systems. Zimm plot. Monodisperse and polydisperse systems. Experimental setup. **Small-angle X-ray scattering (SAXS method)** Rayleigh Debye Gans (RDG) theory. Scattering problem and inverse scattering problem. Dilute monodisperse systems. Radius of gyration, molar mass. Indirect Fourier transformation (ITP

masa. Indirektna Fourierova transformacija - metoda IFT. Parska porazdelitvena funkcija razdalj. Notranja struktura delcev. Koncentrirani sistemi. Posplošena indirektna Fourierova transformacija – metoda GIFT. Eksperimentalni sistem. Aplikacije metode SAXS. Osnove ozkoktnega nevtronskega sipanja: kontrast in variacija kontrasta, selektivno devteriranje. Ozkokotno in širokokotno sipanje rentgenske svetlobe (SWAXS). Računanje rentgenskega sipanja modelnih sistemov z računalniškimi simulacijami. Metoda dopolnjenega sistema.

Dinamično sipanje laserske svetlobe (metoda DLS)

Difuzija in hidrodinamski radij delcev. Avtokorelacijska funkcija. Koncentracijski efekti. Inverzna Laplaceova transformacija avtokorelacijske funkcije. Rotacijski difuzijski koeficient. Ergodijski in neergodijski sistemi. Različne inačice tehnike DLS: 3D-DLS, 'multispeckle DLS' in 'echo DLS'.

Laboratorijske vaje

Projektne vaje: Strukturne raziskave izbranih nano-strukturiranih sistemov z metodami SAXS, SLS in DLS – izvedba eksperimentov ter analiza in interpretacija meritev sipanja.

method). Pair distance distribution function. Internal structure of particles. Concentrated systems. Generalized indirect Fourier transformation (GIFT method). Experimental setup. Applications of SAXS method. Basic of small-angle neutron scattering (SANS method). Contrast variation. Selective deuteration. Small- and wide-angle X-ray scattering (SWAXS). Calculation of the x-ray scattering by computer simulations.
Complemented system approach method.

Dynamic light scattering (DLS method)

Diffusion coefficient and hydrodynamic radius of particles. Autocorrelation function. Concentration effects. Inverse Laplace transformation of autocorrelation function. Rotation diffusion coefficient. Ergodic and non-ergodic (arrested) systems. Variants of DLS technique: 3D-DLS, multispeckle DLS, and echo DLS.

Project works

Structural investigation of chosen nano-systems by SAXS, SLS and DLS – performing experiments and analysis and interpretation of experimental data

Temeljna literatura in viri / Readings:

- O. Glatter, Scattering Methods and their Application in Colloid and Interface Science, Elsevier, (2018), 40 % od 404 str., ISBN 978-0-12-813580-8
- O. Glatter in O. Kratky, Small Angle X-Ray Scattering, Academic Press, 2. izdaja (1983), 30 % od 510 str., ISBN 0-12-286280-5
- B. J. Berne in R. Pecora, Dynamic Light Scattering: With Application to Chemistry, Biology, and Physics, Dover Publications (2000), 20 % od 372 str., ISBN 978-0-486-41155-2
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- **Dopolnilna literatura**
- P. Lindner in T. Zemb, Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter, Elsevier (2002), 541 str., ISBN 0-444-51122-9
- R. J. Roe, Methods of X-Ray and Neutron Scattering in Polymer Science, Oxford University Press (2000), 315 str., ISBN 978-0-19-511321-1
- A. Jamnik, Metode sipanja za določanje strukture in dinamike v nanosistemih, zapiski predavanj.

Cilji in kompetence:

Objectives and Competences:

Cilj predmeta je spoznavanje različnih eksperimentalnih metod, ki temeljijo na sipanju rentgenskih žarkov in nevtronov pod majhnimi koti ter sipanju laserske svetlobe. Te metode se uporabljajo za določevanje strukturnih in dinamičnih značilnosti nanosistemov. Študenti si pri predmetu pridobijo naslednje specifične *kompetence:* - razumevanje teorijskega ozadja sipanja svetlobe - pridobitev eksperimentalnih veščin za merjenje ozkokotnega rentgenskega sipanja ter statičnega in dinamičnega sipanja laserske svetlobe - sistematičnost pristopa pri reševanju projektne naloge - uporaba računalniške programske opreme za analizo meritev sipanja - usposobljenost za samostojno reševanje projektnih nalog in za izdelavo poročil	The aim of the course is to learn the different experimental methods, which are based on the small-angle scattering of X-rays and neutrons, and laser light scattering. These methods are used to determine the structural and dynamic characteristics of nanosystems. Students of the course gain the following specific competences: - Understanding the theoretical background of light scattering - The acquisition of skills for the experimental measurement of small-angle scattering and static and dynamic laser light scattering - A systematic approach to dealing with project tasks - The use of computer software for the analysis of experimental data - Ability to independently solve project tasks and to write scientific reports

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Osnovno teorijsko znanje o interakciji elektromagnetnega valovanja (vidna svetloba, rentgenski žarki) s snovjo. Razumevanje pojava sipanja na posameznih sipalnih centrih ter interference sekundarnih valov. Razumevanje pojmov, ki se uporabljajo pri teorijskih obravnavah sipanja, in zakonitosti, ki sledijo iz teh obravnav. Poznavanje eksperimentalnih sistemov za merjenje rentgenskega in laserskega sipanja. Poznavanje numeričnih metod za obdelavo in interpretacijo meritev sipanja ter možnih zaključkov o strukturnih parametrih, ki sledijo iz te analize.	<u>Knowledge and Comprehension</u> Basic theoretical knowledge of the interaction of electromagnetic radiation (visible light, X-rays) with the matter. Understanding the phenomenon of scattering on the individual scattering centres and the interference of secondary waves. Understanding of the concepts used in theoretical treatments of scattering, and of general laws, which follow from these treatments. Knowledge of the experimental system for measuring the X-ray and laser scattering. Knowledge of numerical methods for the data treatment and interpretation of experimental data, and of possible conclusions about the structural parameters that follow from this analysis.
<u>Uporaba</u> Uporaba metod sipanja za določitev strukturnih in dinamičnih lastnosti zelo različnih sistemov, pri katerih gre za notranjo strukturiranost v koloidnem (nano) območju dimenzij (biološki sistemi - proteini, nukleinske kisline, membrane, makromolekule, polimeri, surfaktanti, mikroemulzije).	<u>Application</u> The use of scattering methods to determine the structural and dynamic properties of very different systems which show internal structure of colloidal (nano) dimensions (biological systems - proteins, nucleic acids, membranes, macromolecules, polymers, surfactants, microemulsions).

Refleksija Občutek za povezavo med splošno teorijo in modelnimi izračuni sipanja, ki iz te sledijo, ter eksperimentalnimi rezultati. Kritično ovrednotenje rezultatov, ki sledijo iz numerične analize meritev sipanja.	Analysis Connection between the general scattering theory and model calculations that follow from this theory, and the experimental results. Critical evaluation of the results arising from the numerical analysis of experimental scattering data.
Prenosljive spretnosti Zbiranje in uporaba znanstvenih člankov pri projektnem (raziskovalnem) delu. Poročanje o predelani literaturi, predstavitev rezultatov projektnih vaj, ter pisanje poročila v obliki znanstvenega članka.	Skill-transference Ability Collection and use of scientific articles in the project research work. Reporting on the used literature, presentation of the results of project work and report writing in the form of a scientific article.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji, projektne laboratorijske vaje.	Lectures, seminars, and laboratory practice.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
- Pisni izpit - Predstavitev rezultatov projektnih vaj	50 50	- Written examination - Presentation of the results of project practical work
Ocenjevanje: 6-10 (pozitivno); 1-5 (negativno).		Marks: 6-10 (positive); 1-5 (negative).

Reference nosilca / Lecturer's references:

- J. Orehek, I. Dogša, M. Tomšič, A. Jamnik, D. Kočar, D. Stopar, Structural investigation of carboxymethyl cellulose biodeterioration by *Bacillus subtilis* subsp. *subtilis* NCIB 3610, Int. Biodeterioration & Biodegradation 77, 2013, 10-17.
- A. Vrhovšek, O. Gereben, A. Jamnik, L. Pusztai, Hydrogen bonding and molecular aggregates in liquid methanol, ethanol, and 1-propanol, J. Phys. Chem. B 115, 2011, 13473-13488.
- 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.
- J. Cerar, A. Jamnik, I. Pethes, L. Temleitner, L. Pusztai, M. Tomšič, Structural, rheological and dynamic aspects of hydrogen-bonding molecular liquids : aqueous solutions of hydrotropic tert-butyl alcohol, Journal of colloid and interface science, 560, 2020, 730-742.
- M. Tomšič, J. Cerar, A. Jamnik, Supramolecular structure vs. rheological properties : 1,4-butanediol at room and elevated temperatures, Journal of colloid and interface science, 557, 2019, 328-335.
- I. Dogsa, J. Cerar, A. Jamnik, M. Tomšič, Supramolecular structure of methyl cellulose and lambda- and kappa-carrageenan in water: SAXS study using the string-of-beads model, Carbohydrate polymers, 172, 2017, 184-196.
- E. Benigar, A. Zupančič-Valant, I. Dogša, S. Sretenović, D. Stopar, A. Jamnik, M. Tomšič,

Structure and dynamics of a model polymer mixture mimicking a levan-based bacterial biofilm of Bacillus subtilis. Langmuir, 32, 2016, 8182-8194.

- A. Lajovic, M. Tomšič, A. Jamnik, The complemented system approach: a novel method for calculating the x-ray scattering from computer simulation, The journal of chemical physics, 333, 2010, 174123.
- M. Tomšič, A. Jamnik, G. Fritz, O. Glatter, L. Vlček, Structural properties of pure simple alcohols from ethanol, propanol, butanol, pentanol, to hexanol: comparing Monte Carlo simulations with experimental SAXS data, The journal of physical chemistry B, 111, 2007, 1738-1751.