UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Karakterizacija sestave in strukture
Course title:	Characterisation of Structure

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Nanoznanosti in nanotehnologije, 3.stopnja	/	1	1
Nanosciences and Nanotechnologies, 3rd cycle	/	1	1

Vrsta predmeta / Course type Izbirni / Elective

Univerzitetna koda predmeta / University course code: NANO-805

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Laboratory work	Druge oblike Others	Samost. delo Individ. work	ECTS
15	**15**			**15**	**105**	**5**

**Navedena porazdelitev ur velja, če je vpisanih vsaj 15 študentov. Drugače se obseg izvedbe kontaktnih ur sorazmerno zmanjša in prenese v samostojno delo. / This distribution of hours is valid if at least 15 students are enrolled. Otherwise the contact hours are linearly reduced and transfered to individual work.*

Nosilec predmeta / Lecturer: Prof. dr. Iztok Arčon

Jeziki / Languages:	**Predavanja / Lectures:**	slovenščina, angleščina / Slovenian, English
	Vaje / Tutorial:	

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisites:**
Zaključena izobrazba druge stopnje ali univerzitetna izobrazba s področja naravoslovja ali tehnologije.	Completed second level education or university education from natural sciences or technology.

Vsebina:	**Content (Syllabus outline):**
Slušatelji se podrobneje seznanijo s posameznimi rentgenskimi absorpcijskimi spektroskopskimi metodami (npr. rentgenske absorpcijske in emisijske spektroskopije, EXAFS, (mikro)XANES, mikroXRF), ki se najpogosteje uporabljajo pri karakterizaciji sodobnih funkcionalnih materialov (v kristaliničnih, nanostrukturnih ali amorfnih oblikah in v obliki tekočih sol-gelov), kot so katalizatorji, Li-ionske baterije in podobni. Predstavljene so lastnosti najpomembnejših, predvsem sinhrotronskih virov svetlobe in žarkovnih linij, ki jih posamezne spektroskopske metode izkoriščajo. Poudarek je na uporabnosti posameznih spektroskopskih metod in njihovem medsebojnem dopolnjevanju ter uporabi v in-situ	Students are acquainted in detail with individual spectroscopic methods (e.g. X-ray absorption and emission spectroscopy EXAFS, (micro)XANES, microXRF), which are most frequently used in the characterization of materials (in crystalline, nanostructured or amorphous state, or liquids and sol-gels), as for example catalysts or Li-Ion batteries. The course presents the properties of the most important, particularly synchrotron radiation sources and experimental stations used by individual spectroscopic methods. Emphasis is placed on the applicability of individual spectroscopic methods and their complementarities and the use of these spectroscopies in-situ and in-operando. Students use real cases to learn basics of

ali in-operando načinu. Študentje se na realnih primerih naučijo osnov analize strukturnih lastnosti materiala.	the analysis of specific material structural properties.

Temeljna literatura in viri / Readings:

Učbeniki in članki / books and articles

- G. Bunker, "Introduction to XAFS: A Practical Guide to X-ray Absorption Fine Structure Spectroscopy", Cambridge University Press, 2010
- X-ray absorption spectroscopy (principles, applications, techniques of EXAFS, SEXAFS and XANES), edited by D. C. Konnigsberger and R. Prins, John Wiley and Sons, NY (1988)
- B. Beckhoff, B. Kanngiesser, N. Langhoff R. Wedell H. Wolff, Handbook of Practical X-Ray Fluorescence Analysis, Springer-Verlag Berlin Heidelberg 2006, ISBN-10 3-540-28603-9 Springer Berlin, Heidelberg
- J. J. Rehr, R. C. Albers, Theoretical approaches to x-ray absorption fine structure, Reviews of Modern Physics, Vol. 72, No. 3, July 2000, 621-654
- Arčon, Introduction to XANES and EXAFS analysis. Nova Gorica: [I. Arčon], 2008. 35 str., ilustr. [COBISS.SI-ID 933883]
- Arčon, X-ray absorption spectroscopy : a practical guide to structural analysis of materials with EXAFS and XANES analysis. Nova Gorica: [I. Arčon], 2008. 51 str., ilustr. [COBISS.SI-ID 934139]
- Katarina Vogel-Mikuš, Iztok Arčon, Peter Kump, Primož Pelicon, Marijan Nečemer, Primož Vavpetič, Špela Koren, Marjana Regvar, Analytical tools for exploring metal accumulation and tolerance in plants.
  Phytotechnologies : remediation of environmental contaminants. Boca Raton (FL): Taylor & Francis, cop. V: Naser A. Anjum, (ed.). (2013) 443-495
- V. Kaučič, N. Zabukovec Logar, I. Arčon,. Characterisation of microporous and mesoporous solids using complementary diffraction and X-ray absorption spectroscopic techniques. V: Characterization techniques for zeolites and related materials : state of the art and recent developments. [S.l.: s.n.], 2008, str. 91-123. 2nd FEZA school 2008, Universite Pierre et marie Curie, Paris, September 1-2, 2008 [COBISS.SI-ID 3992602]

Literatura na svetovnem spletu / Sources on the web:

- I. Arčon: Spletno študijsko gradivo za rentgensko absorpcijsko spektrometrijo / X-ray absorption spectroscopy:
  http://www.p-ng.si/~arcon/xas in http://www.p-ng.si/~arcon/xas-si
- M. Newville and B. Ravel: DEMETER software and documentation for XANES and EXAFS analysis (XAS software 2015) http://bruceravel.github.com/demeter/

Video-predavanja na svetovnem spletu/ Videolectures on the web:

- S. Pascarelli (ESRF), An introduction to X-ray Absorption Spectroscopy and EXAFS, Video, http://indico.ictp.it/event/a13226/session/0/contribution/3/material/video/
- G. Aquilanti (Elettra), XAFS studies in Environmental and Material Sciences, Video, http://indico.ictp.it/event/a13226/session/1/contribution/5/material/video/
- I. Arčon (UNG), In operando XAS analysis of Li-ion and Li-sulphur batteries, Video, http://indico.ictp.it/event/a13226/session/2/contribution/13/material/video
- Bruce Ravel: XAS course 2011
  http://www.diamond.ac.uk/Beamlines/Spectroscopy/Techniques/XAS.html

Cilji in kompetence:	**Objectives and competences:**
Pri predmetu študenti spoznajo osnove sodobne rentgenske spektroskopske (XAS) in mikroskopske metode pri karakterizaciji atomske in elektronske	In this course, the students learn basics of modern X-ray absorption spectroscopic (XAS) and microscopic methods for the characterization of the

strukture materialov s sinhrotronsko svetlobo. Splošne kompetence: • obvladanje raziskovalnih metod, postopkov in procesov, razvoj kritične in samokritične presoje, • sposobnost uporabe znanja v praksi, • razvoj komunikacijskih sposobnosti in spretnosti, posebej komunikacije v mednarodnem okolju, • kooperativnost, delo v skupini (in v mednarodnem okolju) Predmetnospecifične kompetence: Predmet pripravlja študente za uporabna znanja s področja sodobnih rentgenskih absorpcijskih spektroskopskih in mikroskopskih metod s sinhrotronsko svetlobo pri karakterizaciji atomske in elektronske strukture (nano)materialov. Študentje pridobijo osnovna znanja in veščine za načrtovanje in uporabo rentgenske abosorpcijske in fluorescenčne spektroskopije ((mikro) XANES, EXAFS, (mikro)XRF) s sinhrotronsko svetlobo za karakterizacijo materialov.	atomic and molecular structure of materials with synchrotron radiation. General Competences: • The student will master research methods, procedures and processes • The student will develop critical thinking • The student will develop communications skills to present research achievement in the international environment • Work in team (in international environment) Course Specific Competences: Students gain basic applied knowledge about up-to-date X-ray absorption spectroscopic and microscopic methods with synchrotron radiation for the characterization of the atomic and molecular structure of (nano)materials.They gain basic knowledge to plan and use x-ray absorption and fluorescence methods ((mikro) XANES, EXAFS, (mikro)XRF) with synchrotron radiation for material characterization.

Predvideni študijski rezultati:	**Intended learning outcomes:**
Znanje in razumevanje: Razumevanje sodobnih rentgenskih spektroskopskih in mikroskopskih metod (XAS) pri karakterizaciji atomske in elektronske strukture materialov s sinhrotronsko svetlobo. Študentje znajo: - načrtovati XAS experiment s sinhrotronsko svetlobo, - napisati, utemeljiti in upravičiti predlog za meritve XAS na sinhrotronskih žarkovnih linijah po mednarodnih standardih - kvantitativno ovrednotiti rezultate XAS - povezati strukturne rezultate, pridobljene z XAS, z rezultati drugih metod za karakterizacijo preiskovanega materiala	Knowledge and Understanding The student will understand modern X-ray absorption spectroscopic and microscopic methods for the characterization of the atomic and molecular structure of materials with synchrotron radiation Students know how to: • Plan XAS experiment with synchrotron radiation • Write argumentation and justify a proposal for XAS experiment at synchrotron radiation facilitiy following international standards • Quantitatively evaluate XAS results • Connect XAS structural results with results of other methods for the characterisation of the investigated material

Metode poučevanja in učenja:	**Learning and teaching methods:**
• Predavanja in diskusije • Vaje na programski opremi za analizo XAS spektrov na primerih iz raziskovalne prakse pod vodstvom nosilca predmeta.	• Lectures and discussions • Exercises on state of the art software for the analysis of XAS spectra on real data from research practice, under supervision of the the lecturer responsible for the course

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Preverjanje znanja poteka v obliki: 1) individualnih projektnih nalog iz analize rentgenskih absorpcijskih spektrov ter kvantitativnih numeričnih analiz spektrov EXAFS in XANES na realnih primerih iz raziskovalne prakse. 2) zaključnega projekta, pri katerem študentje pripravijo predlog eksperimenta na izbrani sinhrotronski merilni postaji. Projektne naloge in zaključni projekt oddajo v pisni obliki in jih zagovarjajo v ustni obliki v diskusiji z nosilcem predmeta in ostalimi študenti.	50 % 50 %	During the course students prepare: 1) projects on on X-ray absorption spectroscopy and on quantitative EXAFS and XANES analysis on real data from research practice. 2) At the end of the course they prepare a final project, i.e. experiment proposal for beamtime at a selected synchrotron X-ray absoprtion beamline. All projects are prepared in a written form and defended orally in an open discussion with professor and students.

Reference nosilca / Lecturer's references:

1. Arcon I., Paganelli S., Piccolo O., Gallo M., Vogel-Mikus K., Baldi F., XAS analysis of iron and palladium bonded to a polysaccharide produced anaerobically by a strain of Klebsiella oxytoca , Journal of Synchrotron Radiation 22, 1215-1226 (2015)

2. DOMINKO, Robert, VIŽINTIN, Alen, AQUILANTI, Giuliana, STIEVANO, Lorenzo, JOSEPH HELEN, Maria, REDDY MUNNANGI, Anji, FICHTNER, Maximilian, ARČON, Iztok. Polysulfides formation in different electrolytes from the perspective of X-ray absorption spectroscopy. *Journal of the Electrochemical Society*, ISSN 1945-7111. [Online ed.], vol. 165, no. 1, str. A5014-A5019, (2018)

3. VOGEL-MIKUŠ, Katarina, ARČON, Iztok, KUMP, Peter, PELICON, Primož, NEČEMER, Marijan, VAVPETIČ, Primož, KOREN, Špela, REGVAR, Marjana. Analytical tools for exploring metal accumulation and tolerance in plants. V: ANJUM, Naser A. (ur.). Phytotechnologies : remediation of environmental contaminants. Boca Raton (FL): Taylor & Francis, cop., str. 443-495, (2013)

4. PLIEKHOV, Oleksii, ARČON, Iztok, NOVAK TUŠAR, Nataša, LAVRENČIČ ŠTANGAR, Urška. Photocatalytic activity of zirconium- and manganese-codoped titania in aqueous media : the role of the metal dopant and its incorporation site. *ChemCatChem*, ISSN 1867-3899, vol. 8, iss. 12, str. 2109-2118, (2016)

5. ČIŽMAR, Tihana, LAVRENČIČ ŠTANGAR, Urška, ARČON, Iztok. Correlations between photocatalytic activity and chemical structure of Cu-modified TiO2−SiO2 nanoparticle composites. *Catalysis today*, , vol. 287, str. 155-160, (2017)