UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Rentgenska strukturna analiza
Course title:	X-ray Structure Analysis

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

Vrsta predmeta / Course type Izbirni / Elective

Univerzitetna koda predmeta / University course code: NANO3-771

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje work	Druge oblike študija	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 transferred to individual work.*

Nosilec predmeta / Lecturer: Doc. dr. Evgeny Goreshnik

Jeziki / Languages:	
Predavanja / Lectures:	slovenščina, angleščina Slovenian, English
Seminar:	slovenščina, angleščina Slovenian, English

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisits:**
Zaključen študij druge stopnje naravoslovne ali tehniške smeri ali zaključen študij drugih smeri z dokazanim poznavanjem osnov področja predmeta (pisna dokazila, pogovor).	Completed second level studies in natural sciences or engineering or completed second level studies in other fields with proven knowledge of fundamentals in the field of this course (certificates, interview).

Vsebina:	**Content (Syllabus outline):**
Najbolj informativna metoda za določanje kristalnih struktur - rentgenska strukturna analiza, je na široko opisana v knjigah in na spletnih straneh. Na žalost pa so temeljna načela in teoretične osnove rentgenske difrakcije, rešitve in izboljševanje kristalnih struktur, kot tudi rezultati zmanjševanja neidealnosti kristalov, pogosto objavljeni ločeno od praktičnih nasvetov. Tečaj je namenjen: • hitremu pregledu temeljnih načel difrakcijske	The most informative method to study crystal structure – X-ray structure analysis is described widely in both printed books and internet – resources. Unfortunately, fundamental principles and theoretical base of X-ray diffraction, crystal structures solution and refinement, reducing results of crystals imperfectness are published frequently separately from the advices on practical technique. The course is designed to: • quickly touch the basic principles of the

analize atomske strukture kristaliničnih materialov
- razlage fizikalnih osnov interakcije kristalov z rentgenskimi žarki, elektroni in počasnimi nevtroni
- razpravi o točkovnih in prostorskih skupinah ter metodah za določevanje simetrije.
- analize glavnih eksperimentalnih težav, s katerimi se srečujemo pri reševanju kristalnih struktur.

Večji del bo namenjen:
- reševanju in rafiniranju kristalnih struktur različnih spojin z uporabo najpogostejših za te namene uporabnih programskih orodij, (Superflip, Shelxt, SIR, Shelxs in Shelxl) ki se izvajajo v okviru programskega paketa Olex2
- ocenjevanju in interpretacije rezultatov
- prepoznavanju različnih težav in načinov reševanja le-teh.
- pripravi rezultatov za objavo
- preverjanju kakovosti materialov s pomočjo internetnih orodij.

diffraction analysis of the atomic structure of crystalline materials
- explain the physical basis of interaction of X-rays and electrons and slow neutrons with matter
- discuss point and space groups, methods of determining the characteristics of symmetry
- analyze the main experimental problems in diffraction studies of crystal structure.

The major part is devoted to:
- solving and refining crystal structures of various compounds using the most common for these purposes Superflip, Shelxt, SIR, Shelxs and Shelxl software implemented in a program package Olex2
- structures analyses and interpretation
- finding indications of different troubles and the ways how to resolve it
- preparing results for publication
- checking the quality of prepared materials using internet-services.

Temeljni literatura in viri / Readings:

- Werner Massa. Crystal structure determination. Second edition. Springer, 2004. 210 p.
- U. Shmueli. Theories and techniques of crystal structure determination. Oxford University Press, 2007. 269 p.
- Crystal structure analysis: principles and practice, second edition. W. Clegg, editor. Oxford science publication, 2009. 387 p.

Cilji in kompetence:

Glavni cilji predmeta so, da študenti pridobijo praktično znanje, kako rešiti, rafinirati, interpretirati in objaviti kristalno strukturo (majhne molekule) ter rešiti probleme, ki se pogosto pojavijo.

Splošne kompetence:
Praktična sposobnost rešiti in opisati kristalno strukturo, najti in rešiti večino običajnih težav.

Predmetno-specifične kompetence:
Sposobnost za reševanje, opis in razlago kristalne strukture.

Objectives and competences:

The main goals of the course are to give students practical knowledge how to solve, refine, interprete and publish crystal structure (small molecules) and to resolve frequently appeared problems.

General Competences:
Practical abilities to solve and describe crystal structure, find and resolve most usual difficulties.

Course Specific Competences:
Abilities to solve, describe and interpret the crystal structure.

Predvideni študijski rezultati (Izidi):	**Intended learning outcomes:**
Študent pridobi: • praktično sposobnost rešiti in opisati kristalno strukturo, • sposobnost najti in rešiti večino običajnih težav pri reševanju kristalne strukture.	The student will: • be able to solve and describe crystal structure • be able to resolve most common difficulties arising during the solving of the crystal structure

Metode poučevanja in učenja:	**Learning and teaching methods:**
Učenje na realnih nalogah z uporabo pripravljenih podatkov.	Learning on the real tasks using supplied data.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Reševanje kristalnih struktur, pri katerih nastopajo določene težave, z uporabo pripravljenih podatkov.	100 %	Solving the crystal structure with definite troubles using the supplied data

Reference nosilca / Lecturer's references:

- Igor M. Shlyapnikov, Evgeny A. Goreshnik and Zoran Mazej. The cubic [Ti8F36]4– anion found in the crystal structures of K4Ti8F36·8HF and Rb4Ti8F36·6HF. Chem. Commun., 2013, 49, 2703-2705.
- Kristian Radan, Evgeny Goreshnik, Boris Žemva. Xenon(II) Polyfluoridotitanates(IV): Synthesis and Structural Characterization of [Xe2F3]+ and [XeF]+ Salts. Angew. Chem. Int. Ed. 2014, 53, 50, 13715–13719.
- Zoran Mazej, Tomasz Michałowski, Evgeny A. Goreshnik, Zvonko Jagličić, Iztok Arčon, Jadwiga Szydłowska, and Wojciech Grochala. The first example of a mixed valence ternary compound of silver with random distribution of Ag(I) and Ag(II) cations. Dalton Trans., 2015, 44, 10957–10968.
- E.A. Goreshnik, G.Veryasov, D. Morozov, Yu. Slyvka, B. Ardan and M.G. Mys'kiv. Solvated copper(I) hexafluorosilicate π-complexes based on [Cu2(amtd)2]2+ (amtd = 2-allylamino-5-methyl-1,3,4-thiadiazole) dimer. J. Organometallic Chem., 2016, 810, 1-11.
- Zoran Mazej, Evgeny Goreshnik. "Influence of the Increasing Size of the M2+ Cation on the Crystal Structures of XeF5M(SbF6)3 (M = Ni, Mg, Cu, Zn, Co, Mn, Pd), and the Crystal Structure of $(XeF5)3^{[Hg(HF)]_2(SbF_6)_7}$". Eur. J. Inorg. Chem., 2016, 20, 3356-3364.