

# UČNI NAČRT

## UČNI NAČRT PREDMETA / COURSE SYLLABUS

<b>Predmet:</b>	Strukturna karakterizacija materialov
<b>Course title:</b>	Structural characterization of materials

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
MŠP Kemija, 2. stopnja	Materiali za shranjevanje in pretvorbo energije	2	3
USP Chemistry, 2nd Cycle	Materials for Energy Storage and Conversion	2 <sup>nd</sup>	3 <sup>rd</sup>

<b>Vrsta predmeta / Course type</b>	Obvezni / Mandatory
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<b>Univerzitetna koda predmeta / University course code:</b>	
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Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje work	Druge oblike študija	Samost. delo Individ. work	ECTS
20	10	20			50	4

<b>Nosilec predmeta / Lecturer:</b>	prof. dr. Anton Meden / Dr. Anton Meden, Full Professor
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<b>Jeziki / Languages:</b>	<b>Predavanja / Lectures:</b>	Angleški / English
	<b>Vaje / Tutorial:</b>	Angleški / English

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

Predmet imajo opredeljen kot študijsko obveznost študenti, ki so vključeni v projekt "Materiali za shranjevanje in pretvorbo energije +" (MESCS+). Lahko ga vpišejo tudi drugi tuji študenti na mednarodni izmenjavi na UL. Študenti morajo biti vpisani na MŠP Kemija, 2. stopnja, ali imeti podpisan učni sporazum (LA) med UL FKKT in drugimi tujimi izobraževalnimi ustanovami.

### Prerequisites:

This course will be assigned to the students who are part of the "Materials for Energy Storage and Conversion +" (MESCS+) project. It is available to other foreign international exchange students as well. Students must be enrolled to the USP Chemistry, 2nd Cycle or have signed learning agreement between UL FKKT and other foreign educational institution.

### Vsebina:

**Kristalne strukture:** amorfno in kristalinično stanje, primeri struktur.

**Simetrija:** ugotavljanje simetrije na primerih struktur, simetrijski elementi, točkovne skupine, prostorske skupine, kristalni sistemi, osnovna celica, kristalne mreže.

**Difrakcija:** radiacija in njena interakcija s kristali, Braggov zakon, difrakcija na monokristalu in prahu.

**Identifikacija in kvantifikacija faz:** osnove metode, uporaba obstoječega znanja (zbirke podatkov), primer iskalnega programa, osnove in primeri kvantitativne fazne analize.

**Osnove reševanja struktur:** difraktogram in strukturna informacija, metode z monokristali, praškovne metode, koraki določanja strukture iz praškovnih difrakcijskih podatkov.

**Rietveldovo prilagajanje:** informacijska vsebnost praškovnega difraktograma, možne uporabe RP.

**Osnove fizike trdnega stanja in teoretske kemije:** zveza med lastnostmi na atomski skali in makroskopskimi

### Content (Syllabus outline):

**Crystal structures:** amorphous and crystalline state, examples of structures.

**Symmetry:** exploring symmetry in the example structures, symmetry elements, point groups, space groups, crystal systems, unit cell, crystal lattices.

**Diffraction:** radiation and its interaction with crystals, Bragg law, single crystal and powder diffraction.

**Phase identification and quantification:** origin of the method, use of existing knowledge (databases) example of a search-match program, basics and examples of quantitative phase analysis.

**Crystal Structure solution-basics:** diffraction pattern and structural information, single crystal methods, powder methods, steps of structure determination from powder diffraction data.

**Rietveld refinement:** information content in the powder pattern, possible uses of RP.

**Basics in Solid State Physics and**

lastnostmi z nekaj primeri.

**Theoretical Chemistry:** relation between atomic-scale properties and large-scale properties with some examples.

### Temeljni literatura in viri / Readings:

V. K. Pecharsky and P. Z. Zavaliy: Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer, ISBN 0-387-24147-7, New York, USA, 2005.

### Cilji in kompetence:

**Cilji:** Razumevanje strukturnih principov v trdninah, njihove lastnosti in metode njihovega proučevanja, temelječe na difrakciji.

**Kompetence:** Uporaba osnovnih tehnik karakterizacije, temelječih na praškovni difrakciji.

### Objectives and competences:

**Objectives:** Understanding of structural principles of solids, their properties and diffraction-based methods of studying thereof.

**Competences:** Use of basic powder-diffraction-based characterization techniques.

### Predvideni študijski rezultati:

#### Znanje in razumevanje

Poznavanje temeljnih strukturnih principov v anorganskih in organskih trdninah ter razumevanje le-teh. Usvajanje povezave med kristalno strukturo in njeno difrakcijsko sliko ter načinov njene uporabe.

#### Uporaba

Uporaba praškovne difrakcije za temeljno karakterizacijo materialov. Uporaba orodij in podatkov iz kristalografskih podatkovnih zbirk.

### Intended learning outcomes:

#### Knowledge and Comprehension

Knowledge of the basic structural principles of inorganic and organic solids and understanding of structural principles. Comprehension of connection between crystal structure and its diffraction image and pathways of using thereof.

#### Application

Use of powder diffraction for basic characterization of materials. The application of tools and data from crystallographic databases.

### Refleksija

Sposobnost kritičnega pogleda na metode in rezultate praškovne difrakcije v širšem kontekstu karakterizacije materialov.

### Prenosljive spretnosti

Praksa v reševanju problemov. Veščine dela z računalniki. Uporaba zbirk podatkov in branja znanstvenih člankov.

### Analysis

Capability of critical view of powder diffraction methods and their results in a broader scope of materials characterization.

### Skill-transference Ability

Practice in problem-solving. Students get skills in working with computers. The application of databases and reading scientific papers.

### **Metode poučevanja in učenja:**

Predavanja, vodene vaje ob uporabi računalniških programov, vaje v majhnih skupinah in individualno.

### **Learning and teaching methods:**

Lectures, tutorials using computer programs, small group and individual exercises.

Delež (v %) /

### **Načini ocenjevanja:**

Weight (in %)

### **Assessment:**

Ustni izpit, ki vključuje reševanje praktičnega problema	<b>100%</b>	Oral exam including solution of a practical problem
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### **Reference nosilca / Lecturer's references:**

- 1.) STARE, Jernej, MEDEN, Anton, HADŽI, Dušan. Structure determination by joint effort of X-ray powder diffraction and quantum calculations : crystal structure and short hydrogen bonding in pentadecafluorooctanoic acid hydrate. *Croatica chemica acta*, ISSN 0011-1643. [Print ed.], 2018, vol. 91, no. 2, str. 209-220.
- 2.) MEDEN, Anton, RADOSAVLJEVIĆ EVANS, Ivana. Structure determination from powder diffraction data : past, present and future challenges. *Crystal research and technology*, ISSN 1521-4079, 2015, vol. 50, issue 9-10, str. 747-758.
- 3.) POČKAJ, Marta, MEDEN, Anton, ZABUKOVEC LOGAR, Nataša, RANGUS, Mojca, MALI, Gregor, LEZCANO-GONZÁLEZ, Inés, BEALE, Andrew M., GOLOBIČ, Amalija. Structural investigations in pure-silica and Al-ZSM-12 with MTEA or TEA cations. *Microporous and mesoporous materials : zeolites, clays, carbons and related materials*, ISSN 1387-1811, Jun. 2018, vol. 263, str. 236-242.

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