

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet:	Kemija materialov
Course title:	Materials Chemistry

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Znanost o materialih (2. stopnja)	/	1	1-2
Materials Science (2nd level)	/	1	1-2

Vrsta predmeta / Course type obvezni / mandatory

Univerzitetna koda predmeta / University course code: 2ZMA01

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Laboratory work	Teren. vaje Field work	Samost. delo Individ. work	ECTS
60	/	15	30	/	240	12

Nosilec predmeta / Lecturer: prof. dr. Nataša Zabukovec Logar

Jeziki /	Predavanja / Lectures:	slovenski / English
Languages:	Vaje / Tutorial:	slovenski / English

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

/

Prerequisites:

/

Vsebina:

Predmet podaja pregled kemije materialov, s poudarkom na naprednih metodah sinteze različnih tipov materialov. Posebna pozornost je namenjena razumevanju povezave med sestavo in strukturo kovin, keramike, polimerov, tekočih kristalov, poroznih materialov, kompozitov idr. ter njihovimi fizikalno-kemijskimi lastnostmi.

Predmet vključuje naslednja poglavja:

Fizikalne in kemijske lastnosti elementov

- Periodni sistem elementov (elektronska konfiguracija, ionski radij, elektronegativnost, polarizabilnost, magnetni moment, oksidacijsko stanje, idr.)

Kemijske vezi in elektronska struktura

Content (Syllabus outline):

The course provides an overview of the chemistry of materials, with an emphasis on advanced methods of synthesis of different types of materials. Special emphasis is on the relationship between the composition and structure of metals, ceramics, polymers, liquid crystals, porous materials, composites, etc. and their physico-chemical properties.

The course includes the topics of:

Physical and chemical properties of elements

- Periodic table of elements (electronic configuration, ionic radii, electronegativity, polarizability, magnetic moment, oxidation state, etc.)

<ul style="list-style-type: none"> • Klasifikacija kemijskih vezi • Šibke interakcije (H-vezi, Van der Waalove interakcije, idr.) • Elektronska struktura 	<p>Chemical bonds and electronic structure</p> <ul style="list-style-type: none"> • Classification of bonds • Weak interactions (H-bonds, Van der Waals interactions, etc.) • Electronic structure
<p>Kristalinična struktura</p> <ul style="list-style-type: none"> • Koordinacijski poliederi • Vpliv ionskega radija na stabilnost kristala • Polimorfizem • Trdna raztopina • Amorfnost • Strukturne napake in nestehiometričnost 	<p>Crystal structure</p> <ul style="list-style-type: none"> • Atomic packing factor • Influence of ionic radii on the stability of crystal • Polymorphism • Solid solutions • Amorphous phase • Structurally defects and non-stoichiometry
<p>Termodinamika v trdnem</p> <ul style="list-style-type: none"> • Osnovni pristop (ravnotežje, Gibbsovo fazno pravilo) • Difuzija v trdnem • Fazno ravnovesje in fazi diagrami • Kristalizacija in fazne pretvorbe 	<p>Thermodynamics of solid state</p> <ul style="list-style-type: none"> • Basic approach (equilibrium, Gibbs phase rule) • Diffusion in solid state • Phase equilibrium and phase diagrams • Crystallization and phase transformation
<p>Sinteza</p> <ul style="list-style-type: none"> • Sinteza v trdnem, sintranje in mikrostruktura (reakcija v trdnem, mehanizmi sintranja, zrna, meje med zrn in rast zrn) • Sinteza iz raztopin 	<p>Synthesis</p> <ul style="list-style-type: none"> • Solid state synthesis, sintering and microstructure (reaction in solid state, mechanisms of sintering, grain, grain boundary and grain growth) • Synthesis from the solution
<p>Kovine</p> <ul style="list-style-type: none"> • Pridobivanje in predelava kovin • Železo in neželezne kovine • Zlitine • Obdelava (livarstvo, toplotna obdelava, varjenje) • Kemijske lastnosti (korozija in korozijske prevleke) • Mehanske lastnosti kovin in zlitin 	<p>Metals</p> <ul style="list-style-type: none"> • Extraction and recycling of metal • Ferrous and non-ferrous metal • Alloys • Processing (foundry, thermal processes in metallurgy, welding) • Chemical properties (corrosion and corrosion coatings)
<p>Keramični materiali</p> <ul style="list-style-type: none"> • Definicija, klasifikacija, struktura, lastnosti • Steklo • Keramični materiali: ionski prevodniki, dielektriki, superprevodniki, polprevodniki, naprave • Biokeramika • Lastnosti: fizikalne, mehanske, itd • Metode obdelave (mletje, oblikovanje, žganje) 	<p>Ceramic materials</p> <ul style="list-style-type: none"> • Definition, classification, structure types, properties • Glass materials • Functional ceramics: ionic conductors, dielectrics, superconductors, semiconductors, devices • Bioceramics • Properties: physical, mechanical, etc. • Processing methods (milling, forming, firing) • Mechanical properties of metals and alloys
<p>Polimeri</p> <ul style="list-style-type: none"> • Klasifikacija in struktura • Sinteza (adicija/polikondenzacija) • Postopki obdelave polimerov (ekstrudiranje, brizganje, stiskanje, vakuumsko oblikovanje) 	<p>Polymers</p> <ul style="list-style-type: none"> • Classification and structure • Synthesis (addition/polycondensation reactions)

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<p>Termodinamika v trdnem</p> <ul style="list-style-type: none"> • Osnovni pristop (ravnotežje, Gibbsovo fazno pravilo) • Difuzija v trdnem • Fazno ravnovesje in fazi diagrami • Kristalizacija in fazne pretvorbe 	<p>Thermodynamics of solid state</p> <ul style="list-style-type: none"> • Basic approach (equilibrium, Gibbs phase rule) • Diffusion in solid state • Phase equilibrium and phase diagrams • Crystallization and phase transformation
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- Fizikalne in kemijske lastnosti (kemijska stabilnost, toplotna stabilnost, mehanska in kemična razgradnja, razgradnja kot posledica sončnega sevanja, električnih lastnosti, reologija)

Tekoči kristali

- Kemijske lastnosti in sestava
- Fizikalne lastnosti

Porozni materiali

- Klasifikacija in struktura
- Sinteza (hidrotermalna, solvotermalna, ionotermalna, posintezna modifikacija)
- Postopki oblikovanja poroznih materialov (granuliranjem ekstrudiranje, idr.)
- Fizikalne in kemijske lastnosti (kemijska stabilnost, toplotna stabilnost, adsorpcijske in katalitske lastnosti)

Kratek pregled karakterizacijskih metod materialov (meritve mehanske lastnosti, rentgenska difrakcija, termična analiza, mikroskopija, kromatografija, itd.)

- Polymer processing methods (extrusion, injection, compression, vacuum forming)
- Physical and Chemical properties (chemical stability, thermal stability, mechanical and chemical degradation, degradation caused by solar irradiation, electrical properties, rheology)

Liquid crystals

- Chemical properties and composition
- Physical properties

Porous materials

- Classification and structure
- Synthesis (hydrothermal, solvotermalna, ionotermalna, posintezna modifikacija)
- Procedures for shaping of porous materials (extrusion, granulation, etc.)
- Physical and chemical properties (chemical stability, thermal stability, adsorption and catalytic properties)

Short overview of materials characterization methods

(mechanics of materials, X-ray diffraction, microscopy, thermal analysis, chromatography, etc.)

Temeljna literatura in viri / Readings:

- B. D. Fahlman, Materials Chemistry, Springer Netherlands, 2007
- H. R. Allcock, Introduction to materials chemistry, Hoboken, NJ : John Wiley & Sons, 2008
- K. K. Chawla, Composite Materials, Springer-Verlag New York, 2012, DOI: 10.1007/978-0-387-74365-3
- S. Qiu & T. Ben, Porous polymers : design, synthesis and applications, Cambridge : Royal Society of Chemistry, 2016
- D. B. Mitzi (ed.), Solution processing of inorganic materials, Hoboken: Wiley, 2009
- Supporting material from the web will be indicated

Cilji in kompetence:

Cilj predmeta je predstaviti povezavo med sestavo in strukturo materialov in njihovimi lastnosti. Študentje bodo pridobili znanja in praktične izkušnje o mehanizmih in postopkih sinteze materialov in njihove obdelave ter pregled osnovnih karakterizacijskih metod uporabljenih v znanosti o materialih.

Objectives and competences:

The goal of course is presenting the correlation between the composition and structure of materials and properties of materials. The students will gain knowledge and practical experiences on the mechanisms and procedures of materials synthesis and processing as well as an overview of the basic characterization methods used in materials science.

Predvideni študijski rezultati:

Znanje in razumevanje:
Študenti pridobijo znanje kako fizikalne in kemijske lastnosti elementov vplivajo na nastanek vezi in urejanje atomov v kristalni strukturi. Prav tako se naučijo, da ne samo, kemijska sestava, temveč tudi struktura ali kristalna struktura in napake vplivajo na lastnosti materialov. Študenti pridobijo znanja o mehanizmih sinteze in difuzije v trdnem. Študentom je predstavljen širok pregled o različnih naprednih materialih, njihovih sintezi, strukturi, obdelavi, lastnostih in možnostih uporabe. Študenti se naučijo razlikovati med karakterizacijskimi metodami in spoznajo katere metode so najbolj primerne za meritve specifičnih lastnosti materialov. Glavni študijski rezultat za študente je pridobitev znanj za sintezo in karakterizacijo materialov.

Intended learning outcomes:

Knowledge and understanding:
Students learn how the physical and chemical properties of elements influence the formation of bonds and packing of atoms in crystal structure. They also learn that not only the chemical composition but also the structure or crystal structure and defects influence the properties of materials. Students gain knowledge on mechanisms of synthesis and diffusion in solid state. They are introduced to the broad overview on different advanced materials, their synthesis, structure, processing, properties and possible application. Students learn which characterization method is optimal for the analysis of specific material properties. The major learning outcome for students is the development of the skills for synthesis and characterization of materials.

Metode poučevanja in učenja:

- Predavanja
- Seminarske vaje
- Eksperimentalne vaje iz sinteze in obdelave materialov

Learning and teaching methods:

- Lectures
- Tutorial
- Laboratory exercises on synthesis and processing of materials

Delež (v %) /

Načini ocenjevanja:

Weight (in %)

Assessment:

• Pisni izpit	40	• Written exam
• Ustni izpit	40	• Oral examination
• Pisno poročilo iz eksperimentalnih vaj	20	• Written reports on laboratory exercises

Reference nosilca / Lecturer's references:

Prof. dr. Nataša Zabukovec Logar:

Redni profesor za področje kemije na Univerzi v Novi Gorici.
Full Professor of Chemistry at the University of Nova Gorica.

Nataša Zabukovec Logar je vodja Odseka za anorgansko kemijo in tehnologijo na Kemijskem inštitutu v Ljubljani. Trenutno se pri svojih raziskavah osredotoča na razvoj novih kovinsko-organskih in anorganskih poroznih materialov za shranjevanje plinov in toplote ter študiju sorpcijskih mehanizmov kovin na naravne in sintetične zeolite za uporabo pri čiščenju odpadnih vod.

Nataša Zabukovec Logar is a Head of Department for Inorganic Chemistry and Technology at the National Institute of Chemistry in Ljubljana. Her current research focusses are development of new metal-organic and inorganic porous materials for gas and heat storage and studies of sorption mechanisms of metals on natural and synthetic zeolites for water treatment.

Izbrane objave / Selected publications:

1. KRAJNC, Andraž, KOS, Tomaž, ZABUKOVEC LOGAR, Nataša, MALI, Gregor. A simple NMR-based method for studying the spatial distribution of linkers within mixed-linker metal-organic frameworks. *Angewandte Chemie*, ISSN 1433-7851. [Print ed.], Sep. 2015, vol. 54, iss. 36, str. 10535-10538. doi: [10.1002/anie.201504426](https://doi.org/10.1002/anie.201504426). [COBISS.SI-ID [5735962](https://www.cobiss.si/id/5735962)]
2. BIRSA ČELIČ, Tadeja, RANGUS, Mojca, LAZAR, Karoly, KAUČIČ, Venčeslav, ZABUKOVEC LOGAR, Nataša. Spectroscopic evidence for the structure directing role of the solvent in the synthesis of two iron carboxylates. *Angew. Chem. (Int. ed., Print)*. [Print ed.], 2012, vol. 51, iss. 50, str. 12490-12494, ilustr., doi: [10.1002/anie.201204573](https://doi.org/10.1002/anie.201204573). [COBISS.SI-ID [36300805](https://www.cobiss.si/id/36300805)]
3. MAZAJ, Matjaž, BIRSA ČELIČ, Tadeja, MALI, Gregor, RANGUS, Mojca, KAUČIČ, Venčeslav, ZABUKOVEC LOGAR, Nataša. Control of the crystallization process and structure dimensionality of Mg-benzene-1,3,5-tricarboxylates by tuning solvent composition. *Cryst. growth des.*, 2013, vol. 13, iss. 8, str. 3825-3834. doi: [10.1021/cg400929z](https://doi.org/10.1021/cg400929z). [COBISS.SI-ID [5290522](https://www.cobiss.si/id/5290522)]
4. MAZAJ, Matjaž, MALI, Gregor, RANGUS, Mojca, ŽUNKOVIČ, Emanuela, KAUČIČ, Venčeslav, ZABUKOVEC LOGAR, Nataša. Spectroscopic studies of structural dynamics induced by heating and hydration : a case of calcium-terephthalate metal-organic framework. *The journal of physical chemistry. C*, 2013, vol. 117, issue 15, str. 7552-7564, doi: [10.1021/jp311529e](https://doi.org/10.1021/jp311529e). [COBISS.SI-ID [36628485](https://www.cobiss.si/id/36628485)]
5. RISTIČ, Alenka, ZABUKOVEC LOGAR, Nataša, HENNINGER, Stefan K., KAUČIČ, Venčeslav. The performance of small-pore microporous aluminophosphates in low-temperature solar energy storage : the structure-property relationship. *Adv. funct. mater. (Print)*, 2012, vol. 22, iss. 9, str. 1952-1957. [COBISS.SI-ID [4910618](https://www.cobiss.si/id/4910618)]