UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	**MODELIRANJE MATERIALOV NA VEČ RAVNEH**
Course title:	**MULTISCALE MODELLING OF MATERIALS**

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

Vrsta predmeta / Course type	izbirni / elective
Univerzitetna koda predmeta / University course code:	2ZMA16

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje work	Druge oblike študija	Samost. delo Individ. work	ECTS
30	/	30	/	/	100	6

Nosilec predmeta / Lecturer:	**pridr. prof. dr. Miha Grilc in pridr. prof. dr. Matej Huš**

Jeziki / Languages:	**Predavanja / Lectures:**	**Slovenski ali angleški**
	Vaje / Tutorial:	**Slovenski ali angleški**

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisits:**
Potrebna so osnovna visokošolska znanja iz matematike, fizike, kemije, materialov, numeričnih metod ter osnovna znanja uporabe računalnika ter vsaj enega od sodobnih operacijskih sistemov (Windows ali Linux).	Basic university knowledge of mathematics, physics chemistry, materials and numerical methods, and basic skills in using computers with one of the modern operating systems (Windows or Linux) are required.

Vsebina:	Content (Syllabus outline):
Predmet Modeliranje materialov na več ravneh podaja osnovno razumevanje pojavov in numeričnih postopkov, ki jih uporabljamo na širokem področju simulacij materialov od elektronske pa do makroskopske ravni. Poudarek je na formulacijah in modelih osnovnih fizikalnih pojavov na vsakem izmed meril, njihovi sklopitvi in kako z njimi simuliramo specifični material. Študentje pripravijo seminar, ki osvetli eno izmed obravnavanih vsebin.	Course in Multiscale modelling of materials provides a basic understanding of phenomena and numerical approaches used in a broad field of materials simulations from the electronic to macroscopic level. The emphasis is placed on formulations and models of fundamental physical phenomena on each of the scales, their coupling and how to include them in a model of a specific material. Students prepare a seminar that elaborates one of the topics.
1. <u>Uvod</u> • Cilji in namen predmeta • Predstavitev učnega programa • Predstavitev učnih pripomočkov, virov in načina dela • Predstavitev obveznosti študentov • Napotki in sugestije za študij 2. <u>Osnovni pojmi</u> • Kontinuum • Ohranitvene enačbe in kontinuitetna enačba • Ohranitev gibalne količine • Ohranitev vrtilne količine • Ohranitev energije • Prenos sestavin • Entropija • Konstitutivne enačbe • Robni in začetni pogoji 3. <u>Skaliranje in modelske poenostavitve</u> • Osnovna skalirna analiza • Majhni parametri in mejne plasti • Standardne brezdimenzijske grupe 4. <u>Elementi numeričnih algoritmov</u> • Metoda utežnih ostankov (MUO) • Najbolj popularne numerične metode kot posebni primeri MUO. • Metode za generacijo mreže • Načini reševanja posebnih sistemov 5. <u>Računska kvantna mehanika</u> • Osnovne kvantne mehanike in valovna funkcjia • Schrödingerjeva enačba in Hamiltonian • Večdelčni sistemi in sistemi s spinom • Sistemi v 3D prostoru • Metode za računsko reševanje 6. <u>Molekularna dinamika</u> • Področja uporabe in omejitve • Potenciali • Specifični algoritmi molekularne dinamike • Primeri	1. <u>Introduction</u> • Aims and purpose of the course • Syllabus presentation • Presentation of teaching tools, resources and course execution • Students' obligations • Study instructions and suggestions 2. <u>Basic terms</u> • Continuum • Conservation laws and continuity equation • Conservation of momentum • Conservation of angular momentum • Conservation of energy • Transport of species • Entropy • Constitutive equations • Boundary and initial conditions 3. <u>Scaling and model simplifications</u> • Basic scaling analysis • Small parameters and boundary layers • Standard dimensionless groups 4. <u>Elements of numerical algorithms</u> • Weighted residual method (WRM) • Most popular numerical methods as special cases of WRM. • Methods for mesh generation • Methods of solving of special systems 5. <u>Computational quantum mechanics</u> • Fundamental of quantum mechanics and wave function • Schrödinger equation and Hamiltonian • Multiparticle systems and spin systems • Systems in the 3D space • Methods for numerical solutions 6. <u>Molecular dynamics</u> • Areas of applications and limits • Potentials • Specific molecular dynamics algorithms • Examples 7. <u>Kinetic Monte Carlo</u> • Probability and stochastic events

7. Kinetični Monte Carlo • Verjetnost in stohastični dogodki • Isingov model in fazni prehodi • Reakcije in redki dogodki • Teorija prehodnega stanja 8. Mikrokinetični modeli • Reakcije v plinskih zmeseh • Večfazni sistemi 9. Nestisljivi in stisljivi tok • Konstitutivne enačbe, robni pogoji. • Posebnosti numeričnega reševanja • Tlačno-hitrostne sklopitve 10. Newtonski in ne-Newtonski tokovi • Počasni Newtonski tokovi • Proste površine in gibajoči se robovi • Tokovi z veliko inercijo • Ne-Newtonske konstitucijske zveze • Formulacije za modeliranje turbulence 11. Deformacija trdnin • Mikroskopski in makroskopski opis • Konstitucijske enačbe, elastično, plastično, viskoplastično obnašanje • Numerično reševanje 12. Primeri simulacij 13. Praktično delo s simulacijskimi sistemi • Gamess, QuantumEspresso • Zacros • Matlab, Python • OpenFOAM • Itd.	• Ising model and phase transitions • Reactions and rare events • Transition state theory 8. Microkinetic models • Reactions in gaseous mixtures • Multi-phase systems 9. Incompressible and compressible flow • Constitutive equations, boundary conditions. • Specifics of numerical solution • Pressure-velocity couplings 10. Newtonian and non-Newtonian flows • Slow Newtonian flows • Free surfaces and moving boundaries • Flows with large inertia • Non-Newtonian constitutive relations • Formulations for turbulence modelling 11. Deformation of solids • Microscopic and macroscipic description • Constitutive equations, elastic, plastic, viscoplastic behaviour • Numerical solutions 12. Examples of simulations 13. Hands-on work with simulation systems • Gamess, QuantumEspresso • Zacros • Matlab, Python • OpenFOAM • Etc.

Temeljni literatura in viri / Readings:

Z.X. Guo, Multiscale materials modelling, Fundamentals and applications, 1st Edition, Woodhead Publishing, London, 2007

E.B. Tadmor and R.E. Miller, Modeling materials: continuum, atomistic and multiscale techniques, Cambridge University Press, Cambridge, 2011.

E.B. Tadmor, R.E. Miller and R.S. Elliott, Continuum mechanics and thermodynamics: From fundamental concepts to governing equations, Cambridge University Press, Cambridge, 2012.

F. Giustino. Materials modelling using Density Functional Theory: Properties and Predictions, Oxford University Press, Oxford, 2014

C. Pozrikidis, Introduction to theoretical and computational fluid dynamics, Oxford University Press, Oxford, 2011.

Y.C. Fung, P. Tong, Classical and computational solid mechanics, World Scientific Publishing, Singapore, 2001.

QuantumEspresso and Gamess code manual.

Zacros Computer code manual.

Matlab computer code manual.

OpenFOAM manuals from training courses.

Cilji in kompetence:	**Objectives and competences:**
Lastnosti materialov so posledica različnih pojavov na merilih od angstrema do metra in samo obravnava na več merilih lahko poda celovito razumevanje. Raziskovalci materialov morajo zato razumeti osnovne koncepte in tehnike iz različnih področij in te integralno predstavimo v tem predmetu. Računalnik nam omogoča učinkovito reševanje najrazličnejših problemov v znanosti in tehniki materialov. Poglavitni cilj predmeta *Modeliranje materialov na več ravneh* je predstaviti študentom temeljne koncepte, ki se uporabljajo pri simulaciji različnih materialov (kovine, polimeri, keramika in njihovi kompoziti) na različnih merilih (mehanika kontinuuma, fazno polje, statistična mehanika, molekularne in atomističe simulacije, kvantna mehanika). Učni načrt je oblikovan tako, da študente spozna z vsemi osnovnimi koncepti ter jih usposobi za uporabo računalniških programov za reševanje problemov lastnosti materialov, njihovega procesiranja in uporabe. Sposobni bodo reševanja standardnega spektra problemov, povezanih z mikroskopskimi in makroskopskimi problemi mehanike trdnin in tekočin. Razvili pa bodo tudi znanja, potrebna za reševanje težjih, bolj poglobljenih in nestandardnih problemov.	Material properties are a consequence of different phenomena on scales ranging from angstroms to meters, and only a multiscale treatment can provide a complete understanding. Materials scientists have to therefore understand fundamental concepts and techniques from different fields, and these are presented in an integral way in this course. With the help of computers we can efficiently solve a variety of problems in science and engineering of materials. The main objective of the course *Multiscale modelling of materials* is to present the students basic concepts, used in simulation of different materials (metals, polymers, ceramic and their composites) on different scales (continuum mechanics, phase-field, statistical mechanics, molecular and atomistic simulations, quantum mechanics) The syllabus is designed in a way to guide the students through basic concepts and train them how to apply computer programs for solving problems of material characteristics, their processing and use. They will be able to solve a standard spectrum of problems, associated with microscopic and macroscopic fluid and solid mechanics problems. They will also develop skills necessary to solve specific, more involved and non-standard problems.

Predvideni študijski rezultati:	Intended learning outcomes:
Študenti bodo osvojili osnovne koncepte razumevanja in računalniškega modeliranja materialov na različnih merilih. Sposobni bodo samostojnega konceptualnega razvoja ustreznega numeričnega modela in uporabe sodobnih simulacijskih sistemov. Sposobni bodo računalniških optimizacij snovnih lastnosti in procesiranja materialov.	Students will learn the basic concepts of understanding and computer modeling of materials on different scales. They will be able to autonomously conceptually develop a computational model and use a modern simulation systems. They will be able to computationally optimize material properties and materials processing.

Metode poučevanja in učenja:	Learning and teaching methods:
Poučevanje bo sestavljeno iz treh sklopov. Prvi sklop bodo sestavljala predavanja, kjer bodo predstavljene in razložene vse vsebine iz učnega programa. Drugi sklop bo obsegal praktične vaje s simulacijskimi sistemi. Tretji sklop bo obsegal samostojno delo študentov v okviru katerega bodo morali sproti reševati domače naloge ter na koncu izdelati še seminarsko nalogo v obliki primernega numeričnega modela.	Teaching will consist of three parts. The first part will consist of the lectures, where the contents of the syllabus will be presented and explained. The second part will include hands-on training with simulation systems. The third part will consist of individual work where the students will be solving homeworks throughout the course and at the end write a seminar work in the form of an appropriate numerical model.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	Assessment:
Domače naloge.	**25 %**	Homework.
Seminarska naloga z ustnim zagovorom, kjer se preveri zmožnost izdelave numeričnega modela tehničnega problema.	**25 %**	Seminar work with discussion in order to evaluate the ability of making a numerical model of a technical problem.
Pisni ali ustni izpit, kjer se ocenjuje znanje temeljnih konceptov ter zmožnost samostojnega reševanja na podlagi razvitih računalniških programov.	**50 %**	Written or oral exam, which assesses knowledge of the fundamental concepts and ability of problem solving based on existing computer codes.

Reference nosilca / Lecturer's references:

Pridr. prof. dr. **Miha Grilc** je znanstveni sodelavec na Kemijskem inštitutu in vodja Skupine za pretvorbe biomase na Odseku za katalizo in reakcijsko inženirstvo. Njegove raziskave so usmerjene v pretvorbo biomase v gradnike z višjo dodano vrednostjo in opis teh pretvorb na več ravneh. Osredotoča se zlasti na lesno biomaso, kaskadno frakcionacijo in defunkcionalizacijo.

Pridr. Prof. dr. **Matej Huš** je znanstveni sodelavec na Kemijske inštitutu in vodja Skupine za teorijo na Odseku za katalizo in reakcijsko inženirstvo. Njegove raziskave so usmerjene v fundamentalni opis kemijskih pretvorb na ravni kvantne mehanike, kinetičnega Monte Carla in mikrokinetičnega opisa v kontinuumu. Osredotoča se zlasti na kemijo malih molekul, to je valorizacijo CO2, pridobivanje amonijaka, aktivacijo ogljikovodikov in epoksidacijo.

Miha Grilc is a research assistant professor at the National Institute of Chemistry and head of the Group for Biomass Conversions at the Department of Catalysis and Chemical Reaction Engineering. His research is focused on the conversion of biomass into building blocks with higher added value and the description of these conversions at multiple levels. He focuses in particular on lignin biomass, cascade fractionation and defunctionalization.

Matej Huš is a research assistant professor at the National Institute of Chemistry and head of the Theory Group at the Department of Catalysis and Reaction Engineering. His research is focused on the fundamental description of chemical transformations at the level of quantum mechanics, kinetic Monte Carlo and microkinetic description in the continuum. He focuses in particular on small molecule chemistry, i.e. CO_2 valorization, ammonia production, hydrocarbon activation and epoxidation.

Izbrane objave / Selected bibliography

1. KOPAČ, Drejc, LIKOZAR, Blaž, HUŠ, Matej. Metal-doped Cr2O3 as a catalyst for non-oxidative propane and butane dehydrogenation : a multiscale kinetic study. Applied Surface Science. [Print ed.]. 1 Feb. 2022, vol. 575, str. 1-10. ISSN 0169-4332. [COBISS.SI-ID 84726787]
2. HUŠ, Matej, KOPAČ, Drejc, BAJEC, David, LIKOZAR, Blaž. Effect of surface oxidation on oxidative propane dehydrogenation over chromia : an ab initio multiscale kinetic study. ACS catalysis. 3 Sep. 2021, vol. 11, iss. 17, str. 11233-11247, ilustr. ISSN 2155-5435. [COBISS.SI-ID 74972675],
3. HOČEVAR, Brigita, PRAŠNIKAR, Anže, HUŠ, Matej, GRILC, Miha, LIKOZAR, Blaž. H2−free Re-based catalytic dehydroxylation of aldaric acid to muconic and adipic acid esters. Angewandte Chemie : International edition. [Print ed.]. 18 Jan. 2021, vol. 60, iss. 3, str. 1244-1253. ISSN 1433-7851. [COBISS.SI-ID 31739907]
4. BJELIĆ, Ana, GRILC, Miha, HUŠ, Matej, LIKOZAR, Blaž. Hydrogenation and hydrodeoxygenation of aromatic lignin monomers over Cu/C, Ni/C, Pd/C, Pt/C, Rh/C and Ru/C catalysts : mechanisms, reaction micro-kinetic modelling and quantitative structure-activity relationships. Chemical engineering journal. 1 Mar. 2019, vol. 359, str. 305-320.
5. HUŠ, Matej, GRILC, Miha, PAVLIŠIČ, Andraž, LIKOZAR, Blaž, HELLMAN, Anders. Multiscale modelling from quantum level to reactor scale : an example of ethylene epoxidation on silver catalysts. Catalysis today. [Print ed.]. 1 Nov. 2019, vol. 338, str. 128-140. [COBISS.SI-ID 6626074
6. ŠIVEC, Rok, GRILC, Miha, HUŠ, Matej, LIKOZAR, Blaž. Multiscale modeling of (hemi)cellulose hydrolysis and cascade hydrotreatment of 5-hydroxymethylfurfural, furfural, and levulinic acid. Industrial & engineering chemistry research. [Print ed.]. 4 Sep. 2019, vol. 58, iss. 35, str. 16018-16032, ilustr. ISSN 0888-5885. [COBISS.SI-ID 6621210]