UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Molekulsko modeliranje s teorijo gostotnega fukcionala (DFT): molekule, površine in trdnine
Course title:	Molecular modeling using density functional theory (DFT): molecules, surfaces, and bulk solids

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

Vrsta predmeta / Course type Izbirni / Elective

Univerzitetna koda predmeta / University course code: NANO3-905

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 transfered to individual work.*

Nosilec predmeta / Lecturer: Doc. dr. Anton Kokalj

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

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisits:**
Zaključena izobrazba druge stopnje bolonjskega študija ali univerzitetna izobrazba s področja naravoslovja ali tehnologije.	Completed 2nd level cycle degree of the Bologna study or equivalent university education from natural sciences or technology.

Vsebina:	**Content (Syllabus outline):**
1. Uvod v teorijo gostotnega funkcionala (angl. DFT) 2. Translacijska simetrija: Blochov izrek, recipročni »k« prostor, Brillouinova cona 3. Gostota stanj, struktura pasov, Fermijeva energija; kovine, polprevodniki, izolatorji 4. Strukturne optimizacije, molekulska dinamika in izračuni vibracijskih lastnosti 5. Izračun energijskih razlik: jakost vezi, kohezivne, tvorbene, adsorpcijske in reakcijske energije	1. Introduction to Density-Functional-Theory 2. Translational symmetry: Bloch theorem, reciprocal »k« space, Brillouin zone 3. Density-of-states, band-structure, Fermi energy; metals, semi-conductors, insulators 4. Structural relaxations, molecular dynamics simulations, and vibrational calculations 5. Calculation of energy differences: bond strengths, cohesive, formation, adsorption and reactions energies

6. Trdne površine: izračun površinskih energij in izstopnega dela; problem polarnih površin 7. Analiza kemijskih vezi: molekulske orbitale, razlika elektronskih gostot, »projicirana« gostota stanj, donacija in povratna donacija naboja 8. Simulacija slik STM 9. Kako modelirati kemijske reakcije: prehodna stanja in aktivacijske energije 10. Praktični uvod v molekulsko modeliranje z računalnikom: narediti simulacijo z uporabo prosto dostopne programske opreme in odprtokodnih orodij	6. Solid surfaces: calculation of surface-free energies and work functions; problem of polar surfaces 7. Analysis of chemical bonding: molecular orbitals, charge density differences, projected density-of-states, charge donation and back-donation 8. Simulation of STM images 9. How to model chemical reactions: transition-states and activation energies 10. Practical introduction to molecular modeling with a computer: do a simulation yourself using free-software and open-source tools

Temeljni literatura in viri / Readings:

R. O. Jones, "**Density functional theory: Its origins, rise to prominence, and future**", *Reviews of Modern Physics*, Vol. 87, pp. 897–923, 2015.

Roald Hoffmann, "**Solids and surfaces: A chemist's view of bonding in extended structures**", (Wiley-VCH, New York, 1988). ISBN 0-471-18710-0

R. M. Martin, "**Electronic Structure: Basic Theory and Practical Methods**", (Cambridge University Press, Cambridge. 2004). ISBN 978-0-521-78285-2

C. D. Taylor and P. Marcus (Eds.) "**Molecular modeling of corrosion processes**", (Wiley, Hoboken, New Jersey, 2015). ISBN 978-1-118-26615-1

B. Hammer, J. K. Norskov, "**Theoretical surface science and catalysis – Calculations and concepts**", *Advances in Catalysis*, Vol. 45 (2000) 71–129.

Cilji in kompetence:	**Objectives and competences:**
Študent se bo najprej seznanil z osnovami teorije gostotnega funkcionala (angl. DFT) in tako pridobil osnovna znanja, potrebna za praktično molekulsko modeliranje. Namen tega predmeta je naučiti študenta samostojno »poganjati« molekulske simulacije in analizirati rezultate simulacij. Poudarek bo na uporabi prosto dostopnih in odprtokodnih programskih paketov in orodij, kot je npr. Quantum ESPRESSO ali kateri koli drug programski paket po izboru študenta. V okviru tega predmeta bomo obravnavali tako (1) molekulske (molekule, nanodelce) kot (2) periodične sisteme (površine in trdnine) in razložili specifičnosti pri modeliranju obeh vrst sistemov. Obravnavali bomo praktični primer modeliranja površine in molekulske adsorpcije.	Students will be first introduced to the fundamentals of Density-Functional-Theory as to gain the basic knowledge needed for practical molecular modeling. The purpose of this course is to teach the students how to make molecular simulations with a computer on their own and how to analyze the results. The emphasis will be given to free-software and open-source tools, such as Quantum ESPRESSO or any other software package of student's preference. This course will provide a link between (1) finite (molecules, clusters, nanoparticles) and (2) extended systems (surfaces and bulk solids) by teaching the student about specifics in modeling the two kinds of systems. A practical example of modeling surfaces and adsorption thereon will be given.

Splošne kompetence:	General competences:
• obvladanje raziskovalnih metod, pomembnih za molekulsko modeliranje • sposobnost uporabe molekulskega modeliranja na svojem specifičnem področju raziskav • razvoj komunikacijskih veščin in komunikacije v mednarodnem okolju • sposobnost samostojnega dela in timskega dela v skupini (v mednarodnem okolju) Predmetnospecifične kompetence: • študent se bo naučil, kako samostojno uporabljati molekulsko modeliranje, tj. kako zgraditi adekvaten model iz osnovnih gradnikov v nizu korakov molekulskega modeliranja in kako »poganjati« molekulske simulacije	• the student will learn research methods relevant for ab initio molecular modeling • the student will learn how to exploit molecular modeling in her/his specific area of research • the student will develop communication skills to present research achievements in an international environment • the student will learn to work independently and in a team (in an international environment) Course-specific competences: • the student will learn how to start a molecular modeling project from scratch, that is, to build a fully-fledged model from basic constituents in a series of molecular modeling steps

Predvideni študijski rezultati:	**Intended learning outcomes:**
Funkcionalno znanje o metodah molekulskega modeliranja in o tehnikah, ki jih uporabljamo pri molekulskih simulacijah. Študenti bodo sposobni samostojno “poganjati” molekulske simulacije. Študenti bodo sposobni uporabljati molekulsko modeliranje na svojem specifičnem področju raziskav.	The students will obtain an overview of the DFT molecular modeling methods and simulation techniques. The students will acquire a functional know-how to make a molecular modeling simulation from scratch. The students will be able to apply molecular modeling in their specific area of research.

Metode poučevanja in učenja:	**Learning and teaching methods:**
• Predavanja • Seminar • Laboratorijsko delo (praktično delo z računalnikom – simulacije) • Konzultacije	• Lectures • Seminar • “Virtual laboratory” work, i.e., practical computer simulations • Consultations

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Seminar	50 %	Seminar
Ustni izpit	50 %	oral exam

Reference nosilca / Lecturer's references:

- POBERŽNIK, Matic, COSTA, Dominique, HEMERYCK, Anne, KOKALJ, Anton. Insight into the bonding of silanols to oxidized aluminum surfaces. *The Journal of Physical Chemistry. C, Nanomaterials and*

interfaces, ISSN 1932-7447, 2018, vol. 122, no. 17, str. 9417-9431, doi: 10.1021/acs.jpcc.7b12552. [COBISS.SI-ID 31359783]

- POBERŽNIK, Matic, KOKALJ, Anton. Origin of surprising attractive interactions between electronegative oxygen adatoms on aluminum surfaces. *The Journal of Physical Chemistry. C, Nanomaterials and interfaces*, ISSN 1932-7447, 2016, vol. 120, no. 45, str. 25915-25922, doi: 10.1021/acs.jpcc.6b08894. [COBISS.SI-ID 29992743]

- KOKALJ, Anton. Ab initio modeling of the bonding of benzotriazole corrosion inhibitor to reduced and oxidized copper surfaces. *Faraday Discussions*, ISSN 1359-6640, 2015, vol. 180, str. 415-438, doi: 10.1039/C4FD00257A. [COBISS.SI-ID 28748327]

- KOKALJ, Anton, COSTA, Dominique. Molecular modeling of corrosion inhibitors. V: WANDELT, Klaus (ur.). *Encyclopedia of interfacial chemistry : surface science and electrochemistry*. Oxford: Elsevier. 2018, str. 332-345, doi: 10.1016/B978-0-12-409547-2.13444-4. [COBISS.SI-ID 31421735]

- KOKALJ, Anton. Computer-aided design of the reaction site in heterogeneous catalysis. V: MEYERS, Robert A. (ur.). *Encyclopedia of complexity and systems science*, (SpringerLink). New York: Springer, 2014, str. 1-41, doi: 10.1007/978-3-642-27737-5_89-3. [COBISS.SI-ID 28690215]