



Univerza v Mariboru

Fakulteta za naravoslovje
in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet:	Atomistične simulacije biomolekul
Course title:	Atomistic simulations of biomolecules

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
FIZIKA, 3. stopnja		1. ali 2.	1., 2. ali 4.
PHYSICS, 3 rd cycle		1. or 2.	1., 2. or 4.

Vrsta predmeta / Course type

Izbirni za vse module

Univerzitetna koda predmeta / University course code:

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Lab. vaje Laboratory work	Terenske vaje Field work	Samost. delo Individ. work	ECTS
10	5				165	6

Nosilec predmeta / Lecturer:

Franci Merzel

**Jeziki /
Languages:**

**Predavanja /
Lectures:**
Vaje / Tutorial:

slovenski/Slovenian in/and angleški s slovenskim
prevodom/English with translation in Slovenian

slovenski/Slovenian in/and angleški s slovenskim
prevodom/English with translation in Slovenian

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

Vsaka obveznost študenta v načinih ocenjevanja mora biti opravljena s pozitivno oceno. Opravljena seminarska naloga je pogoj za pristop k ustnemu izpitu.

Prerequisites:

Each student requirement within the assessment methods must be completed with a passing grade. Completed seminar paper is a prerequisite for taking the oral exam.

Vsebina:

- Opis kvantnih in klasičnih prostostnih stopenj ter interakcij pri biomolekularnih sistemih
- Simulacije različnih statistično-mehanskih porazdelitev

Content (Syllabus outline):

- Description of quantum and classical degrees of freedom and corresponding interactions in biomolecular systems

- Napredne metode in algoritmi za simulacije
- Struktura, dinamika in funkcija biomolekul
- Analiza normalnih načinov nihanja
- Povezava z glavnimi eksperimentalnimi tehnikami za določanje strukture (rentgenska kristalografija, NMR spektroskopija) in dinamike (IR in nevtronska spektroskopija)
- Računanje proste energije pri biokemijskih procesih (vezava ligandov)
- Problem zvijanja proteinov
- Simulacije agregacije polipeptidov

- Simulating various statistical-mechanical ensembles - Advanced simulation methods and algorithms
- Structure, dynamics and function of biomolecules
- Normal mode analysis
- Simulation methods versus experimental techniques for structure determination (X-ray crystallography, NMR) and for studying dynamics (light and neutron spectroscopy)
- Calculating free energies in biochemical processes (ligand binding)
- Protein folding problem
- Simulating polypeptide aggregation

Temeljni literatura in viri / Readings:

- 1) Frenkel, D. (2002). *Understanding Molecular Simulation : From Algorithms to Applications*. Academic Press. **Celotno besedilo dostopno v EBSCOhost Ebook Academic Collection - World Wide**
- 2) *Multiscale molecular methods in applied chemistry* (Let. 307). (2012). Springer. <http://dx.doi.org/10.1007/978-3-642-24968-6>
- 3) SEVER, Marko, MERZEL, Franci. Influence of SGLT1 sugar uptake inhibitors on water transport. *Molecules*. 8 Jul. 2023, vol. 28, iss. 14, art. 5295, str. 1-15, ilustr. ISSN 1420-3049. <https://www.mdpi.com/1420-3049/28/14/5295>, <https://dirros.openscience.si/lzpisGradiva.php?id=16768>, DOI: 10.3390/molecules28145295. [COBISS.SI-ID 159826435]

Dodatna:

- 4) A. R. Leach, *Molecular Modelling: Principles and Applications*, Prentice Hall, 2001.
- 5) M. Daune, *Molecular biophysics: Structures in motion*, Oxford, University Press, 1999.

Cilji in kompetence:

Študenti poglobijo znanje s področja modeliranja v molekularni biofiziki. Študenti so sposobni uporabiti metode molekularnega modeliranja pri konkretnih problemih iz molekularne biofizike. Spoznajo pomembnost povezanosti računalniških simulacij z eksperimentalnimi metodami.

Objectives and competences:

Students acquire advanced knowledge in the field of modeling in molecular biophysics. Students are able to apply methods of molecular modeling to solve various problems in molecular biophysics. They learn about the importance of the link between computer simulations and experimental methods.

Spoznajo najnovejše raziskave in delo raziskovalnih skupin na tem področju po svetu in v regiji.

Students get familiar with up-to-date research work and research teams working in that field in the region and worldwide.

Predvideni študijski rezultati:

Znanje in razumevanje:

Poglobljeno razumevanje in sposobnost formulacije problemov iz molekularne biofizike na atomskem nivoju ter njihovo reševanje s sodobnimi računalniškimi metodami.

Prenosljive/ključne spretnosti in drugi atributi:

Sposobnost razvoja in uporabe izvirnih znanstvenih rešitev pri konstruiranju matematičnih modelov molekularne biofizike ter njihova predstavitev v mednarodni znanstveni periodiki.

Intended learning outcomes:

Knowledge and understanding:

Deeper understanding of - and abilities to formulate - problems in molecular biophysics on atomic-detail level and solving these problems using modern computational methods.

Transferable/Key Skills and other attributes:

Skills for development and implementation of original scientific solutions in constructing mathematical models of molecular biophysics. Presentation of acquired knowledge and research results in international scientific journals.

Metode poučevanja in učenja:

Predavanja, seminar in izdelava samostojnih raziskovalnih/seminarskih nalog.

Learning and teaching methods:

Lectures, seminar and work out of individual research seminars.

Načini ocenjevanja:

Seminarska naloga
Ustni izpit

Delež (v %) /

Weight (in %)

Assessment:

Seminar paper
Oral exam

50
50

Reference nosilca / Lecturer's references:

1. GRDADOLNIK, Jože, MERZEL, Franci, AVBELJ, Franc. Origin of hydrophobicity and enhanced water hydrogen bond strength near purely hydrophobic solutes. *Proceedings of the National Academy of Sciences of the United States of America*, ISSN 0027-8424, Jan. 2017, vol. 114, iss. 2, str. 322-327 <http://www.pnas.org/content/early/2016/12/23/1612480114.full.pdf?sid=4d626f7e-b9fa-446e-aeb6-b9080c59ce6a>, doi: 10.1073/pnas.1612480114. [COBISS.SI-ID 6068250]
2. MIRTič, Andreja, MERZEL, Franci, GRDADOLNIK, Jože. The amide III vibrational circular dichroism band as a probe to detect conformational preferences of alanine dipeptide in

water. *Biopolymers*, ISSN 0006-3525, Jul. 2014, vol. 101, iss. 7, str. 814-818, ilustr. <http://onlinelibrary.wiley.com/doi/10.1002/bip.22460/pdf>, doi: 10.1002/bip.22460. [COBISS.SI-ID 5482522]

3. PODOBNIK, Marjetka, SIDDIQUI, Nida, REBOLJ, Katja, NAMBI, Subhalaxmi, MERZEL, Franci, VISWESWARIAH, Sandhya S. Allostery and conformational dynamics in cAMP-binding acyltransferases. *The Journal of biological chemistry*, ISSN 0021-9258, Jun. 2014, vol. 289, iss. 23, str. 16588-16600. <http://www.jbc.org/content/289/23/16588.abstract>, doi: 10.1074/jbc.M114.560086. [COBISS.SI-ID 5463578]

4. NANDI, Sisir, MONESI, Alessandro, DRGAN, Viktor, MERZEL, Franci, NOVIČ, Marjana. Quantitative structure-activation barrier relationship modeling for Diels-Alder ligations utilizing quantum chemical structural descriptors. *Chemistry central journal*, ISSN 1752-153X, Oct. 2013, vol. 7, str. 1-13, ilustr. <http://journal.chemistrycentral.com/content/pdf/1752-153X-7-171.pdf>, doi: 10.1186/1752-153X-7-171. [COBISS.SI-ID 5382426]

5. GODEC, Aljaž, SMITH, Jeremy C., MERZEL, Franci. Soft collective fluctuations governing hydrophobic association. *Physical review letters*, ISSN 0031-9007. [Print ed.], Sep. 2013, vol. 111, iss. 12, str. 127801-1 - 127801-5. <http://link.aps.org/doi/10.1103/PhysRevLett.111.127801>, doi: 10.1103/PhysRevLett.111.127801. [COBISS.SI-ID 36953605]