Univerza v Mariboru

Fakulteta za naravoslovje in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	**Simulacijske metode v fiziki kondenzirane snovi**
Course title:	**Simulation methods in condensed matter physics**

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, 3rd cycle		**1. or 2.**	**1., 2. or 4.**

Vrsta predmeta / Course type	Izbirni za vse module/ Optional for all modules
Univerzitetna koda predmeta / University course code:	

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje work	Druge oblike študija	Samost. delo Individ. work	ECTS
15					165	6

Nosilec predmeta / Lecturer:	**Victor Teboul**

Jeziki / Languages:	**Predavanja / Lectures:**	angleško/English
	Vaje / Tutorial:	angleško/English

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisits:**
Pogojev ni. Priporočljiva znanja so: predznanje klasične fizike, moderne fizike, osnovnih numeričnih metod, matematičnih metod v fiziki.	None. Recommended is knowledge of classical physics, modern physics, basic numerical methods, and mathematical methods in physics.

Vsebina:	**Content (Syllabus outline):**

- Fizikalne osnove simulacij. Prednosti in slabosti.
- Poglavitne simulacijske metode: Monte Carlo in molekularna dinamika.
- Principi naprednih simulacijskih metod (disipativna dinamika delcev, metoda zrnjenja, ograjenost...).
- Statistika »surovih« rezultatov.
- Naprednejše metode.

Primeri in aplikacije.

- The physics behind the simulations. Advantages and drawbacks.
- The main simulation methods: Monte Carlo and Molecular Dynamics.
- Principles of advanced simulations methods (dissipative particle dynamics. coarse graining, confinement, ...).
- Statistics from the raw results.
- More advanced technics.

Examples and applications.

Temeljni literatura in viri / Readings:

1. Allen, M. P., & Tildesley, D. J. (2001). Computer simulation of liquids (Reprinted ed.). Oxford: Clarendon Press. ISBN 0-19-855645-4. [COBISS.SI-ID 11371784] https://plus.cobiss.net/cobiss/si/sl/bib/pefmb/11371784
2. Griebel, M., Knapek, S., & Zumbusch, G. (2007). Numerical simulation in molecular dynamics: Numerics, algorithms, parallelization, applications [e-knjiga]. Berlin; Heidelberg: Springer. ISBN 978-3-540-68095-6. [COBISS.SI-ID 33072133] https://plus.cobiss.net/cobiss/si/sl/bib/pefmb/33072133
3. Frenkel, D., & Smit, B. (2002). Understanding molecular simulation: From algorithms to applications (2nd ed.). San Diego: Academic Press. ISBN 0-12-267351-4. [COBISS.SI-ID 11320328] https://plus.cobiss.net/cobiss/si/sl/bib/pefmb/11320328
4. Landau, D. P., & Binder, K. (2000). A guide to Monte Carlo simulations in statistical physics. Cambridge: Cambridge University Press. ISBN 0-521-65314-2; 0-521-65366-5. [COBISS.SI-ID 1232484] https://plus.cobiss.net/cobiss/si/sl/bib/pefmb/1232484
5. Introduction to the basic concepts of modern physics: Special relativity, quantum and statistical physics [e-knjiga]. (2007). Milano: Springer. ISBN 978-88-470-0607-2. [COBISS.SI-ID 33217541] https://plus.cobiss.net/cobiss/si/sl/bib/pefmb/33217541
6. Teboul, V., Ciobotarescu, S. (2021). Orientation of motion of a flat folding nano-swimmer in soft matter. *Physical Chemistry Chemical Physics*, 23(14), 8836–8846. https://doi.org/10.1039/D1CP00136A

Dodatna literatura / Additional readings:

1. Leach, A. R. (2001). Molecular modelling: Principles and applications (2nd ed.). Harlow [etc.]: Prentice Hall. [COBISS.SI-ID 15988775]

Cilji in kompetence:

Objectives and competences:

Študenti pridobijo napredna znanja s področja simulacij v fiziki kondenzirane materije.	Students acquire advanced knowledge on simulations in condensed matter physics.

Predvideni študijski rezultati:	**Intended learning outcomes:**
Znanje in razumevanje: Razumevanje simulacijskega modeliranja različnih fizikalnih problemov. Pridobitev naprednih znanj na področju računalniških metodologij za reševanje fizikalnih problemov. Prenesljive/ključne spretnosti in drugi atributi: Reševanje problemov z numeričnimi metodami.	Knowledge and understanding: Understanding of simulation modeling of various problems in physics. Knowledge of computational methodologies for physics problem solving. Transferable/Key Skills and other attributes: Solving of problems with numerical methods.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Predavanja in reševanje zastavljenih problemov.	Lectures and solving of defined problems.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
~~Seminar.~~	**50%**	~~Seminar.~~
~~Ustni izpit.~~	**50%**	~~Oral exam.~~
Seminarska naloga		Seminar paper
Ustni izpit		Oral exam

Reference nosilca / Lecturer's references:

~~Teboul, V. (2023). Dynamic phase transition induced by active molecules in a supercooled liquid. Physical Review E, 108(2), 024605~~ ~~https://doi.org/10.1103/PhysRevE.108.024605~~

~~V Teboul, S. Ciobotarescu. Orientation of motion of a flat folding nano-swimmer in soft matter. Physical Chemistry Chemical Physics 14 (2021) DOI~~ ~~https://doi.org/10.1039/D1CP00136A~~

~~V Teboul, G Rajonson, Temperature dependence of the violation of Purcell's theorem experienced by a folding molecular motor. Physical Chemistry Chemical Physics 21 (5), 2472-2479 (2019)~~

- TEBOUL, Victor. Dynamic phase transition induced by active molecules in a supercooled liquid. Physical Review E, 2023, vol. 108, no. 2, 024605. doi: 10.1103/PhysRevE.108.024605

- TEBOUL, Victor, CIOBOTARESCU, Simona. Orientation of motion of a flat folding nano-swimmer in soft matter. Physical Chemistry Chemical Physics, 2021, vol. 23, no. 14, str. 8259–8264. doi: 10.1039/D1CP00136A

  MERCIER, Felix, DELHAYE, Gaetan, TEBOUL, Victor. Activation induced fluidization of a confined viscous liquid, Journal of Molecular Liquids 360 (2022) 119545, doi: 10.1016/j.molliq.2022.119545