



Univerza v Mariboru

Fakulteta za naravoslovje
in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet:	Statistična termodinamika
Course title:	Statistical thermodynamics

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Fizika 2. st.		1	1
Physics 2 nd degree		1	1

Vrsta predmeta / Course type

Univerzitetna koda predmeta / University course code:

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje work	Druge oblike študija	Samost. delo Individ. work	ECTS
30		45			165	8

Nosilec predmeta / Lecturer:

Jeziki / Languages:	Predavanja / Lectures:	<input type="text" value="slovenski/Slovenian"/>
	Vaje / Tutorial:	<input type="text" value="slovenski/Slovenian"/>

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

Pogojev ni. Priporočljiva znanja so: formalno oziroma neformalno osvojeno znanje iz vsebin predmetov Mehanika, Termodinamika, Elektromagnetizem, Nihanje in valovanje, Moderna fizika.

Prerequisites:

None. Recommended knowledge: formal or informal knowledge from subjects Mechanics, Thermodynamics, Electromagnetism, Vibrational and Wave motion, Modern Physics.

Vsebina:

Content (Syllabus outline):

Predavanja

1. Termodinamika. Makroskopska stanja in termodinamične spremenljivke. Enačbe stanja. Zakoni termodinamike. Termodinamični potenciali. Fazne spremembe.
2. Osnovni pojmi teorije verjetnosti. Diskretne in zvezne porazdelitve verjetnosti.
3. Statistična mehanika. Mikroskopska stanja in princip maksimalne entropije. Teorija ansamblov: mikrokanoničen, kanoničen in veleanoničen ansambel ter ustrezne porazdelitvene funkcije. Primeri: idealni plin, idealna raztopina, kristal; toplotna kapaciteta idealnega plina in trdne snovi, paramagnetizem, enačba stanja realnega plina, kemijske reakcije.
4. Osnove kvantne statistične mehanike. Idealni Bosejevi in Fermijevi sistemi. Primeri: harmonski oscilator, idealni plin, sevanje črnega telesa, elektroni v kovini.
5. Kinetična teorija transportnih procesov. Difuzija snovi, prevajanje toplote, viskoznost.
6. Osnove neravnovesne termodinamike in izbrani primeri iz biologije in kemije. Kinetika in termodinamika encimskih reakcij, farmakokinetika.

Seminarska raziskovalna naloga

Študent se s seminarsko raziskovalno nalogo poglobi v zahtevnejši problem na področju statistične termodinamike in predlaga (ali v literaturi poišče) njegovo rešitev v obliki teoretičnega fizikalnega modela. O rezultatih poroča v obliki pisne seminarske naloge in ustne predstavitve.

Lectures:

1. Thermodynamics. Macroscopic states and thermodynamic variables. Equations of state. The laws of thermodynamics. Thermodynamic potentials. Phase transitions. Introduction to non-equilibrium thermodynamics.
2. Principles of probability. Probability distribution functions.
3. Statistical mechanics. Microstates and the principle of maximum entropy. The ensemble theory: microcanonical, canonical and grand canonical ensemble and partition functions. Boltzmann statistics. Examples and applications: ideal gas and ideal solution, solids; heat capacity; paramagnetism, equation of state of real gases, chemical reactions.
4. Introduction to quantum statistics. Ideal Bose and Fermi systems. Examples and applications: ideal gas, harmonic oscillator, black-body radiation, the electron gas in metals.
5. Kinetic theory of transport processes. Diffusion, heat conduction, viscosity.
6. Introduction to non-equilibrium thermodynamics and selected examples from biology and chemistry. Chemical kinetics and thermodynamics, enzymatic reactions, pharmacokinetics.

Seminar work

In scope of the seminar work student studies an advanced specific problem in statistical thermodynamics and propose its solution in the form of physical theoretical model. The results of the seminar work are presented in the form of written work and oral presentation.

Temeljni literatura in viri / Readings:

1. W. Greiner, L. Neise, H. Stöcker: Thermodynamics and Statistical Mechanics, Springer, New York 1997.
2. S. J. Blundell, K. M. Blundell: Concepts in Thermal Physics, Oxford University Press, Oxford 2006.
3. I. Kuščer, S. Žumer: Toplota (Termodinamika, statistična mehanika, transportni pojavi), DMFA, Ljubljana 2017.
4. K.A. Dill, S. Bromberg: Molecular Driving Forces, Statistical Thermodynamics in Chemistry and Biology, Garland Science, New York 2003.

Cilji in kompetence:

Podati metode in koncepte fizikalnega opisa sistemov na mikroskopski in makroskopski ravni s poudarkom na njuni medsebojni povezanosti.

Objectives and competences:

Students gain methods and concepts of description of systems on the micro and macroscopic scales with the interrelationship between the two levels emphasized.

Predvideni študijski rezultati:**Znanje in razumevanje:**

Razumevanje procesov v naravi (primeri iz fizike, kemije in biologije) na makroskopski in mikroskopski ravni. Pri tem študentje osvojijo kvantitativne matematično fizikalne pristope in metode opisa teh pojavov.

Študent razume povezavo med makroskopsko obravnavo termodinamike in statistično termodinamiko in zna uporabiti analogije, tako da matematični model na nekem fizikalnem področju kritično prenese na nova področja (elektronski plin itd.).

Študent razume, analizira in sintetizira tista področja iz fizike in kemije, ki jih povezuje statistična termodinamika.

Prenesljive/ključne spretnosti in drugi atributi:

Celosten pristop k reševanju problemov in izdelavi matematičnih modelov. Osvojiti znanja uporabne matematike.

Sposobnost prepoznati problem in ga teoretično obravnavati v okviru konceptov in metod statistične termodinamike.

Uporaba informacijske tehnologije: uporaba različnih simulacijskih programskih orodij za izvedbo zahtevnejših fizikalnih simulacij.

Intended learning outcomes:**Knowledge and understanding:**

Understanding of processes in nature (examples from physics, chemistry and biology) on the macroscopic as well as microscopic scales. The students acquire to use quantitative mathematical and physical methods in comprehensive description of these phenomena.

The student understands the relation between the macroscopic treatment of physical phenomena in thermodynamics and microscopic treatment in statistical thermodynamics. The student is able to use analogies and critically translate the mathematical model from specific physical area to new areas (electronic gas etc.).

The student understands, analyses and synthesises those areas in physics and chemistry that are connected with statistical thermodynamics.

Transferable/Key Skills and other attributes:

An integral approach to solving problems and elaborating the corresponding mathematical models. To gain advanced mathematical tools. Ability to identify problems and describe them theoretically within the scope of methods and concepts of statistical thermodynamics.

Use of information technology: use of different computer simulation tools in demanding physical simulations.

Metode poučevanja in učenja:**Learning and teaching methods:**

<ul style="list-style-type: none"> - Predavanja (razlaga, razgovor) - Seminarska raziskovalna naloga (individualizacija poučevanja) - Računske vaje (razlaga, razgovor) 	<ul style="list-style-type: none"> - Lectures (explanation, discussion) - Seminar research work (individualization of teaching) - Tutorials (explanation, discussion)
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Delež (v %) /

Weight (in %) /

Načini ocenjevanja:

Assessment:

Način:	Delež (v %) / Weight (in %)	Type:
pisni izpit (lahko se opravi z 2 pisnima kolokvijema)	40	written exam (can be done with 2 written tests)
ustni izpit	30	oral exam
seminarska naloga	30	seminar work
<p>Opravljena seminarska naloga je pogoj za pristop k izpitu. Za uspešno zaključeno učno enoto mora vsak del posebej biti pozitiven.</p>		<p>Completed seminar work is necessary to approach the oral exam. Each part of the examination must be successfully completed for final and successful completion of the course.</p>

Reference nosilca / Lecturer's references:

Andrej Dobovišek:

1. ŠTERK, Marko, MARKOVIČ, Rene, MARHL, Marko, FAJMUT, Aleš, **DOBOVIŠEK, Andrej**. Flexibility of enzymatic transitions as a hallmark of optimized enzyme steady-state kinetics and thermodynamics. *Computational biology and chemistry*. [Print ed.]. Apr. 2021, vol. 91, str. 1-10. ISSN 1476-9271. DOI: [10.1016/j.compbiolchem.2021.107449](https://doi.org/10.1016/j.compbiolchem.2021.107449). [COBISS.SI-ID [52543491](https://www.cobiss.si/id/52543491)], financier: ARRS, Programi, P1-0055, SI, Biofizika polimerov, membran, gelov, koloidov in celic

2. JURETIĆ, Davor, BONAČIĆ LOŠIĆ, Željana, KUIĆ, Domagoj, SIMUNIĆ, Juraj, **DOBOVIŠEK, Andrej**. The maximum entropy production requirement for proton transfers enhances catalytic efficiency for β -lactamases. *Biophysical chemistry*. [Print ed.]. Jan. 2019, vol. 244, str. 11-21, ilustr. ISSN 0301-4622. DOI: [10.1016/j.bpc.2018.10.004](https://doi.org/10.1016/j.bpc.2018.10.004). [COBISS.SI-ID [24237832](https://www.cobiss.si/id/24237832)], financier: ARRS, Programi, P1-0055 (B), SI, Biofizika polimerov, membran, gelov, koloidov in celic

3. VITAS, Marko, **DOBOVIŠEK, Andrej**. Towards a general definition of life. *Origins of life and evolution of the biospheres*. 2019, vol. 49, iss. 1/2, str. 77-88, graf. prikazi. ISSN 0169-6149. DOI: [10.1007/s11084-019-09578-5](https://doi.org/10.1007/s11084-019-09578-5). [COBISS.SI-ID [24634376](https://www.cobiss.si/id/24634376)], financier: ARRS, Programi, P1-0055 (B), SI, Biofizika polimerov, membran, gelov, koloidov in celic

4. VITAS, Marko, **DOBOVIŠEK, Andrej**. In the beginning was a mutualism : on the origin of translation. *Origins of life and evolution of the biospheres*. 2018, vol. 48, iss. 2, str. 223-243, ilustr. ISSN 0169-6149. DOI: [10.1007/s11084-018-9557-6](https://doi.org/10.1007/s11084-018-9557-6). [COBISS.SI-ID [23839496](https://www.cobiss.si/id/23839496)], financier: ARRS, Programi, P1-0055 (B), SI, Biofizika polimerov, membran, gelov, koloidov in celic

5. **DOBOVIŠEK, Andrej**, MARKOVIČ, Rene, BRUMEN, Milan, FAJMUT, Aleš. The maximum entropy production and maximum Shannon information entropy in enzyme kinetics. *Physica. A, Statistical mechanics and its applications*. [Print ed.]. 2018, vol. 496, str. 220-232. ISSN 0378-4371. DOI: [10.1016/j.physa.2017.12.111](https://doi.org/10.1016/j.physa.2017.12.111). [COBISS.SI-ID [23601416](https://www.cobiss.si/id/23601416)], financier: ARRS, Programi, P1-0055 (B), SI, Biofizika polimerov, membran, gelov, koloidov in celic

