

Subject card

Subject name and code	Statistical mechanics of biological macromolecules, PG_00119777						
Field of study	Chemistry						
Date of commencement of studies	October 2025		Academic year of realisation of subject		2026/2027		
Education level	Master's studies		Subject group		Optional subject group		
Mode of study	full-time studies		Mode of delivery		at the university		
Year of study	2		Language of instruction		English		
Semester of study	3		ECTS credits		2.0		
Learning profile	academic		Assessment form		credit		
Conducting unit	Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Józef Liwo				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	30.0	0.0	0.0	0.0	30
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours		Self-study	SUM
	Number of study hours	30		5.0		15.0	50
Subject objectives	The aim of the course is to familiarize students with the basics of statistical mechanics of biopolymers, with particular emphasis on the conditions and mechanisms their structure formation.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_U11] Communicates in English in accordance with the requirements specified for level B2 of the Common European Framework of Reference for Languages.	The student learns English vocabulary in statistical physics and the physical chemistry of biological macromolecules.	[SU1] oral statement/conversation/discussion
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	The student knows the limitations of her/his knowledge in calculus, statistical physics, and the physical chemistry of biological molecules and knows the ways of completing it.	[SK4] test/exam - oral or written [SK5] implementation of a problem task
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	The student critically evaluates applications of statistical mechanics in the description of the structure and energetics of biological macromolecules.	[SU1] oral statement/conversation/discussion [SU5] implementation of a problem task
	[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student applies calculus to statistical mechanical description of macromolecules.	[SW4] test/exam - oral or written [SW1] oral statement/conversation/discussion [SW5] implementation of a problem task
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	The student applies extended knowledge in the statistical mechanics of biological macromolecules.	[SW4] test/exam - oral or written [SW1] oral statement/conversation/discussion
	[CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.	The student applies statistical mechanics in the description of biological macromolecules.	[SK1] oral statement/conversation/discussion [SK4] test/exam - oral or written [SK5] implementation of a problem task
Subject contents	Elements of statistical mechanics: ensembles, ensemble averages, thermodynamic connection. Statistical-mechanical models of polymers chains. Potentials of mean force. Structure formation and self-organization in biopolymers as a phase transition. One-dimensional case: helix-coil transition. Solvent-mediated interactions in the formation and stabilization of biopolymer structure. Polymers in a good and in a bad solvent. Global minimum of a potential and of the free energy and stability of polymer structure. Foldability. Simple lattice models to study foldability. Free-energy landscapes of biological macromolecules and methods for their investigation. Coarse-grained force fields for biopolymer simulations as potentials of mean force.		
Prerequisites and co-requisites	Knowledge of the applications of statistical mechanics in chemistry.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Test	51.0%	50.0%
	Completing assignments	51.0%	50.0%
Recommended reading	Basic literature	D. McQuarrie: Statistical mechanics	
		A. Leach: Molecular modeling: principles and applications	
	Supplementary literature	T. Schlick: Molecular dynamics and simulations	
	eResources addresses		
Example issues/ example questions/ tasks being completed	1. Calculate the energy of a protein molecule represented by the HP model on cubic lattice. 2. Using UNRES server run energy minimization of the crambin molecule and interpret the deviations from the experimental structure. 3. Using UNRES server determine the thermal heat-capacity profile of tryptophan cage and interpret the maximum in this profile.		
Work placement	Not applicable		

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