University of Gdańsk

Subject card

Subject name and code	Statistical mechanics of biological macromolecules, PG_00119777						
Field of study	Chemistry						
Date of commencement of studies	October 2026			Academic year of realisation of subject		2027/2028	
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	(see table below)

Course outcome	Subject outcome	Method of verification
[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 descritption of biological macromolecules.	[SK1] oral statement/conversation/ discussion [SK4] test/exam - oral or written [SK5] 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_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_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	The student criticlally 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_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_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

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	Knowlege of the applications of statistical mechanics in chemistry.
Assessment methods and criteria	(see table below)

Subject passing criteria	Passing threshold	Percentage of the final grade
Completing assignments	51.0%	50.0%
Test	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 miminization 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