GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	MOLECULAR PHYSICOCHEMISTRY OF SOLUTIONS, PG_00064404		
Field of study	Chemistry		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2028/2029
Education level	first-cycle studies	Subject group	Optional subject group Subject group related to scientific research in the field of study
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	3	Language of instruction	Polish
Semester of study	5	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Maciej Śmiechowski	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	15.0	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	2.0	18.0	50

Subject objectives

The aim of the subject is to introduce the students to the molecular basis of the physicochemical phenomena associated with the formation of solutions.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U03] operates typical laboratory apparatus and carries out analyses to identify chemical compounds and materials, integrating computational methods and application software	performs molecular dynamics or Monte Carlo simulations to predict the structure and physicochemical properties of solutions.	[SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task [SU1] Assessment of task fulfilment
[K6_W05] recognises methods, techniques and tools of computer aided design for solving engineering tasks in chemistry, chemical engineering and technology, mechanical engineering, in the design and analysis of technological processes	can utilise selected open-source programs for conducting simulations using molecular dynamics and Monte Carlo methods and analyzing the obtained results.	[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects
[K6_W03] demonstrates knowledge in the area of theoretical chemistry and related engineering disciplines, necessary to predict structures, design and conduct basic process operations using molecular mechanics tools	knows the basics of molecular mechanics, including molecular dynamics and the Monte Carlo method, to the extent necessary to conduct computer simulations in the field of physicochemistry of solutions.	[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects
[K6_U01] gathers information from literature, databases and other sources, interpreting, critically evaluating, summarising, formulating and justifying opinions, independently analyses and produces technical drawings with the use of computer assistance	is able to relate the observed macroscopic properties of various types of solvents used in technological processes with their molecular structure and microscopic physical properties.	[SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject

Subject contents	Course content – lecture Resume of phenomenological thermodynamics: conditions of spontaneity and equilibrium, laws of thermodynamics, thermodynamic potentials, Gibbs-Duhem equation, partial quantities, apparent quantities; Resume of probabilistics: probability, law of large numbers, discrete and continuous random variables, measures of location and dispersion, probability distributions, normal distribution, central limit theorem; Fundamentals of classical statistical thermodynamics: phase space, density of states, Liouville's theorem, microcanonical, canonical, grand canonical ensembles, sum of states, ergodic hypothesis, equilibrium fluctuations; Molecular theory of solutions: distribution functions, Kirkwood-Buff theory; Solvation theory and preferential solvation; Dynamic properties: linear response theory, correlation functions, Green-Kubo relations. Course content – laboratory Computer exercises in the field of molecular dynamics of solutions: 1. Hydrotropic Solubilization in a Two-Phase Water-Chloroform System Using Ethanol 2. Determination of the Molar Volume of Ionic Liquids in Molecular Solvents 3. Determination of the Induced Dipole Moment of Halogen Ions in Polar Solvents
Prerequisites and co-requisites	Successfully finished subjects: Mathematics, Physics, Physical chemistry, Theoretical chemistry

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Final lecture test	50.0%	50.0%
Laboratory reports	60.0%	50.0%

Recommended reading

Basic literature	K. Zalewski, Wykłady z mechaniki i termodynamiki statystycznej dla chemików, PWN, Warszawa, 1982. N. A. Smirnowa, Metody termodynamiki statystycznej w chemii fizycznej, PWN, Warszawa, 1980.
Supplementary literature	H. Buchowski, Elementy termodynamiki statystycznej, WNT, Warszawa 1998. A. Ben-Naim, Molecular Theory of Solutions, Oxford University Press, New York, 2006. D. A. McQuarrie, Statistical Mechanics, Harper & Row, New York, 1976. M. E. Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford University Press, New York, 2010.
eResources addresses	

Example issues/ example questions/ tasks being completed	Give the relationship between the heat capacity of a system and its energy fluctuations. Give the relationship between the isothermal compressibility of a system and fluctuations in the number of particles. Describe the ergodic hypothesis. Discuss the concept of activity in the context of statistical thermodynamics. State the physical meaning of the radial distribution function and its relationship to the number of particles at a given distance. Give the definition of the Kirkwood-Buff integral. Give the Ben-Naim definition of the free energy of solvation. Define the concept of preferential solvation. Prove that the Einstein's formula for the diffusion coefficient and the corresponding Green-Kubo relation are interrelated.
Practical activites within the subject	Not applicable

Document generated electronically. Does not require a seal or signature.