GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Molecular Physicochemistry of Solutions , PG_00053220		
Field of study	Chemistry		
Date of commencement of studies	October 2020	Academic year of realisation of subject	2022/2023
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	6	ECTS credits	4.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Maciej Śmiechowski	
	Teachers		

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	15.0	0.0	15.0	60

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	60	5.0	35.0	100

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_W03	The student performs molecular dynamics or Monte Carlo simulations to predict the structure and physicochemical properties of solutions.	[SW3] Assessment of knowledge contained in written work and projects
[K6_U03] can make detailed documentation of the results of self-conducted experiments and prepare a report describing these results	The student conducts computer simulations in the field of physical chemistry of solutions using various techniques and is able to document and interpret their results.	[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task
[K6_U05] can, on the basis of the collected experimental or source material, prepare an oral communication with a multimedia presentation	The student presents a multimedia presentation on a given topic related to the molecular basis of physicochemical phenomena occurring in solutions.	[SU5] Assessment of ability to present the results of task [SU1] Assessment of task fulfilment
[K6_U01] knows how to get information from literature, databases and other sources, can integrate the information obtained, interpret and critically evaluate it, and draw conclusions, and to formulate and justify the opinions	The student 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.	[SU3] Assessment of ability to use knowledge gained from the subject [SU2] Assessment of ability to analyse information

Subject contents	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, Ornstein-Zernike and Percus-Yevick integral equations; Solvation theory and preferential solvation; Dynamic properties: linear response theory, correlation functions, fluctuation-dissipation theorem, Green-Kubo relations; Fundamentals of thermodynamics of irreversible processes: source of entropy, local equilibrium hypothesis, local Gibbs equation, substance balance of entropy, thermodynamic stimuli and flows, Onsager's principle, Curie's principle, cross-effects, stationary states. Laboratory: Computer exercises in the field of molecular dynamics of solutions and the Monte Carlo method. Seminar: Presentations extending the lecture topics.
Prerequisites and co-requisites	Successfully finished subjects: Mathematics, Physics, Physical chemistry, Theoretical chemistry, Modeling in chemistry

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Multimedia presentation	50.0%	30.0%
Laboratory reports	60.0%	30.0%
Final lecture test	50.0%	40.0%

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. B. Baranowski, Nierównowagowa termodynamika w chemii fizycznej, PWN, Warszawa, 1974.
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	Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed	
Work placement	Not applicable