



Subject card

Subject name and code	Physical Chemistry, PG_00048936						
Field of study	Chemistry						
Date of commencement of studies	February 2024		Academic year of realisation of subject		2023/2024		
Education level	second-cycle studies		Subject group		Obligatory subject group in the field of study 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	1		Language of instruction		Polish		
Semester of study	1		ECTS credits		4.0		
Learning profile	general academic profile		Assessment form		exam		
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. Aneta Panuszko				
	Teachers		dr inż. Joanna Grabowska				
			dr hab. Aneta Panuszko				
			dr hab. inż. Piotr Bruździak				
			dr hab. inż. Dorota Warمیńska				
			dr hab. inż. Joanna Krakowiak				
		dr hab. inż. Jarosław Wawer					
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	30.0	0.0	0.0	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		10.0		30.0	100
Subject objectives	The aim of the course is to familiarize the student with various techniques, both experimental and theoretical, used to study the physicochemical properties of solutions and complex systems.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	K7_W05		The student is able to build simple simulation systems and simulate them using molecular dynamics methods. The student analyzes the results obtained using molecular dynamics methods and draws conclusions based on them.		[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge		
	K7_U01		ability of critical evaluation of information sources, available in the literature		[SU2] Assessment of ability to analyse information [SU1] Assessment of task fulfilment		
	K7_W02		The student knows and understands the principles of the operation of measuring equipment used to test the physicochemical properties of solutions and complex systems. The student develops and interprets the results of physicochemical experiments.		[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge		

Subject contents	The subject of the course covers the following issues: <ol style="list-style-type: none">1. Infrared spectroscopy in the study of intermolecular interactions: methods of developing spectra, selected chemometric methods in the analysis of spectral series in solving chemical problems. Analysis of the structure and energy of water hydrogen bonds around a solute: isotope dilution technique, difference spectra method, OD band spectral parameters, Badger-Bauer rule, empirical function correlating the oxygen-oxygen intermolecular distance with the position of the band.2. Intermolecular interactions in electrolyte solutions containing solvents with different donor properties and spatial structure and in aqueous solutions of non-electrolytes using precise measurements of density and sound speed: determining the limit values of apparent volumes and molar compressibility, division of standard partial volumes and molar compressibility of electrolytes into ionic shares , determination of solvation numbers of ions based on adiabatic compressibility and standard partial molar volume, coefficient of thermal expansion, Hepler's relation, standard partial volumes and molar compressivities of solute transfer, McMillan and Mayer equation.3. Study of the particle aggregation process using atomic force microscopy; characterization of colloidal solutions containing aggregates of macromolecules or nanoparticles by measuring dynamic light scattering.4. Heterogeneous redox reactions - calculation of the absolute value of the standard hydrogen electrode potential using the thermodynamic cycle. Standard potential of reduction reactions - determination, application and correlations with parameters reflecting the electronic structure of the molecule.5. Basics of molecular modeling methods: models of intermolecular interactions, taking into account constraints; problem of boundaries of simulation systems, periodic boundary conditions; molecular dynamics, numerical solution of equations of particle motion; different simulation conditions (NVT, NpT); results analysis methods: liquid structure, radial distribution functions, time correlation functions, diffusion.		
Prerequisites and co-requisites	Mathematics, Physics, Physical Chemistry,		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	computer laboratory	60.0%	25.0%
	practical elements of the lecture	60.0%	25.0%
	exam	60.0%	50.0%
Recommended reading	Basic literature	<ol style="list-style-type: none">1. H. Mark, J. Workman, Jr. , "Chemometrics in spectroscopy", 2007, Elsevier2. J. Stangret, <i>Zeszyty Naukowe Politechniki Gdańskiej</i>, Chemia XLV (578), 2000.3. Z. Jia, J. Li, L. Gao, D. Yang, A. Kanaev, Dynamic Light Scattering: A Powerful Tool for In Situ Nanoparticle Sizing, <i>Colloids Interfaces</i> 7, (2023) 154. Malvern Instruments, technical note, "Dynamic Light Scattering: An Introduction in 30 Minutes" MRK656-015. S. Liu, Y. Wang, Application of AFM in Microbiology: A Review <i>Scanning</i> 32, (2010) 61736. Organic Electrochemistry: Revised and Expanded (pp.229-259), Edition: 5th, Chapter: 6, Publisher: CRC Press, Taylor and Francis Group, Editors: Ole Hammerich, Bernd Speiser7. M.J. Abraham, D. van der Spoel, E. Lindahl, B. Hess, and the GROMACS Development Team. GROMACS 2023.4 Manual	
	Supplementary literature	<ol style="list-style-type: none">1. M. Śmiechowski, J. Stangret, Vibrational spectroscopy of semiheavy water (hdo) as a probe of solute hydration, <i>Pure Appl. Chem.</i> 82 (10) (2010) 18691887.2. M. Szklarczyk, <i>Mikroskopia chemiczna i analityczne techniki wielowymiarowe oraz sprzężone</i> PWN 2020	
	eResources addresses	Adresy na platformie eNauczanie:	
Example issues/ example questions/ tasks being completed	<ol style="list-style-type: none">1. What are the purposes of chemometric analysis methods for spectral data?2. Discuss the Badger-Bauer rule with a simple example.3. What fractions make up the standard partial molar volume of an electrolyte?4. How is the correlation function obtained in DLS measurements?5. Carrying out a computer simulation of argon gas under conditions of constant pressure and constant volume.		
Work placement	Not applicable		

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