



Subject card

Subject name and code	Applied physical chemistry, PG_00066089						
Field of study	Chemistry						
Date of commencement of studies	February 2025	Academic year of realisation of subject			2024/2025		
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			3.0		
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. Aneta Panuszko					
	Teachers	dr hab. Aneta Panuszko dr hab. inż. Piotr Bruździak dr inż. Joanna Grabowska dr hab. inż. Dorota Warmińska dr hab. inż. Joanna Krakowiak					
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	30.0	15.0	0.0	45
	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	45		5.0		25.0	75
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_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation	The student develops and delivers technical reports in the form of text documents and spreadsheets. The student creates charts and diagrams for result analysis. The student prepares a multimedia presentation and presents the results in the form of a public speech.	[SU5] Assessment of ability to present the results of task [SU4] Assessment of ability to use methods and tools [SU3] Assessment of ability to use knowledge gained from the subject
	[K7_W03] recognizes and describes phenomena in the field of physics, including elements of quantum mechanics, solid state physics and nuclear physics, necessary to predict the course of physical phenomena and to solve technical problems	The student builds simple simulation systems and conducts their simulations using molecular dynamics methods. The student analyzes the results obtained through molecular dynamics methods and draws conclusions based on them.	[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects
	[K7_U02] prepares detailed documentation of the results of independently conducted experiments and analyzes the obtained results, uses professional vocabulary with understanding and prepares and communicates information	The student develops and interprets the results of independently conducted physicochemical experiments. The student presents the results in the form of a report.	[SU5] Assessment of ability to present the results of task [SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfilment
[K7_K02] is able to cooperate and work in a group, taking on different roles	The student effectively collaborates in a team, assuming various roles to accomplish common tasks and projects. The student takes responsibility for specific tasks and engages in communication and problem-solving within the group.	[SK4] Assessment of communication skills, including language correctness [SK1] Assessment of group work skills [SK5] Assessment of ability to solve problems that arise in practice	
Subject contents	<p>The subject of the course covers the following issues:</p> <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 compressibilities of solute transfer, McMillan and Mayer equation. 3. 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. 4. 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
	reports (project)	60.0%	50.0%
	tests + reports (laboratory)	60.0%	50.0%
Recommended reading	Basic literature	<ol style="list-style-type: none"> 1. H. Mark, J. Workman, Jr., "Chemometrics in spectroscopy", 2007, Elsevier 2. J. Stangret, <i>Zeszyty Naukowe Politechniki Gdańskiej</i>, Chemia XLV (578), 2000. 3. Organic Electrochemistry: Revised and Expanded (pp.229-259), Edition: 5th, Chapter: 6, Publisher: CRC Press, Taylor and Francis Group, Editors: Ole Hammerich, Bernd Speiser 4. 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. 	
	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. Carrying out a computer simulation of argon gas under conditions of constant pressure and constant volume.
Work placement	Not applicable

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