GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Physical Chemistry, PG_00048936		
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	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		

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_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.	[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects
K7_U01	ability of critical evaluation of information sources, available in the literature	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information
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.	[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects

Subject contents

The subject of the course covers the following issues:

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
exam	60.0%	50.0%
practical elements of the lecture	60.0%	25.0%
computer laboratory	60.0%	25.0%

Recommended reading

Basic literature

1. H. Mark, J. Workman, Jr. , "Chemometrics in spectroscopy", 2007, Elsevier
2. J. Stangret, *Zeszyty Naukowe Politechniki Gdańskiej*, 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, Colloids Interfaces 7, (2023) 15
4. Malvern Instruments, technical note, "Dynamic Light Scattering: An Introduction in 30 Minutes" MRK656-01
5. S. Liu, Y. Wang, Application of AFM in Microbiology: A Review Scanning 32, (2010) 6173
6. Organic Electrochemistry: Revised and Expanded (pp.229-259), Edition: 5th, Chapter: 6, Publisher: CRC Press, Taylor and Francis Group, Editors: Ole Hammerich, Bernd Speiser
7. M.J. Abraham, D. van der Spoel, E. Lindahl, B. Hess, and the GROMACS Development Team. GROMACS 2023.4 Manual

Supplementary literature

1. M. Śmiechowski, J. Stangret, Vibrational spectroscopy of semiheavy water (hdo) as a probe of solute hydration, Pure Appl. Chem. 82 (10) (2010) 18691887.
2. M. Szklarczyk, Mikroskopia chemiczna i analityczne techniki wielowymiarowe oraz sprzężone PWN 2020

eResources addresses

Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed

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

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