

## 。 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	Subject supervisor		dr hab. Aneta Panuszko					
of lecturer (lecturers)	Teachers							
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Projec	t	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 ir classes includ plan		a didactic Participation in consultation hours		Self-study SU		SUM	
	Number of study 60 hours			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		

1.         Inferred spectroscopy in the study of intermolecular interactions: methods of devolution technique, selected chornenterin, methods in the analysis of percent arents. Bodge: Boards arents and solute: isotope dilution technique, difference spectra method. OD band spectral parentses. Bodge: Boards with different door properties and spatial structure and in express system intermolecular distance with the position of the band.           2.         Intermolecular interactions: intervolves using prestame measurements of within of solution numbers of ioms based on adiabatic compressibility of descriptions in the ion starts of descriptions in the ion starts of an expective system. The ion is starts of adiabatic compressibility of descriptions in the ion starts of molecular molecular on the solution and the adiabatic compressibility of descriptions in the ion starts of molecular molecular on adiabatic sequences. Start and partial adiabatic partial molecular interactions. Lating of the standard partial volumes and malar compressibility of descriptions in the ion starts of the mean of the standard partial volumes and malar compressibility of descriptions in starts of the mean electrone spectra and start and the mean electrone control of the standard private light scattering.           3.         Study of the partial signification control of the attradent by the partial starts of the mean electrone study of the starts of the mean electrone study of the standard partial volumes and malar compressibility of descriptions in spectroscopy of the standard partial volumes and malar compressibility of the standard partial volumes and malar compressibility of the standard partial volumes and malar volumes and malar volumes and malar compressibility of the standard partial volumes and malar volume and the partial volumes and malar volume and malar volumes anad volume trestressibility of themeandecular interactions. Lange v	Subject contents	The subject of the course covers the following issues:						
Prerequisites       Mathematics, Physics, Physical Chemistry,         Assessment methods and criteria       Subject passing criteria       Passing threshold       Percentage of the final grade         Assessment methods and criteria       Subject passing criteria       Passing threshold       Percentage of the final grade         exam practical elements of the lecture       60.0%       50.0%         Recommended reading       Basic literature       1. H. Mark, J. Workman, Jr., "Chemometrics in spectroscopy", 2007, Elsevice         2. J. Stangert, Zeszyly Naukowe Politechniki Gdańskie, Chemia XLV (578), 2000.       2. J. Stangert, Zeszyly Naukowe Politechniki Gdańskie, Chemia XLV (578), 2000.         3. Z. Ja, J. Li, L. Go n. Stunoparticel Szing, Colloids Interfaces 7, (2023) 15       Matvem 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       S. Liu, Y. Wang, Application of AFM in Microbiology: A Review Scanning 32, (2010) 16173         Supplementary literature       1. M. Smiechowski, J. Stangert, Vibrational spectroscopy of semileavy water (hdo) as a probe of solute hydration, Pure Appl. Chem. 82 (10) (2010) 16801887.         Supplementary literature       1. M. Smiechowski, J. Stangert, Vibrational spectroscopy of semineavy water (hdo) as a probe of solute hydration, Pure Appl. Chem. 82 (10) (2010) 16801887.         Example issues/ example questions/ tasks being completed       1. What are the purposes of chemometric analysis me		<ol> <li>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.</li> <li>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.</li> <li>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.</li> <li>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.</li> <li>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: l</li></ol>						
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. Stangert, 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. Lindani, B. Hess, and the GROMACS Development Team. GROMACS 2023 Manual         Supplementary literature       1.       M. Skiterskopia chemiczna i analityczne techniki wielowymiarowe oraz sprzężone PWN 2020         example issues/ example questions/ tasks being completed       1.       What rac the purposes of chemometric analysis methods for spectral data?         2.	Prerequisites and co-requisites	Mathematics, Physics, Physical Chemistry,						
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Image: 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. Ju, J. L. 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: A normal tool for In Situ Nanoparticle Sizing, Colloids Interfaces 7, (2023) 15           5. 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, Berd Speiser           7. M.J. Abraham, D. van der Spoel, E. Lindahl, B. Hess, and the GROMACS Development Team. GROMACS Development Team. GROMACS Development Team. GROMACS 2023.4 Manual           Supplementary literature         1. M. Smiechowski, J. Stangret, Vibrational spectroscopy of semiheavy water (hdo) as a probe of solute hydration, Pure Appl. Chem. 82 (10) (2010) 18691887.           example issues/ example questions/ tasks being completed         1. What are the purposes of chemometric analysis methods for spectral data?           9. Usita tractic state completer simulation obtained in DLS measurements?         5. Carrying out a computer simulation of argon gas under conditions of constant pressure and constant volume.		practical elements of the lecture	60.0%	25.0%				
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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	Recommended reading	Basic literature	<ol> <li>H. Mark, J. Workman, Jr., "Chemometrics in spectroscopy", 2007, Elsevier</li> <li>J. Stangret, <i>Zeszyty Naukowe Politechniki Gdańskiej</i>, Chemia XLV (578), 2000.</li> <li>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</li> <li>Malvern Instruments, technical note, "Dynamic Light Scattering: An Introduction in 30 Minutes" MRK656-01</li> <li>S. Liu, Y. Wang, Application of AFM in Microbiology: A Review Scanning 32, (2010) 6173</li> <li>Organic Electrochemistry: Revised and Expanded (pp.229-259), Edition: 5th, Chapter: 6, Publisher: CRC Press, Taylor and Francis Group, Editors: Ole Hammerich, Bernd Speiser</li> <li>M.J. Abraham, D. van der Spoel, E. Lindahl, B. Hess, and the GROMACS Development Team. GROMACS 2023.4 Manual</li> <li>M. Śmiechowski, J. Stangret, Vibrational apostroscopy of</li> </ol>					
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		Supplementary literature	<ol> <li>M. Śmiechowski, J. Stangret, Vibrational spectroscopy of semiheavy water (hdo) as a probe of solute hydration, Pure Appl. Chem. 82 (10) (2010) 18691887.</li> <li>M. Szklarczyk, Mikroskopia chemiczna i analityczne techniki wielowymiarowe oraz sprzężone PWN 2020</li> </ol>					
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	Work placement	Not applicable						

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