GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	, PG_00037601		
Field of study	Green Technologies		
Date of commencement of studies	October 2020	Academic year of realisation of subject	2023/2024
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	4	Language of instruction	Polish
Semester of study	7	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. inż. Maciej Śmiechowski	
	Teachers	dr hab. inż. Maciej Śmiechowski	

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	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	3.0	27.0	75

Subject objectives

The aim of the course is to familiarize students with the phenomenon of hydration from the physicochemical perspective, paying particular attention to intermolecular interactions occurring in aqueous solutions.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_W03] has a basic knowledge of soil, air and water pollutants, design and supervision of environmentally friendly technologies and technologies which do not produce waste, knows technology of cleaning and neutralization of industrial waste and wastewater management, has a basic understanding of the theoretical basis of methods and types of apparatus used in chemical analysis of environmental pollutants	The student understands the concept of hydration at the microscopic level and is able to describe characteristic phenomena accompanying the dissolution of pollutants, especially organic ones, in water.	[SW1] Assessment of factual knowledge
[K6_U05] can formulate and solve engineering tasks analytical methods, simulation as well as experimental, able to apply knowledge of basic physics and mathematics to analyze the results of experiments, is able to analyze and assess existing technical solutions	The student applies knowledge of the physical chemistry of solutions to predict phenomena occurring in aqueous environment and uses physicochemical laws in the analysis and interpretation of experimental results.	[SU5] Assessment of ability to present the results of task [SU1] Assessment of task fulfilment

Subject contents

LECTURES

Introduction: necessary thermodynamics. Theory of intermolecular interactions: the role of electron density, non-covalent interactions from quantum chemistry. Intermolecular interactions vs charge distribution: electrostatic (charge-charge), dipolar (dipole-charge, dipole-dipole, dipole-induced dipole), London dispersion (induced dipole-induced dipole). Hydrogen bonding: definition and properties, types of hydrogen bonds, strengths of hydrogen bonds, C-H hydrogen bonds, salt bridges. Investigating intermolecular interactions & hydration: spectroscopy, thermophysical measurements, computational chemistry. Water properties: "anomalies" of liquid water, water vs seawater. Non-ionic hydration: hydration of non-ionized molecules, hydrogen bond stabilization of polar groups, thermodynamics, properties of non-electrolyte solutions. Ionic hydration: cations vs anions, ionic activity, properties of electrolyte solutions, ion solution thermodynamics. Hydrophobic hydration: thermodynamics of hydrophobic hydration, water structure around hydrophobic particles, clathrates, hydrophobic interactions, hydrophobic effect, hydrophobicity scales, superhydrophobicity. Biomolecule hydration: osmolytes, polyelectrolytes in water, water-soluble polymers, hydration of proteins & protein folding, hydration of other natural polymers, colloids, "internal" water

LABORATORIES

1. Spectrophotometric determination of complex formation constant in aqueous solutions
2. Determination of partial molar volumes in water-organic solvent systems
3. Application of infrared spectroscopy in investigating hydration

Prerequisites and co-requisites

Completed the basic physical chemistry course.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Final lecture test	50.0%	65.0%
Lab entry tests and lab reports	60.0%	35.0%

Recommended reading

Basic literature	1. P. Atkins, J. de Paula, J. Keeler. Atkins' physical chemistry. Oxford University Press, Oxford 2018. 2. B. E. Conway. Ionic hydration in chemistry and biophysics. Elsevier Scientific Publishing Company, Amsterdam 1981. 3. A. Ben-Nairn. Hydrophobic Interactions. Plenum Press, New York 1980.
Supplementary literature	1. L. Piela. Ideas of quantum chemistry. Elsevier, Amsterdam 2007. 2. A. Ben-Naim. Molecular theory of water and aqueous solutions. Pt. 1, Understanding water. World Scientific, Singapore 2009.
eResources addresses	Podstawowe https://water.lsbu.ac.uk - M. Chaplin, Water Structure and Science https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Topics_in_Thermodynamics_of_Solutions_and_Liquid_Mixtures - M. J. Blandamer, J. C. R. Reis, Topics in Thermodynamics of Solutions and Liquid Mixtures Adresy na platformie eNauczanie: Hydration of molecules and intermolecular interactions 2023 - Moodle ID: 32060 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=32060

Example issues/ example questions/ tasks being completed

1. Describe the usefulness of reduced density gradient for detecting non-covalent interactions.
2. Show the experimental procedure enabling the obtaining of absolute hydration enthalpy of proton (H+).
3. Describe the types of interactions collectively known as van der Waals forces and their distance dependence.
4. Enumerate the hydrophobibity scales used for amino acids and their physical basis.
5. What are salt bridges and what is their role in stabilizing protein structure?
6. Define an osmolyte. Describe the difference between stabilizing and destabilizing osmolytes.
7. Show a scale of kosmotropic/chaotropic ions and define the notion of kosmo-/chaotropicity.
8. What thermodynamic mechanism causes hydrophobic particles to aggregate in water?
9. Enumerate the factors determining gas solubility in water.
10. Define a clathrate and discuss the relevance of clathrates to economy and the environment.

Work placement

Not applicable