



Subject card

Subject name and code	PROGRAMMING, PG_00064382						
Field of study	Chemistry						
Date of commencement of studies	October 2024		Academic year of realisation of subject			2024/2025	
Education level	first-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	2		ECTS credits			2.0	
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 inż. Mateusz Kogut				
	Teachers		dr inż. Mateusz Kogut				
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	15.0	0.0	0.0	30
	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	30		5.0		15.0	50
Subject objectives	The goal of the course is to introduce students to the basics of programming in the context of chemistry, including the creation of scripts for chemical data analysis, automation of calculations and the basics of structured and object-oriented programming. Students will gain skills to use programming tools to analyze experimental data and model chemical processes.						
Learning outcomes	Course outcome		Subject outcome			Method of verification	
	[K6_U02] determines the time required for the task, plans and organises the work of both the individual and the small team in such a way as to ensure that the task is completed within the set time limit		The student is able to analyze the requirements in software projects related to chemical analysis, identify the needed functions and divide the related tasks.			[SU5] Assessment of ability to present the results of task [SU2] Assessment of ability to analyse information	
	[K6_W05] recognises methods, techniques and tools of computer aided design for solving engineering tasks in chemistry, chemical engineering and technology, mechanical engineering, in the design and analysis of technological processes		The student knows the basics of the Python language and how to use it to analyze chemical data.. The student is able to write scripts for laboratory data processing and simulation of chemical processes.			[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge	
	[K6_K01] understands the need for continuous learning, can inspire and organise learning and others, understands the importance of group and team activities		The student is aware of the dynamic development of software tools and knows how to search for new solutions.			[SK5] Assessment of ability to solve problems that arise in practice [SK2] Assessment of progress of work	

Subject contents	<ol style="list-style-type: none">1. Introduction to programming (Python, syntax basics and data types).2. Control structures and operations on chemical data.3. File handling and analysis of experimental data.4. Use of NumPy, Pandas and Matplotlib libraries in chemistry.5. Automation of chemical calculations (e.g., reaction balancing, spectroscopic analysis).6. Introduction to object-oriented programming and its application in chemistry.7. Interfaces to computational programs used in chemistry.8. Basics of molecular modeling in Python.9. Numerical elements in chemistry: interpolation, solving nonlinear equations, numerical integration.10. Statistics in chemistry: data analysis, linear regression, statistical tests.		
Prerequisites and co-requisites	Students should have basic knowledge of mathematics and physical chemistry. Knowledge of basic computer and spreadsheet skills will be an asset.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Performance of 4 numerical tasks on labs	100.0%	70.0%
	Final exam colloquium	50.0%	30.0%
Recommended reading	Basic literature	Eric Matthes, Python. Instrukcje dla programisty. Wydanie III, Helios, 2023 Luciano Ramalho, Fluent Python: Clear, concise, and effective programming. O'Reilly Media, Inc., 2015 Christian Hill, Python for Chemists: Practical Programming for Chemical Applications, Cambridge University Press, 2022	
	Supplementary literature	Brett Slatkin, Efektywny Python. 90 sposobów na lepszy kod. Wydanie II, Helios, 2020 Lee Vaughan, Python Tools for Scientists: An Introduction to Using Anaconda, JupyterLab, and Python's Scientific Libraries, No Starch Press, 2023	
	eResources addresses	Adresy na platformie eNauczanie: Programowane (lato 2024_25, Chemia sem.2) - Moodle ID: 43879 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=43879	
Example issues/ example questions/ tasks being completed	<ul style="list-style-type: none">• Writing scripts for the analysis of NMR spectra.• Automating the balancing of chemical equations.• Analysis of large experimental data sets.• Modeling the kinetics of chemical reactions.• Solving nonlinear equations by numerical methods.• Implementation of interpolation and numerical integration methods.• Statistical analysis of the results of chemical experiments.		
Work placement	Not applicable		

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