GDAŃSK UNIVERSITY OF TECHNOLOGY

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

<table>
<tr><td>Subject contents</td><td>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.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>Students should have basic knowledge of mathematics and physical chemistry. Knowledge of basic computer and spreadsheet skills will be an asset.</td></tr>
<tr><td>Assessment methods and criteria</td><td><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Performance of 4 numerical tasks on labs</td><td>100.0%</td><td>70.0%</td></tr>
<tr><td>Final exam colloquium</td><td>50.0%</td><td>30.0%</td></tr>
</table></td></tr>
<tr><td>Recommended reading</td><td><table>
<tr><td>Basic literature</td><td>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</td></tr>
<tr><td>Supplementary literature</td><td>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</td></tr>
<tr><td>eResources addresses</td><td>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</td></tr>
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<tr><td>Example issues/ example questions/ tasks being completed</td><td>• 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.</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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