GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	AI in the chemistry lab, PG_00069259		
Field of study	Chemical Technology, Chemistry, Biotechnology, Engineering and Technologies of Energy Carriers, Corrosion , Green Technologies, InfoBioChem		
Date of commencement of studies	February 2026	Academic year of realisation of subject	2026/2027
Education level	second-cycle studies	Subject group	
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	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Agnieszka Gajewicz-Skrętna	
	Teachers	dr hab. Agnieszka Gajewicz-Skrętna	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	30.0	0.0	0.0	45

E-learning hours included: 0.0

eNauczanie source address: https://enauczanie.pg.edu.pl/2025/course/view.php?id=5994

Moodle ID: 5994 AI w laboratorium chemicznym https://enauczanie.pg.edu.pl/2025/course/view.php?id=5994

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	5.0	25.0	75

Subject objectives

The course aims to introduce students to the practical applications of AI-based tools in the chemical sciences. It has a practical focus and covers the effective, critical and responsible use of modern AI tools, such as *ChatGPT, Perplexity AI, SciSpace, ResearchRabbit* and *LM Studio*, for planning experiments, supporting data analysis processes, preparing documentation and automating repetitive tasks.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_K04] is aware of the responsibility for decisions made, observing and developing the principles of professional ethics and working to ensure compliance with these principles	is aware of the responsibility associated with the use of AI tools in the chemical sciences, particularly with regard to the reliability of generated content, the risk of AI hallucinations, data security, intellectual property protection, and the ethical and transparent use of AI in scientific and professional work.	[SK5] Assessment of ability to solve problems that arise in practice [SK4] Assessment of communication skills, including language correctness
[K7_W02] identifies analytical techniques appropriate for solving specific analytical tasks – also in the production plant	can identify the appropriate analytical techniques for solving specific research and practical problems, and explain how AI tools can be used to search for information, compare analytical methods, support data interpretation and select the most suitable analytical approach.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects
[K7_U02] prepares detailed documentation of the results of independently conducted experiments and analyzes the obtained results, uses professional vocabulary with understanding and prepares and communicates information	is able to use AI tools to support the analysis of experimental data, the visualisation of results, and the preparation of laboratory documentation, reports, and scientific summaries, using appropriate specialist terminology and critically assessing the accuracy, completeness, and reliability of AI-generated content.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task
[K7_U101] is able to formulate complex research problems and adopts appropriate methods, obtaining innovative solutions, cooperating with other people, both as a leader and a team member	can formulate complex research problems in chemistry and related sciences, and select the most appropriate AI tools and prompting strategies to solve them. This includes experimental planning, the automation of repetitive tasks, data analysis and generating innovative solutions. The student can work independently and collaboratively in different team roles.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task
[K7_K02] is able to cooperate and work in a group, taking on different roles	collaborates in a group when designing and applying AI-based solutions, taking on different team roles.	[SK1] Assessment of group work skills [SK3] Assessment of ability to organize work [SK4] Assessment of communication skills, including language correctness
[K7_W01] recognizes problems of modern chemistry, including properties and obtaining chemical compounds, necessary for making calculations, including the dependence of the compound's structure and its reactivity	knows and recognises the ways in which artificial intelligence tools can support the analysis of chemical compound properties, the planning of synthetic approaches, the interpretation of structure–reactivity relationships and the performance and verification of chemical calculations in contemporary chemistry.	[SW3] Assessment of knowledge contained in written work and projects [SW2] Assessment of knowledge contained in presentation

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<tr><td>Subject contents</td><td>Course content – lecture

The lecture will cover the following areas:
- Concepts and introduction to generative AI and large language models (LLMs): architecture, operating mechanisms, and application of language models such as ChatGPT, LLaMA, Claude, and Gemini in the context of the chemical and natural sciences.
- Prompt engineering: the principles of effective prompting; techniques for formulating queries; and the importance of context, structure, and precision in obtaining relevant answers.
- AI hallucinations and the reliability of generated information: the mechanisms behind errors in generated content, how to recognise and minimise their impact, and how to improve the quality of training data, the contextualisation of prompts, and fact-checking.
- The principles of the ethical and safe use of AI in the chemical sciences are also covered, including user responsibility, transparency of sources, copyright, and the limits of AI use in scientific work.
- The theoretical foundations for creating AI gems, assistants, and agents, their tasks, and their cooperation within multi-assistant systems for automating repetitive activities.
- The future of AI in the chemical sciences will be explored, including directions of development and examples of AI tools such as ChatGPT, Perplexity AI, Elicit, SciSpace and ResearchRabbit. Examples of the use of AI in chemistry and related sciences will be given, including its application to the analysis of HPLC results, spectroscopy and experimental statistics.

Course content – laboratory

The laboratory course covers the following areas of content:

- An overview of the most popular language models, such as ChatGPT, LLaMA, Claude and Gemini.
- Crafting effective prompts: practical training in writing scientific, technical and analytical queries, and modifying them to achieve better results.
- A practical introduction to designing Gems AI, AI assistants and AI agents for specific tasks, including defining OKRs (Objectives and Key Results), creating a list of rules and a personality, and selecting the level of creativity.
- Analysis and visualisation of research results using AI, including generating charts, tables and infographics for presenting results.
- Creating chatbots.
- Case study: solving a real research problem using AI, from concept to final report. Work individually or in teams using various AI tools.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td></td></tr>
<tr><td>Assessment methods and criteria</td><td>
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<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Lecture: written exam consisting of multiple-choice test questions and open-ended questions</td><td>50.0%</td><td>60.0%</td></tr>
<tr><td>Laboratory classes: project-based assignment</td><td>50.0%</td><td>40.0%</td></tr>
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<tr><td>Recommended reading</td><td>
<table>
<tr><td>Basic literature</td><td>- Andrzej Kacprzak. Prompt engineering i ChatGPT. Poradnik skutecznej komunikacji ze sztuczną inteligencją. Wydawnictwo: ISBN: 978-83-289-1362-2.
- Olivier Caelen, Marie-Alice Blete. Tworzenie aplikacji z wykorzystaniem GPT-4 i ChatGPT. Buduj inteligentne chatboty, generatory treści i fascynujące projekty. Helion 2024, ISBN: 978-83-289-1044-7</td></tr>
<tr><td>Supplementary literature</td><td>- James Phoenix Taylor Mike. Skuteczna inżynieria promptów. Przyszłościowe rozwiązania dla rzetelnych wyników generatywnej AI. Helion 2025, ISBN: 978-83-289-1904-4.</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
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Example issues/ example questions/ tasks being completed	Examples of theoretical topics: - What is generative artificial intelligence, and how does it differ from traditional AI? - Explain how transformer architecture forms the basis of large language models. - What are the fundamental differences between ChatGPT, Claude and Gemini? - How does the 'learning' process of a large language model work? - List and characterise example applications of LLMs in chemistry. - What is tokenisation in language models? - Explain the term 'prompt engineering' and its importance when working with AI. - What elements should an effective scientific prompt contain? - Explain the differences between Zero-Shot, One-Shot and Few-Shot Prompting. - Describe the difference between open-ended, closed-ended and contextual prompts. - How should a prompt be formulated to obtain a summary of scientific literature from AI? - Why is it important to provide context in prompts? - What is 'prompt leakage' and how does it affect the response generated by AI? - Propose a prompt for analysing HPLC results using ChatGPT. - Explain what are known as 'AI hallucinations' and why they are problematic in scientific work. - Which factors increase the risk of hallucinations in responses generated by AI? - How can an unreliable response from a language model be recognised? - Discuss the role of training data quality in the context of AI hallucinations. - What tools or techniques can be used to fact-check information generated by AI? - How can a personality and communication style be assigned to an AI agent? - How are the goals and operating principles for a single AI agent defined? - How is cooperation between AI agents organised in a multi-agent system? - How can OKRs be defined for an AI agent analysing UV-Vis spectroscopy results? - How does choosing a creativity level affect the behaviour of an AI agent? - How can a team of AI agents be used to automate the reporting of research results? - In what ways does a data-searching agent differ from a data-analysing agent?
Practical activites within the subject	Not applicable

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