University of Gdańsk

Subject card

Subject name and code	Introduction to digital chemistry, PG_00054862		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2024/2025
Education level	postgraduate studies	Subject group	Obligatory subject group in the field of study
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	English English
Semester of study	1	ECTS credits	1.0
Learning profile	academic	Assessment form	
Conducting unit	Pracownia Chemoinformatyki Środowiska -> Katedra Chemii i Radiochemii Środowiska -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Tomasz Puzyn	
	Teachers	prof. dr hab. Tomasz Puzyn dr hab. Rafał Ślusarz dr Lidia Chomicz-Mańka dr Jakub Brzeski	

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	10.0	0.0	0.0	0.0	0.0	10
	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	10	2.0	13.0	25

Subject objectives

The aim of the course is to introduce the student to the world of digital chemistry:

- overview on the main methods divided into (i) physics-based methods (based on classical and quantum physics) and (ii) data-driven methods;
- showing the areas of application of both groups of methods to design new chemical compounds and materials.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_U03] Finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry.	Student finds necessary information in specialist literature, databases, and other sources, lists basic scientific journals in chemistry	[SU4] test/exam - oral or written
[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	Student selects experimental and theoretical techniques to the extent necessary to understand the description and modeling of extended complexity chemical processes	[SW4] test/exam - oral or written
[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Student knows the limitations of her/his own knowledge; understands the need for further education	[SK1] oral statement/conversation/ discussion
[CHEMMU2_W04] Applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis.	Student applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis, and analysis	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	Student demonstrates in-depth knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
[CHEMMU2_U06] Presents the results of scientific discoveries in chemistry and related disciplines in an understandable way.	Student presents the results of scientific discoveries in chemistry and related disciplines in an understandable way	[SU4] test/exam - oral or written
[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	Student applies acquired knowledge of chemistry and related scientific disciplines	[SU1] oral statement/conversation/ discussion [SU4] test/exam - oral or written
[CHEMMU2_W09] Classifies specialist IT tools used in statistical evaluation of experiment results.	Student classifies specialist IT tools used in statistical evaluation of experiment results	[SW4] test/exam - oral or written

Subject contents

Review of the most important aspects of digital chemistry, including the latest progress in advanced materials science, advances in big-data, molecular modelling, artificial intelligence, and machine learning methods used across academia and industry for design and synthesis of advanced materials.

Prerequisites and co-requisites

Basic knowledge in chemistry and physics

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Written test exam	51.0%	100.0%

Recommended reading

Basic literature

J. D. Lee Concise inorganic chemistry

L. Jones, P. Atkins Chemical principle

S. D. Brown, R. Tauler, B. Walczak (ed): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009

R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005

Molecular Modelling: Principles and Applications, Andrew Leach, Prentice Hall 2001

Ideas of quantum chemistry, Lucjan Piela, Elsevier 2006

	Supplementary literature	L. Pauling General chemistry J. Leszczynski, A. Kaczmarek-Kedziera, T. Puzyn, M. G. Papadopulos, H. Reis, M. Shukla (ed): Handbook of Computational Chemistry (2nd Edition). Springer 2016. Volume 5: Chemoinformatics, Puzyn T (ed.). T. Puzyn, J. Leszczynski, M. T. D. Cronin (ed): Recent Advances in QSAR Studies: Methods and Applications. Springer 2010. ISBN: 978-1-4020- 9782-9. K. Roy, S. Kar, R. Narayan Das (ed): A Primer on QSAR/QSPR Modeling - Fundamental Concepts. Springer 2015. ISBN: 978-3-319-17281-1.
	eResources addresses	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	Describe current trends in material chemistry or machine learning.	
Work placement	Not applicable	

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