University of Gdańsk

Subject card

Subject name and code	Computational methods for designing advanced materials, PG_00117803						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject	2027/2028			
Education level	Master's studies		Subject group	Optional subject group			
Mode of study	full-time studies		Mode of delivery	at the university			
Year of study	2		Language of instruction	English			
Semester of study	4		ECTS credits	2.0			
Learning profile	academic		Assessment form	credit			
Conducting unit	Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		dr Alicja Mikołajczyk				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	30.0	0.0	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 aim of the course is ability to design of advanced materials with the use of computational methods.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_U06] Presents the results of scientific discoveries in chemistry and related disciplines in an understandable way.	Ability to build regression and classification models	[SU2] presentation/project/paper/ report [SU4] test/exam - oral or written
[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	Understanding the idea of computer chemistry research	[SW4] test/exam - oral or written [SW2] presentation/project/paper/ report
[CHEMMU2_K04] Correctly identifies and resolves dilemmas related to the profession of a chemist.	Ability to critically evaluate experimental results and understand the necessity of their control	[SK2] presentation/project/paper/ report [SK4] test/exam - oral or written
[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	correctly prepares data (including molecular models and data matrix) for the design of advanced materials	[SW4] test/exam - oral or written [SW2] presentation/project/paper/ report
[CHEMMU2_U05] Presents the results of research in the form of an independently written paper containing a description and justification of the purpose of the work, adopted methodology, results and their significance in comparison to other similar research.	Independently presents the results of the work in the form of a report, prepared in accordance with the guidelines	[SU2] presentation/project/paper/ report [SU4] test/exam - oral or written
[CHEMMU2_K07] Can think and act in an entrepreneurial manner.	Performs chemoinformatic analyses that allow to reduce costs and time of research.	[SK2] presentation/project/paper/ report [SK4] test/exam - oral or written
[CHEMMU2_W04] Applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis.	Development of regression and classification models, correct validation of models and use of models to predict the toxicity and/ or functionality of designed materials uses computational methods as tools to support the design of advanced materials with specific properties	[SW4] test/exam - oral or written [SW2] presentation/project/paper/ report
[CHEMMU2_K03] Understands the need for systematic work on various projects of a long-term nature and knows how to set priorities for the implementation of undertaken tasks.	Understanding the need for deeper learning as a method supporting the design of advanced materials	[SK2] presentation/project/paper/ report [SK4] test/exam - oral or written

Subject contents

The concept of computational methods used for designing of advanced materials. The review of the latest progress in materials science and computational tools used to design of advanced chemicals and materials with desired properties and safety. Introduction to nanotechnology. Application of advanced materials in nanotechnology, photocatalysis, and nanomedicine. Safe and sustainability design (SSbD) strategy for the design of advanced materials which present of an optimal combination of specific features, functionality, and safety. The methods used for physic- based and data-based models development used for describing and predicting the quantitative relationship between structure, properties, and toxicity of designed advanced materials (reverse modeling, Structure-Activity Prediction Networks, SAPNet).

Prerequisites and co-requisites

basic knowledge in chemistry

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
report	51.0%	100.0%

Recommended reading

Basic literature	I. A. Parinov, S.-H. Chang, V. K. Gupta: Advanced Materials. Springer 2017. ISBN: 978-3-319-78918-7 A. Tiwari; N. A.Murugan; R. Ahuja. Advanced Engineering Materials and Modeling. Scrivener Publishing. ISBN-13: 9781119242468 S. Thomas, N. Kalarikkal, A.M. Stephan, B. Raneesh, Advanced Nanomaterials, Synthesis, Properties, and Applicationsm, Academic Press, ISBN 9781774633090
Supplementary literature	-
eResources addresses	

Example issues/ example questions/ tasks being completed

Work placement	Not applicable

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