University of Gdańsk

Subject card

Subject name and code	Advanced nanoinformatics, PG_00051249						
Field of study	Chemistry						
Date of commencement of studies	October 2024		Academic year of realisation of subject	2025/2026			
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	3		ECTS credits	2.0			
Learning profile	academic		Assessment form				
Conducting unit	Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		mgr inż. Michał Kałapus				
	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	familiarizing the students with the current status, challenges and recent efforts in application of computational approaches in nanomaterials characterization, analysis and modelling presenting the benefits of using nanoinformatics for modelling activity and toxicity, properties, interactions and fate of nanomaterials (NMs)						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	The student is able to critically evaluate the results of nanoinformatics experiments, observations and theoretical calculations, identifying potential sources of errors and measurement uncertainties. The student is able to perform error analysis and assess the impact of errors on the reliability of results. The student is also able to discuss the results and conclusions of research in a constructive and substantive manner.	[SU1] oral statement/conversation/ discussion [SU2] presentation/project/paper/ report
[CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.	The student consciously and responsibly plans and implements research projects in nanoinformatics, taking into account the potential impact of research results on society and the environment. The student is able to identify and evaluate the ethical and social implications associated with the development and application of nanotechnology.	[SK2] presentation/project/paper/ report [SK8] observation of student's independent or team work
[CHEMMU2_W09] Classifies specialist IT tools used in statistical evaluation of experiment results.	The student is able to classify and select appropriate computer tools (e.g., statistical packages, data analysis software) for statistical evaluation of the results of nanoscience experiments, taking into account the specifics of the data and the purpose of the analysis. The student is able to conduct statistical analysis of the results of the experiment, interpret the results and evaluate their statistical significance.	[SW1] oral statement/ conversation/discussion [SW2] presentation/project/paper/ report
[CHEMMU2_K02] Works in a team taking on various roles in it.	The student is able to work effectively in a team in the implementation of nanoinformatics projects, assuming different roles (leader, performer, reviewer) and adapting his/her actions to the needs of the team. The student is able to communicate with other team members, share knowledge and skills, and resolve conflicts.	[SK8] observation of student's independent or team work
[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student is able to apply basic mathematical methods (e.g., differential and integral calculus, linear algebra, statistics) to analyze and interpret experimental data and theoretical models in nanoinformatics. The student is able to use mathematics to describe and model chemical processes occurring at the nanoscale.	[SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	The student is able to apply in-depth theoretical knowledge of computational and computer methods (e.g., molecular modeling, molecular dynamics simulations, quantum chemical methods) to solve problems in chemistry, especially those related to nanomaterials. The student is able to select appropriate methods for a specific research problem, carry out calculations, interpret the results and assess their reliability.	[SW1] oral statement/ conversation/discussion [SW2] presentation/project/paper/ report

	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.	The student is able to independently search and analyze scientific information in the field of nanoinformatics, using a variety of sources such as databases (e.g. Web of Science, Scopus, PubMed), scientific journals (e.g. Nature Nanotechnology, ACS Nano, Nano Letters, Small) and professional literature. The student is able to evaluate the reliability and usefulness of the information found.	[SU1] oral statement/conversation/ discussion [SU3] text preparation/written work
Subject contents	The course covers practical issues in nanoinformatics which includes: introduction to nanotechnology, nanoscience and nanomaterials areas, introduction to nanoinformatics and statistical modelling (data collection, curation, metadata and ontologies in nanoinformatics; nanodescriptors; unsupervised techniques for similarity analysis, profiling, and grouping; supervised techniques for filling data gaps), application of computational models/tools/software packages to compute/model activity and toxicity, properties, (bio)interactions and fate of NMs, application of the combination of modeling approaches for selected case study nanoparticles (e.g., carbon nanostructures, metal oxide nanoparticles), group discussions on selected computational nanoscience papers, published in top journals.		
Prerequisites and co-requisites	Introduction to Python programming · Introduction to R programming · Quantum chemistry in practice · Exploratory analysis of multidimensional chemical space · Machine learning in chemistry Molecular descriptors		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	observation of the student's behavior during classes and during consultations	50.0%	20.0%
	oral presentation and argumentation during the discussion	50.0%	80.0%
Recommended reading	Basic literature	The EU US Nanoinformatics 2030 Roadmap: https://www.nanosafetycluster.eu/outputs/eu-us-roadmap-nanoinformatics-2030/	
	Supplementary literature	Nanoscience and Advancing Computational Methods in Chemistry: Research Progress (Eds.) Eduardo A. Castro and A.K. Haghi, 2012	
	eResources addresses	Adresy na platformie eNauczanie:	
Example issues/ example questions/ tasks being completed	data collection, curation, metadata and ontologies in nanoinformatics; nanodescriptors; unsupervised techniques for similarity analysis, profiling, and grouping; supervised techniques for filling data gaps) application of computational models/tools/software packages to compute/model activity and toxicity, properties, (bio)interactions and fate of NMs application of the combination of modeling approaches for selected case study nanoparticles (e.g., carbon nanostructures, metal oxide, nanoparticles)		
Work placement	Not applicable		

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