GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Artificial Intelligence in materials science and nanotechnology, PG_00070928		
Field of study	Nanotechnology		
Date of commencement of studies	February 2027	Academic year of realisation of subject	2027/2028
Education level	second-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	1.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Division of Theoretical Physics and Quantum Informaton -> Institute of Physics and Applied Computer Science -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Paweł Syty	
	Teachers	dr inż. Paweł Syty	

Lesson types							
	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	0.0	0.0	15
	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	15	1.0	9.0	25

Subject objectives	The aim of the course is to deepen students' knowledge of advanced artificial intelligence methods used in materials science and nanotechnology, with particular emphasis on the integration of machine learning models with physical and chemical knowledge. The course aims to develop students' ability to critically analyse the possibilities and limitations of AI methods in modelling, analysing and designing materials and nanostructures. Students will acquire the skills necessary to consciously use AI tools in scientific research and development work in the field of nanotechnology.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[K7_U06] is able to apply acquired specialist knowledge to problems in other physical, natural, or technical sciences and to critically analyze and evaluate the functioning of the adopted solutions	The student is able to use artificial intelligence and machine learning methods to analyse, model and design materials and nanostructures, integrating knowledge in the fields of physics, chemistry and materials engineering, and critically assesses the correctness, reliability and limitations of the models obtained and predictive results.	[SU1] Assessment of task fulfilment [SU3] Assessment of ability to use knowledge gained from the subject
	[K7_W05] has in-depth knowledge of mathematical, numerical, and simulation methods - both classical and quantum - used in the modeling of nanostructures	The student has an in-depth knowledge of the mathematical and numerical foundations of machine learning methods and knows how to apply them in simulation and multiscale modelling of the properties of materials and nanostructures, including classical and quantum approaches.	[SW1] Assessment of factual knowledge
	[K7_W01] has broadened and well-structured knowledge in the field of materials science, including material fabrication or control of processes accompanying fabrication, with particular emphasis on materials and structures at the nanoscale.	The student understands the possibilities of applying artificial intelligence in materials research and nanotechnology, in particular in: discovering new materials, analysing experimental and simulation data, optimising synthesis and manufacturing processes, predicting the structure, properties and stability of nanostructures, and is able to select the appropriate AI tools for a specific engineering or research problem.	[SW1] Assessment of factual knowledge

Subject contents	Course content – lecture 1. The role of artificial intelligence (AI) in modern materials science - AI as the fourth paradigm of science after theory, experiment and simulation - The specificity of materials and nanotechnology problems - Overview of current trends 2. Representation of materials and nanostructures in ML models - Material descriptors - Atomistic representations - Challenges specific to the nanoscale 3. Deep learning in materials science - Neural networks for materials data - Sequential models and attention in structure analysis - Transfer learning in materials problems - Limitations in the context of small data sets 4. Physics-Informed Machine Learning - Integration of physics laws with ML models - Hybrid models - The role of interpretability and physical consistency 5. Modelling the properties of materials and nanostructures - Property prediction - Multi-task learning - Prediction uncertainty and error propagation - Probabilistic models and Bayesian ML 6. Designing materials and nanostructures using AI - Inverse problem - Generative algorithms - Material optimisation - Design space exploration 7. Experimental data analysis - AI in data analysis from microscopy (SEM, TEM, AFM) and spectroscopy - Segmentation, denoising, super-resolution - Automation of experiment interpretation - Active learning in experiment planning 8. Integration of AI with numerical simulations - Simulation acceleration - Learning interatomic potentials - Reduction of large-scale computation costs - Coupling MLMDDFT 9. Interpretability, reliability and ethics of AI in engineering sciences - Explainable AI (XAI) - Model validation in a physical context - Reproducibility of AI-based research - Risks of black-box models 10. Future directions - Autonomous laboratories - AI as a tool for humanalgorithm collaboration - Competencies of the future nanotechnology engineer
Prerequisites and co-requisites	Knowledge of basic methods of artificial intelligence and machine learning.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Oral examination	50.0%	70.0%
Assessment of homework (written)	50.0%	30.0%

Recommended reading

Basic literature	- Stuart Russell, Peter Norvig, Artificial Intelligence: A Modern Approach, Pearson, 2020 - Chip Huyen, Designing Machine Learning Systems: An Iterative Process for Production-Ready Applications, OReilly Media, 2022
Supplementary literature	- Tongyi Zhang, An Introduction to Materials Informatics: The Elements of Machine Learning, Springer, 2024 - Olexandr Isayev, Alexander Tropsha, Stefano Curtarolo, Materials Informatics: Methods, Tools, and Applications, Wiley VCH, 2019
eResources addresses	

Example issues/ example questions/ tasks being completed	- Explain the specifics of artificial intelligence applications in materials science and nanotechnology compared to classical machine learning problems. - Discuss the importance of material data representation in AI models. How does the choice of descriptors affect the model's ability to generalise results? - Compare classical machine learning methods and deep learning methods in the context of material property modelling. In which situations is each of them more justified? - What is the physics-informed machine learning approach? Give examples of the benefits and potential limitations of this approach in nanotechnology. - Explain the inverse design problem in materials design. What classes of AI algorithms are most commonly used to solve it?

Practical activites within the subject	(Additional task for those interested, related to, for example, a thesis in preparation). Proposing an appropriate model for selected data from real-life experience or simulations, e.g. conducted in the Nanotechnology Laboratory (collected as part of a thesis, research project or other course).

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