GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Quantum modeling of electronic materials, PG_00070894		
Field of study	Informatics		
Date of commencement of studies	February 2025	Academic year of realisation of subject	2025/2026
Education level	second-cycle studies	Subject group	
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	2	Language of instruction	Polish
Semester of study	3	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Optoelectronics -> Faculty of Electronics Telecommunications and Informatics -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Bartłomiej Dec	
	Teachers	dr inż. Bartłomiej Dec	

Lesson types							
	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	15.0	0.0	0.0	45
	E-learning hours included: 0.0						
	eNauczanie source address: https://enauczanie.pg.edu.pl/2025/course/view.php?id=4697 Moodle ID: 4697 Kwantowe modelowanie materiałów elektronicznych https://enauczanie.pg.edu.pl/2025/course/view.php?id=4697						

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	3.0	27.0	75

Subject objectives	The aim of this course is to introduce students to modern methods of quantum modeling of electronic materials, with particular emphasis on the practical use of simulation software (e.g., QuantumATK). Students will acquire the skills to plan and conduct quantum simulations of materials used in electronics, analyze the results, and interpret the electronic, optical, and transport properties of materials in the context of broadly understood technological applicationsfrom semiconductors to advanced functional materials.

Learning outcomes			
	Course outcome	Subject outcome	Method of verification
	[K7_U04] can apply knowledge of programming methods and techniques as well as select and apply appropriate programming methods and tools in computer software development or programming devices or controllers using microprocessors or programmable elements or systems specific to the field of study, making assessment and critical analysis of the prepared software as well as a synthesis and creative interpretation of information presented with it	Student can design and perform quantum computations using Python and dedicated simulation software, selecting and applying appropriate programming methods and tools (k-point grid, cutoff energy, exchange-correlation functionals) depending on the type of material being studied. Can evaluate and critically analyze written computational scripts, and creatively interpret DFT simulation results (band structures, density of states, transport properties) in the context of electronics applications.	[SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information
	[K7_W02] knows and understands, to an increased extent, selected laws of physics and physical phenomena, as well as methods and theories explaining the complex relationships between them, constituting advanced general knowledge in the field of technical sciences related to the field of study	Student knows and understands advanced concepts of density functional theory (DFT) and quantum modeling methods of the electronic structure of electronic materials. Has knowledge of approximations used in ab initio calculations, wave function representation methods (LCAO, plane waves), and the theoretical foundations of computational simulation of materials used in electronics. Knows the principles of modeling electronic, optical, and transport properties of materials – from semiconductors to advanced functional materials – using computational tools.	[SW1] Assessment of factual knowledge

Subject contents	
	Course content – lecture An introduction to quantum methods for modeling electronic materials and devices. Density functional theory (DFT) and its application to the calculation of electronic structures. Approximations and approximation methods in quantum computations. Modeling the electronic, optical, and magnetic properties of materials. Application of quantum methods to the design of nanoelectronic and spintronic devices.
	Course content – laboratory Practical use of software for modeling the atomic structures and electronic properties of materials. Building atomic models, configuring DFT calculation parameters, conducting simulations, and analyzing the results. Visualizing electronic structures, calculating band structures, electronic density of states, and transport properties. Modeling interfaces and nanostructures.
Prerequisites and co-requisites	

Assessment methods and criteria			
	Subject passing criteria	Passing threshold	Percentage of the final grade
		50.0%	50.0%
		50.0%	50.0%

Recommended reading		
	Basic literature	1. Newman, M. "Computational Physics", wyd. 2, CreateSpace/ University of Michigan (2013) 2. Martin, R.M. "Electronic Structure: Basic Theory and Practical Methods", Cambridge University Press (2020) 3. QuantumATK User Manual and Tutorials, Synopsys Documentation 4. Kohanoff, J. "Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods", Cambridge University Press (2006) 5. Frenkel, D., Smit, B. "Understanding Molecular Simulation: From Algorithms to Applications", wyd. 3, Academic Press/Elsevier (2023)
	Supplementary literature	nie dotyczy
	eResources addresses	

Example issues/ example questions/ tasks being completed	
Practical activites within the subject	Not applicable