



Subject card

Subject name and code	Quantum modeling of electronic components, PG_00069760						
Field of study	Informatics, Hydrogen Technologies and Electromobility						
Date of commencement of studies	February 2026		Academic year of realisation of subject		2026/2027		
Education level	second-cycle studies		Subject group				
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		2.0		
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	15.0	0.0	15.0	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		2.0		18.0	50
Subject objectives	The aim of this course is to introduce students to modern methods of quantum modeling of materials and electronic devices, with particular emphasis on the practical use of simulation software (e.g., QuantumATK). Students will acquire the skills to plan and conduct quantum simulations, analyze the results, and interpret the electronic properties of materials in the context of technological applications.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[K7_U08] while identifying and formulating engineering tasks specifications and solving these tasks, can: - apply analytical, simulation and experimental methods, - notice their systemic and non-technical aspects, - make a preliminary economic assessment of suggested solutions and engineering work		Students can design and perform quantum computations, selecting appropriate computational parameters (k-point grid, cutoff energy, exchange-correlation functionals) depending on the type of material being studied. Students can analyze DFT simulation results (band structures, density of states, transport properties) and interpret them in the context of electronic device design. They can assess the accuracy and limitations of various computational methods and make a preliminary assessment of the computational costs of proposed simulations.		[SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task		
	[K7_W03] knows and understands, to an increased extent, the construction and operating principles of components and systems related to the field of study, including theories, methods and complex relationships between them and selected specific issues - appropriate for the curriculum		Students will understand advanced concepts of density functional theory (DFT) and quantum methods for modeling the electronic structure of materials. They will be familiar with the approximations used in ab initio calculations and wave function representation methods (LCAO, plane waves). They will also be familiar with the principles of modeling the electronic, optical, and transport properties of nanostructures and electronic devices at the atomic scale.		[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%	30.0%
		50.0%	70.0%
Recommended reading	Basic literature	1. Szabo, A., Ostlund, N.S. "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", Dover Publications (2012) 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. Marder, M.P. "Condensed Matter Physics", Wiley (2010)	
	Supplementary literature	nie dotyczy	
	eResources addresses		
Example issues/ example questions/ tasks being completed			
Practical activities within the subject	Not applicable		

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