GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Quantum modeling of electronic components, PG_00069760		
Field of study	Kwantowe modelowanie elementów elektronicznych		
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	1	Language of instruction	Polish
Semester of study	2	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Katedra Optoelektroniki -> Faculty of Electronics Telecommunications and Informatics -> Wydziały Politechniki Gdańskiej		
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

eNauczanie source addresses:

Moodle ID: 1887 Kwantowe modelowanie elementów elektronicznych
https://enauczanie.pg.edu.pl/2025/course/view.php?id=1887

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	0.0	0.0	30

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_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] Ocena wiedzy faktograficznej
[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.	[SU5] Ocena umiejętności zaprezentowania wyników realizacji zadania [SU4] Ocena umiejętności korzystania z metod i narzędzi

Subject contents

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.

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%	70.0%
	50.0%	30.0%

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 activites within the subject

Not applicable

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