GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Materials Science - quantum particle approach, PG_00052037		
Field of study	Nanotechnology		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2025/2026
Education level	second-cycle studies	Subject group	Specialty subject group 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	2	Language of instruction	English
Semester of study	3	ECTS credits	6.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Division of Physics of Disordered Systems -> Institute of Nanotechnology and Materials Engineering -> Faculty of Applied Physics and Mathematics -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Maciej Bobrowski	
	Teachers	dr hab. Maciej Bobrowski	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	45.0	0.0	0.0	75

E-learning hours included: 0.0

Additional information:
In-person, online - if necessary.

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	75	5.0	70.0	150

Subject objectives

Purposes:

1.Pass the knowledge on application of quantum methods for issues of change of electronic structure present in molecules and crystals.

2. Teaching axioms of quantum mechanics and their applications.

3. Teaching of commonly utilized quantum methods based on wave functions and electron densities: HF, CI, MCSCF, CC, MPn, DFT.

4. Teaching of utilization of commonly applied basis sets in quantum calculations

Learning outcomes

Course outcome	Subject outcome	Method of verification

Subject contents

application of quantum methods in cases of solving of electronic-structure change for systems of molecules and crystals, axioms of quantum mechanics and their applications, commonly utilized quantum methods based on wave functions and electron densities: HF, CI, MCSCF, MPn, CC, DFT, basis sets.

Prerequisites and co-requisites

Base knowledge on physics, mathematics and chemistry.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
sprawozdanie	51.0%	50.0%
exam	51.0%	50.0%

Recommended reading	Basic literature	1. Frank Jensen, Introduction to Computational Chemistry, Wydawnictwo Wiley, 2007, 2. C. J. Ballhausen, H. B. Gray, Molecular Orbital Theory, Wydawnictwo W. A. Benjamin Inc. 1964,
	Supplementary literature	Yung-Kuo Lim, Problems and Solutions on Quantum Mechanics, Wydawnictwo World Scientific, 2005,
	eResources addresses	
Example issues/ example questions/ tasks being completed	1.Calculate given commutators in cartesian and spherical coordinates, 2. Normalize given wavefunctions, 3. Orthogonalize given basis stes, 4. Calculate energies of given electron configurations 5. What atomic and molecular orbitals should be taken into account in the case of given electron states of given molecules and given spins. 6. Calculate CI coefficients for hydrogen molecule for given electron configuration.	
Work placement	Not applicable	

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