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 2023	Academic year of realisation of subject	2024/2025
Education level	second-cycle studies	Subject group	Optional 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 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		
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
K7_W05	Student has deep knowledge on: operators' definitions in spherical coordinates, matrix representation and diagonalization and orthogonalization methods, normalization of wavefunctions, Slater and Gaussian basis sets, Hartree-Fock-Roothan approach, atomic and molecular orbitals, CI methods, perturbation methods, methods of finding and characterizing stationary states.	[SW3] Assessment of knowledge contained in written work and projects [SW2] Assessment of knowledge contained in presentation
K7_W02	Student has a deep knowledge on quantum methods which can be applied to computations of electronic structure's change of chemical systems which build nanostructures, as well as on capabilities and limitations of such method.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation
K7_U06	Sudent can for himself, solve the problems given by the teacher by means of software for quantum calculations.	[SU5] Assessment of ability to present the results of task [SU4] Assessment of ability to use methods and tools [SU3] Assessment of ability to use knowledge gained from the subject
K7_U03	Student can maintain software for quantum calculations on many-processor computer along with advanced visualization software which is used for displaying partial results and for building the structures.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools

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
exam	51.0%	50.0%
sprawozdanie	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	Adresy na platformie eNauczanie: Materials science. Quantum particle approach. 2024 - Moodle ID: 40233 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=40233

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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