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 2025	Academic year of realisation of subject	2026/2027
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 -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Maciej Bobrowski	
	Teachers	dr hab. Maciej Bobrowski	

Lesson types

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

eNauczanie source address: https://enauczanie.pg.edu.pl/2025/course/view.php?id=1343

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_W02] has enhanced, theoretically supported, detailed knowledge of selected branches of nanotechnology and, according to the needs, within the scope of related fields of science and technology.	The student has in-depth knowledge of quantum methods used in calculations to change the electronic structure of chemical systems that build nanosystems as well as the possibilities and limitations of such methods.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects
	[K7_U06] can plan and conduct theoretical and numerical calculations, simulations of phenomena and processes, critically analyze their results, draw conclusions and formulate reasoned conclusions – within their specialization.	A student can solve a problem assigned by the instructor using quantum computing software. A student can solve the problems assigned by the instructor for themselves using quantum calculation software.	[SU3] Assessment of ability to use knowledge gained from the subject [SU5] Assessment of ability to present the results of task [SU4] Assessment of ability to use methods and tools
	[K7_W05] has enhanced knowledge of mathematical, numerical, simulation, classical and quantum methods, applied in modeling nanostructures.	The student has in-depth knowledge of mathematical, numerical, and simulation methods, both classical and quantum, used in modeling nanostructures. The student has in-depth knowledge of: the definition of quantum-mechanical operators in spherical coordinates, the matrix representation of operators, diagonalization and orthogonalization, wave function normalization, as well as: Slater and Gaussian basis sets, the Hartree-Fock-Roothan approximation, atomic and molecular orbitals, CI methods, perturbation methods, and methods for finding and characterizing stationary states.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects
	[K7_U03] has enhanced abilities of using advanced specialist software packages	The student can operate a quantum computation program on a multiprocessor computer along with advanced visualization software used for displaying partial results and building structures.	[SU4] Assessment of ability to use methods and tools [SU2] Assessment of ability to analyse information [SU5] Assessment of ability to present the results of task

Subject contents	Course content – lecture The lecture hours are divided below: 1--2. Examples of the application of quantum methods in research projects focused on: the search for and characterization of new, complex materials for applications in electrochemistry, optics, energy, and electronics. 3--6. Schrodinger solutions for a rigid rotor and the hydrogen atom: spherical harmonics, atomic orbitals, eigenvalues, properties. 7--11. Variational methods: nonlinear and linear parameters. Matrix representation. 12--14. Multi-electron systems: the Slater determinant, the Hartree-Fock method, the SCF algorithm. 15. Configuration mixing methods and basis functions. The labs are divided as follows (by week): 1. Information about the Linux operating system, network organization, including access to the computational server and external data access, and setting up accounts on the computational server. 2. Molecular geometry and molecular coordinates: Cartesian and internal, as well as assistance from the Molden program. 3. Sample calculations on the computational server for cases assigned by the instructor. 4. Discussion of a common project problem and division of tasks (a different task for each student). 5-15. Individual calculations conducted independently by each student on a given problem.
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	

Example issues/ example questions/ tasks being completed	Lectures: 1. Calculate given commutators in Cartesian and spherical coordinates, 2. Normalize given wave functions, 3. Orthogonalize given basis functions, 4. Calculate the electronic energies of given electronic configurations, 5. Which atomic and molecular orbitals will be considered when calculating given electronic states of molecules with a given multiplicity? 6. Calculate the CI expansion coefficients for a hydrogen molecule in a given electronic state. Laboratories: 1. Calculate the polymerization reaction mechanism for a given polymer. 2. Compare the energies of the electronic states of ferromagnetic iron(III) oxides.
Practical activites within the subject	Not applicable

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