



Subject card

Subject name and code	Theoretical methods of materials design, PG_00071147						
Field of study	Technical Physics, Mathematics, Nanotechnology, Nanotechnology						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2025/2026		
Education level	second-cycle studies	Subject group			Optional subject group		
Mode of study	Full-time studies	Mode of delivery			at the university		
Year of study	2	Language of instruction			Polish		
Semester of study	4	ECTS credits			1.0		
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	15.0	0.0	0.0	0.0	0.0	15
	E-learning hours included: 0.0						
	eNauczenie source address: https://enauczenie.pg.edu.pl/2025/course/view.php?id=3646						
	Moodle ID: 3646 Metody teoretyczne projektowania materiałów 2026 https://enauczenie.pg.edu.pl/2025/course/view.php?id=3646						
Additional information:							
Lecture. On-site. If necessary, online classes.							
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	15	2.0	8.0	25		
Subject objectives	Presentation of the diversity and often irreplaceability of theoretical methods in the design of new functional materials. Presentation of numerous examples of their application in the design of polymeric, electrochemical, liquid, gas, and solid-state materials, also in the context of ongoing European projects (with the participation of industrial entrepreneurs). Presentation of the general physical and mathematical principles of the computational methods used: classical, quantum, and hybrid. General differences between methods, more specific algorithms and computational problems in various methods. Main principles of the applicability of given classes of methods in general types of cases, with examples. Software. Where possible, live presentation of calculations, results, and analysis.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[K7_K101] acknowledges the importance of knowledge related to the field of study in solving cognitive and practical problems, critically assessing the information obtained	The student is familiar with the available computational methods and is able to select appropriate ones to study given processes in systems of a given complexity.	[SK5] Assessment of ability to solve problems that arise in practice
	[K7_W101] is able to make an in-depth identification of key objects and phenomena related to the field of study, as well as theories that describe them and applicable analytical and design methods	The student is able to define theoretical models, which in the next step he or she works on using theoretical methods and obtains a systematic and comparable set of analytical data.	[SW2] Assessment of knowledge contained in presentation [SW1] Assessment of factual knowledge
	[K7_U101] is able to formulate complex research problems and adopts appropriate methods, obtaining innovative solutions, cooperating with other people, both as a leader and a team member	The student is able to define a complex research problem, e.g. in electrochemistry, in the context of obtaining a better material, e.g. a better electrochemical cell, by finding factors that directly influence the cell's efficiency and then searching for a better material structure in order to improve the properties of this cell.	[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 [SU1] Assessment of task fulfilment
Subject contents	<p>Course content – lecture</p> <ol style="list-style-type: none"> 1. Organization, overview of the subject and issues, grading rules. References. Proposals for implementing own projects using theoretical methods, including at the master's thesis level. Presentation of the complexity of theoretical issues. 2. Example one of the application of theoretical methods: chemical reactions, polymers produced by CVD technology, functionalization of polymers during CVD, application in liquid lenses. 3. Example two of the application of theoretical methods: the diversity of spatial structures and electronic structure in metal oxides from the smallest stoichiometrically to nanometric molecules. Reference to ferrofluids based on ionic liquids, used in thermoelectric systems. 4. Classical force field methods: energy components, force field parameterization, coarse graining, advantages and limitations. 5-6. Quantum methods: axioms of quantum mechanics (wave function, operators, Schrödinger equation, spin). 7. Quantum methods: from the rigid rotor model to spherical harmonics. 8. Quantum methods: from the hydrogen atom model to atomic orbitals. 9-10. Quantum methods: linear and nonlinear variational methods (including the HFR method), the SCF algorithm. 11. The 3-electron system: a complete calculation to obtain an energy expression for any electron configuration. 12. The hydrogen molecule: configurations, spin, and full energy derivations for all configurations. 13. Multiconfiguration methods: complexity, method diversity, quality, examples. 14. Perturbative methods: derivation of formulas, corrections. 15. Selected systems: calculations, molecular orbitals, molecular properties, practical tips. 		
Prerequisites and co-requisites	Basics of chemistry, physics and mathematics.		
Assessment methods and criteria	Subject passing criteria passing the exam at the end of the course.	Passing threshold 51.0%	Percentage of the final grade 100.0%

Recommended reading	Basic literature	<ol style="list-style-type: none"> 1. Lucjan Piela, Idee Chemii Kwantowej, Warszawa, wydanie 2, 2011, PWN, 2. Frank Jensen, Introduction to Computational Chemistry, 3rd Edition ISBN: 978-1-118-82599-0
	Supplementary literature	<ol style="list-style-type: none"> 1. Włodzimierz Kołos, Quantum Chemistry, PWN, Warsaw, 1978. 2. Teacher's materials: derivations, lectures, sample input and output data in PDF format.
	eResources addresses	
Example issues/ example questions/ tasks being completed	<p>What does a chemical reaction profile look like without and with a spin change during the process?</p> <p>Normalize the wave function given by the formula.</p> <p>Describe the electronic configurations of the given radicals/ions of the given atoms.</p> <p>Describe the Slater determinant for the given configurations of the hydrogen molecule.</p> <p>Draw the energy diagram for the given diatomic molecule.</p> <p>Present the electronic energy formula for two given electronic configurations of the two isomers of the molecule.</p> <p>Describe the SCF algorithm. When are relativistic methods needed? Explain why relativistic electrons influence the behavior of valence electrons.</p> <p>How can polymer flexibility be improved and how can this be investigated using theoretical methods (classical and quantum).</p> <p>How can one find a way to chemically functionalize a given system, including how to identify the structural factors responsible for functionalization.</p>	
Practical activities within the subject	Not applicable	

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