

Subject card

Subject name and code	Quantum chemistry, PG_00082079						
Field of study	Chemistry						
Date of commencement of studies	October 2025		Academic year of realisation of subject		2025/2026		
Education level	Bachelor's studies		Subject group		Obligatory subject group in the field of study 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	1		Language of instruction		Polish		
Semester of study	2		ECTS credits		2.0		
Learning profile	academic		Assessment form		credit		
Conducting unit	Laboratory of Quantum Chemistry -> Department of Theoretical Chemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. Sylwia Freza				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	30.0	0.0	0.0	0.0	30
	E-learning hours included: 0.0						
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		5.0		15.0	50
Subject objectives	Familiarize students with the concepts of quantum chemistry, basic approximations, and selected quantum chemical computational methods.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[CHEML3_W08] Demonstrates knowledge of basic computational methods to solve problems in chemistry, physics, mathematics.		describes the boundary surfaces of orbitals, explains Pauli's exclusion principle and Hund's rule.		[SW4] test/exam - oral or written		
	[CHEML3_U01] Identifies, analyses and solves problems in the field of broadly understood chemistry on the basis of the acquired knowledge.		solves eigenvalue equations with observable operators.		[SU4] test/exam - oral or written		
	[CHEML3_U08] Presents in an understandable way the basic facts about chemistry using a scientific language typical of chemical sciences.		predicts the measurability of physical quantities,		[SU4] test/exam - oral or written		
	[CHEML3_K07] Appreciates the need for understandable presentation of selected chemical issues to the public.		The student is cautious and critical in expressing opinions and shows openness to innovative concepts.		[SK4] test/exam - oral or written		
	[CHEML3_U09] Is able to learn independently.		plans the selection of appropriate computational methods, recognizes the symmetry of the wave function		[SU4] test/exam - oral or written		
Subject contents	Operators, eigenvalue equation, Jordan's rules, orbital angular momentum, quantum numbers, orbitals, determination of atomic terms, spin operators, symmetry of the wave function, construction of the Slater determinant, calculation of electronic energy						

Prerequisites and co-requisites	basic knowledge of linear algebra, differential and integral calculations		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	tests	51.0%	100.0%
Recommended reading	Basic literature	1. Włodzimierz Kołos Chemia kwantowa A 2. Alojzy Gołębiewski Elementy mechaniki i chemii kwantowej	
	Supplementary literature	1. Lucjan Piela Idee chemii kwantowej 2. P.W. Atkins Molekularna mechanika kwantowa	
	eResources addresses		
Example issues/ example questions/ tasks being completed	1. Find the eigenvalues 2. Calculate the commutators 3. Calculate the electronic energy		
Work placement	Not applicable		

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