University of Gdańsk

Subject card

Subject name and code	Quantum chemistry, PG_00082078						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject	2026/2027			
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	3.0			
Learning profile	academic		Assessment form	exam			
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	30.0	0.0	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		40.0	75
Subject objectives	The aim of the lecture is to present 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.	student lists the basic methods of quantum chemistry, explains simple applications of quantum chemistry, recognizes the symmetry of the wavefunction, describes the postulates of quantum mechanics, explains the tunnel effect,	[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.	student estimates the probability of finding an electron in a specific area, calculates the electron energy of molecules	[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.	student predicts the measurability of physical quantities, classifies the multiplicity of states, discusses the basic approximations used in quantum chemistry	[SU4] test/exam - oral or written
[CHEML3_U09] Is able to learn independently.	student solves eigenvalue equations with quantum mechanical operators, student constructs a determinant wavefunction, student plans the appropriate choice of calculation method	[SU4] test/exam - oral or written
[CHEML3_K07] Appreciates the need for understandable presentation of selected chemical issues to the public.	student is careful and critical in expressing opinions, student is open to innovative concepts	[SK1] oral statement/conversation/ discussion

Subject contents

wave-particle dualism, postulates of quantum mechanics, solution of the Schrödinger equation for a free particle, a particle in a potential box, a rigid rotator, a harmonic oscillator and a hydrogen atom; electron spin; atomic terms; approximate methods of quantum chemistry: perturbation and variational methods, Ritz method, Hartree-Fock method, CI method, MCSCF, CASSCF, coupled cluster method;

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
exam	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. What is the one-electron approximation? 2. Describe Heisenberg's uncertainty principle. 3. Discuss quantum numbers.

Work placement

Not applicable

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