University of Gdańsk

Subject card

Subject name and code	Quantum chemistry, PG_00082079		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2024/2025
Education level	Bachelor's studies	Subject group	Obligatory subject group 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	dr hab. Sylwia Freza dr Jakub Brzeski	

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_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
[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_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_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_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

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

<table>
<tr><td>Prerequisites and co-requisites</td><td colspan="3">basic knowledge of linear algebra, differential and integral calculations</td></tr>
<tr><td>Assessment methods and criteria</td><td colspan="3"><table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>tests</td><td>51.0%</td><td>100.0%</td></tr></table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td colspan="2">1. Włodzimierz Kołos Chemia kwantowa A

2. Alojzy Gołębiewski Elementy mechaniki i chemii kwantowej</td></tr>
<tr><td>Supplementary literature</td><td colspan="2">1. Lucjan Piela Idee chemii kwantowej

2. P.W. Atkins Molekularna mechanika kwantowa</td></tr>
<tr><td>eResources addresses</td><td colspan="2"></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="3">1. Find the eigenvalues

2. Calculate the commutators

3.Calculate the electronic energy</td></tr>
<tr><td>Work placement</td><td colspan="3">Not applicable</td></tr>
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