GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	THEORETICAL CHEMISTRY, PG_00037381		
Field of study	Chemistry		
Date of commencement of studies	October 2021	Academic year of realisation of subject	2022/2023
Education level	first-cycle 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	2	Language of instruction	Polish
Semester of study	4	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Inorganic Chemistry -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Andrzej Okuniewski	
	Teachers	dr inż. Andrzej Okuniewski	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	30.0	0.0	0.0	45

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	45	5.0	25.0	75

Subject objectives

The aim of the course is to acquaint students with the basics of theoretical chemistry and quantum mechanics.

Learning outcomes

Course outcome	Subject outcome	Method of verification
K6_W03	understands and is able to use the terminology and designations used in theoretical chemistry, knows the history and modern ideas in the field of quantum chemistry, analyzes the model quantum-mechanical problems and can qualitatively discuss their applications in chemistry, is prepared to continue learning of theoretical methods in chemistry	[SW1] Assessment of factual knowledge
[K6_U05] can, on the basis of the collected experimental or source material, prepare an oral communication with a multimedia presentation	N/A	[SU5] Assessment of ability to present the results of task
[K6_W05] knows and understands the chemical processes and algorithms of mathematical models which are necessary for the design of technological processes, knows chemical structure of contemporary materials and its relation to their properties, enabling the selection of the materials for sustainable development technology and material-efficient and energy-efficient methods	uses computer software to determine selected properties of atoms, interprets the obtained results and confronts them with literature experimental results	[SW3] Assessment of knowledge contained in written work and projects

<table>
<tr><td>Subject contents</td><td>Lecture: History of quantum mechanics. Wave-particle duality. The postulates of quantum mechanics. Uncertainty. Functions of many variables. Differential equations. Particle in a one-dimensional potential well. Quantum tunnelling. Harmonic oscillator. Particle in a ring. Particle in a two-dimensional potential well. Rigid rotor. Hydrogen atom and hydrogen-like ions. Multielectronic systems.

Computer labs: Verification of the validity of Aufbau principle. Determining the energy of the electronic excitation. Determination of ionization energy. Determination of Mulliken electronegativity and Pearson's hardness. Study of electronegativity and hardness variability in the periodic table. The charge of the nucleus and its shielding.

A detailed program of the course as well as the laboratory are regularly updated and posted on the eNauczanie platform.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>The student must have mastered the following courses at the undergraduate level: mathematics, physics, general chemistry.</td></tr>
<tr><td>Assessment methods and criteria</td><td><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Final test</td><td>60.0%</td><td>50.0%</td></tr>
<tr><td>Computer labs</td><td>60.0%</td><td>50.0%</td></tr>
</table></td></tr>
<tr><td>Recommended reading</td><td><table>
<tr><td>Basic literature</td><td>D. O. Hayward: Mechanika kwantowa dla chemików, PWN, Warszawa 2007.</td></tr>
<tr><td>Supplementary literature</td><td>R. F. Nalewajski: Podstawy i metody chemii kwantowej, PWN, Warszawa 2001.

L. Piela: Idee chemii kwantowej. PWN, Warszawa 2011.

W. Kołos, J. Sadlej: Atom i cząsteczka, WNT, Warszawa 1998.

H. Haken, H. Ch. Wolf: Fizyka molekularna z elementami chemii kwantowej, PWN, Warszawa 1998.</td></tr>
<tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:
Chemia teoretyczna 2022/23 - Moodle ID: 25080
https://enauczanie.pg.edu.pl/moodle/course/view.php?id=25080</td></tr>
</table></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td>Available on the "eNauczanie" platform.</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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