



## Subject card

Subject name and code	THEORETICAL CHEMISTRY, PG_00037381						
Field of study	Chemistry						
Date of commencement of studies	October 2022	Academic year of realisation of subject			2023/2024		
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						
Lesson type and method 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_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_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_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		

Subject contents	<p><b>Lecture:</b> 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.</p> <p><b>Computer labs:</b> 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.</p> <p>A detailed program of the course as well as the project and seminar topics are regularly updated and posted on the Department of Inorganic Chemistry webpage: <a href="http://chem.pg.edu.pl/kchn/ch-chemia-teoretyczna">chem.pg.edu.pl/kchn/ch-chemia-teoretyczna</a></p>											
Prerequisites and co-requisites	The student must have mastered the following courses at the undergraduate level: mathematics, physics, general chemistry, physical chemistry.											
Assessment methods and criteria	<table border="1" data-bbox="448 546 1487 651"> <thead> <tr> <th data-bbox="448 546 794 577">Subject passing criteria</th> <th data-bbox="794 546 1141 577">Passing threshold</th> <th data-bbox="1141 546 1487 577">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="448 577 794 609">Final test</td> <td data-bbox="794 577 1141 609">60.0%</td> <td data-bbox="1141 577 1487 609">50.0%</td> </tr> <tr> <td data-bbox="448 609 794 651">Computer labs</td> <td data-bbox="794 609 1141 651">60.0%</td> <td data-bbox="1141 609 1487 651">50.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	Final test	60.0%	50.0%	Computer labs	60.0%	50.0%
Subject passing criteria	Passing threshold	Percentage of the final grade										
Final test	60.0%	50.0%										
Computer labs	60.0%	50.0%										
Recommended reading	Basic literature	D. O. Hayward: <i>Mechanika kwantowa dla chemików</i> , PWN, Warszawa 2007.										
	Supplementary literature	R. F. Nalewajski: <i>Podstawy i metody chemii kwantowej</i> , PWN, Warszawa 2001.  L. Piela: <i>Idee chemii kwantowej</i> . PWN, Warszawa 2011.  W. Kołos, J. Sadlej: <i>Atom i cząsteczka</i> , WNT, Warszawa 1998.  H. Haken, H. Ch. Wolf: <i>Fizyka molekularna z elementami chemii kwantowej</i> , PWN, Warszawa 1998.										
	eResources addresses											
Example issues/ example questions/ tasks being completed	<a href="http://chem.pg.edu.pl/kchn/ch-chemia-teoretyczna">chem.pg.edu.pl/kchn/ch-chemia-teoretyczna</a>											
Work placement	Not applicable											