

Subject card

Subject name and code	Diploma lecture - Disputes about molecular structure: From electron clouds to biological macromolecules, PG_00081854						
Field of study	Chemistry						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2026/2027		
Education level	Bachelor's studies	Subject group			Obligatory subject group in the field of study Optional subject group		
Mode of study	full-time studies	Mode of delivery			at the university		
Year of study	3	Language of instruction			Polish		
Semester of study	6	ECTS credits			2.0		
Learning profile	academic	Assessment form			credit		
Conducting unit	Department of Theoretical Chemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Iwona Anusiewicz					
	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		15.0	50
Subject objectives	Introducing students to selected ab initio and molecular dynamics methods in the study of basic chemical problems; Introducing students to modern applications of quantum chemistry.						
Learning outcomes	Course outcome	Subject outcome			Method of verification		
	[CHEML3_W02] Describes the properties of elements and the most important chemical compounds, enumerates the methods of their preparation and methods of analysis.	Student describes the basic physical properties of the most important chemical compounds; knows the most important methods of computational chemistry and knows the basic functional bases used in chemical calculations;			[SW4] 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 chooses the appropriate theoretical method for various chemical molecules.			[SU4] test/exam - oral or written		
	[CHEML3_K01] Identifies the level of her/his own knowledge and skills and the need for continuous learning and personal development.	Student understands the need for further education, keeps caution and criticism when expressing opinions, and demonstrates openness to innovative concepts.			[SK4] test/exam - oral or written		
	[CHEML3_W03] Explains the relationship between the structure of matter and its observed properties.	Student knows the relationship between the geometric and electronic structure of matter and its observed properties.			[SW4] test/exam - oral or written		
Subject contents	Selected methods based on density functional theory and ab initio methods in the study of basic chemical problems. A practical introduction to the use of computational methods in quantum chemistry and the study of the electronic structure of molecules. Electron correlation. Study of reaction mechanisms. Examples of modern applications of quantum chemistry. Structures of peptides and proteins. Introduction to molecular modeling - from experiment to the spatial structure of proteins.						

Prerequisites and co-requisites	basic knowledge of linear algebra, differential and integral calculus		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	written test	51.0%	100.0%
Recommended reading	Basic literature	Ideas of Quantum Chemistry (L. Piela)	
	Supplementary literature	Molecular Quantum Mechanics (P. Atkins, R. Friedman)	
	eResources addresses		
Example issues/ example questions/ tasks being completed	Give a method for determining the geometric structures of dichloroethylene isomers and determine which isomer corresponds to the global minimum.		
Work placement	Not applicable		

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