University of Gdańsk

Subject card

Subject name and code	Diploma lecture - Disputes about molecular structure: From electron clouds to biological macromolekules, PG_00081854		
Field of study	Chemistry		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2028/2029
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.

<table>
<tr><td>Prerequisites and co-requisites</td><td colspan="3">basic knowledge of linear algebra, differential and integral calculus</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>written test</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">Ideas of Quantum Chemistry (L. Piela)</td></tr>
<tr><td>Supplementary literature</td><td colspan="2">Molecular Quantum Mechanics (P. Atkins, R. Friedman)</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">Give a method for determining the geometric structures of dichloroethylene isomers and determine which isomer corresponds to the global minimum.</td></tr>
<tr><td>Work placement</td><td colspan="3">Not applicable</td></tr>
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