University of Gdańsk

Subject card

Subject name and code	Introduction to molecular modeling, PG_00033259		
Field of study	Chemistry		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2027/2028
Education level	Bachelor's studies	Subject group	Optional subject group
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	2	Language of instruction	Polish
Semester of study	3	ECTS credits	2.0
Learning profile	academic	Assessment form	credit
Conducting unit	Laboratory of Carbohydrate Chemistry -> Department of Organic Chemistry -> Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Rafał Ślusarz	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	0.0	30.0	0.0	0.0	30

E-learning hours included: 0.0

Additional information:

- experiment designing
- analysis of critical events (cases)
- conducting experiments
- blended learning (on-line and stationary classes)

Methods:

- problem study with issues for independent learning
- discussion in the course forum
- exercises in the computer lab (stationary)

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

Introduction of the student to the subject of molecular modeling.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEML3_U05] Uses basic statistical methods and IT techniques to describe chemical processes and analyse experimental data.	student names the projection methods and defines the scope of the transmitted information in selected molecular systems	[SU2] presentation/project/paper/ report
[CHEML3_W09] Describes the practical applications of IT tools (computer programmes) for chemical calculations and data analysis.	student illustrates changes occurring in systems, selects tools specialized in measurement, construction or analysis of collected data	[SW2] presentation/project/paper/ report
[CHEML3_W08] Demonstrates knowledge of basic computational methods to solve problems in chemistry, physics, mathematics.	student calculates simple profiles of energy changes, constructs correct queries to bioinformatics databases, indicates the causes of conformation changes	[SW2] presentation/project/paper/ report
[CHEML3_U09] Is able to learn independently.	student assesses the usefulness of types of representations in the presentation of results, proposes the best methods of visualization of chemical compounds, shows creativity in the preparation of chemical presentations	[SU2] presentation/project/paper/ report

Subject contents

- learning to visualize chemical structures in various computer programs
- preparation of two- and three-dimensional representations of structures of chemical compounds
- simple computer simulations of dynamics and geometry optimization of modeled chemical compounds

Prerequisites and co-requisites

A basic knowledge of English and a general understanding of the structure of chemical compounds is required.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
student prepares a report for each exercise performed; each such report is assessed separately; the final grade is the arithmetic mean of the partial grades obtained	51.0%	100.0%

Recommended reading

Basic literature	none
Supplementary literature	none
eResources addresses	

Example issues/ example questions/ tasks being completed

- identify and measure all valence angles in an aspirin molecule
- prepare 1,2-dichloroethane z-matrix
- draw up and interpret selected bond-rotation energy profile

Work placement

Not applicable

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