

**Subject card**

<b>Subject name and code</b>	Molecular mechanics & dynamics, coarse-grain modeling, PG_00117807						
<b>Field of study</b>	Chemistry						
<b>Date of commencement of studies</b>	October 2024	<b>Academic year of realisation of subject</b>			2024/2025		
<b>Education level</b>	postgraduate studies	<b>Subject group</b>			Obligatory subject group in the field of study		
<b>Mode of study</b>	full-time studies	<b>Mode of delivery</b>			at the university		
<b>Year of study</b>	1	<b>Language of instruction</b>			English		
<b>Semester of study</b>	2	<b>ECTS credits</b>			3.0		
<b>Learning profile</b>	academic	<b>Assessment form</b>					
<b>Conducting unit</b>	Faculty of Chemistry						
<b>Name and surname of lecturer (lecturers)</b>	<b>Subject supervisor</b>		prof. dr hab. Cezary Czaplewski				
	<b>Teachers</b>						
<b>Lesson types</b>	<b>Lesson type</b>	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	<b>Number of study hours</b>	30.0	0.0	0.0	0.0	0.0	30
	E-learning hours included: 0.0						
<b>Learning activity and number of study hours</b>	<b>Learning activity</b>	Participation in didactic classes included in study plan		Participation in consultation hours		Self-study	SUM
	<b>Number of study hours</b>	30		5.0		40.0	75
<b>Subject objectives</b>	Practical introduction to the techniques and tools of computational chemistry used in molecular modeling. Teaching students how to choose the right methods of computational chemistry depending on the system under study						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	The student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently using the workstations connected to the Internet. Develops the responsibility for his/her personal account on the workstation. Develops the ability to work in a team.	[SK8] observation of student's independent or team work
	[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	The student classifies molecular modeling methods used to determine the structure, spectral characteristics, properties of chemical compounds in different states of concentration and selects the appropriate method of computational chemistry to support experimental work.	[SW4] test/exam - oral or written [SW2] presentation/project/paper/report
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	Student analyzes the results of computer simulations, compares the results of calculations with experimental data.	[SU2] presentation/project/paper/report
	[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	Student defines and describes basic molecular modeling methods. Distinguishes between methods of quantum chemistry and methods of molecular mechanics as well as deterministic and stochastic methods of computer simulations.	[SW4] test/exam - oral or written [SW2] presentation/project/paper/report
	[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	Student conducts calculations and computer simulations using selected computational chemistry programs,	[SU2] presentation/project/paper/report [SU8] observation of student's independent or team work
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Student characterizes approximations used in quantum chemistry methods and empirical force fields.	[SW4] test/exam - oral or written [SW2] presentation/project/paper/report	
Subject contents	Visualization of chemical molecules and macromolecules. Molecular mechanics, determining the structure and conformational changes of chemical molecules. Empirical force fields and their application in conformational analysis. Introduction to computer simulation methods: Monte Carlo and molecular dynamics (MD). Parameterization of empirical force fields used in molecular mechanics and molecular dynamics. Application of ab initio and semi-empirical methods in parametrization of empirical forcefields. Modeling of macromolecules: DNA, RNA, proteins, and their complexes. Protein structure prediction. Molecular docking. Protein-peptide, and protein-protein docking. CASP and CAPRI initiatives. Coarse-grain modeling of macromolecules.		
Prerequisites and co-requisites	ability to use the LINUX operating system, basics of organic chemistry		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	test exam	51.0%	100.0%
Recommended reading	Basic literature	Molecular Modelling: Principles and Applications, Andrew Leach, Prentice Hall 2001  Ideas of quantum chemistry, Lucjan Piela, Elsevier 2006	
	Supplementary literature	Graham Patrick An Introduction to Medicinal Chemistry, Oxford University Press 2023	
	eResources addresses	Adresy na platformie eNauczanie:	
Example issues/ example questions/ tasks being completed			
Work placement	Not applicable		

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