University of Gdańsk

Subject card

Subject name and code	Molecular mechanics & dynamics, coarse-grain modeling, PG_00117808						
Field of study	Chemistry						
Date of commencement of studies	October 2024		Academic year of realisation of subject		2024/2025		
Education level	postgraduate studies		Subject group		Obligatory subject group in the field of study		
Mode of study	full-time studies		Mode of delivery		at the university		
Year of study	1		Language of instruction		English		
Semester of study	2		ECTS credits		3.0		
Learning profile	academic		Assessment form				
Conducting unit	Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Cezary Czaplewski				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	45.0	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		8.0		22.0	75
Subject objectives	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.	[SW2] presentation/project/paper/report
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Student characterizes approximations used in quantum chemistry methods and empirical force fields.	[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_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_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.	[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
reports	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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