

Subject card

Subject name and code	Monographic lecture - Computational chemistry software, PG_00129556						
Field of study	Chemistry						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2025/2026		
Education level	Master'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	2	Language of instruction			Polish		
Semester of study	4	ECTS credits			3.0		
Learning profile	academic	Assessment form			credit		
Conducting unit	Faculty of Chemistry -> Rector						
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	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	40.0	75		
Subject objectives	Introduction to the available software for quantum chemistry calculations as well as molecular mechanics and molecular dynamics simulations.						
Learning outcomes	Course outcome	Subject outcome			Method of verification		
	[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	The student recognizes and characterizes the available software for quantum chemistry as well as molecular mechanics and molecular dynamics calculations.			[SW2] presentation/project/paper/report		
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Learns the principles of safe, responsible and effective work on supercomputers in data centers.			[SK2] presentation/project/paper/report		
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Distinguishes between programs for quantum chemistry calculations and programs using molecular mechanics methods			[SW2] presentation/project/paper/report		
	[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	The student recognizes and characterizes the available software for simulations of infrared, visible and ultraviolet spectra as well as nuclear magnetic resonance (NMR).			[SW2] presentation/project/paper/report		
Subject contents	Using UNIX shell scripts. The sed stream editor and awk scripts, their application to the analysis of results obtained from computational chemistry software. Running tasks in high performance computer centers. Queuing systems: PBS, LSF and NQS. Software for ab initio and semi-empirical quantum chemistry calculations: GAMESS, GAUSSIAN, MOPAC, MOLPRO, TURBOMOLE packages. Software for molecular mechanics and molecular dynamics simulations: AMBER, GROMACS, TINKER, NAMD, ECEPPAK packages. Molecular editors and visualization software: Avogadro, Molden, MolMol, RasMol, Pymol, VMD, Chimera, Sirius. CSDS database of crystallographic structures of small molecules and PDB database of biomolecular structures and their use.						

Prerequisites and co-requisites	Information technology, Quantum Chemistry, Teoretical Chemistry		
	Ability to work in the Unix system, knowledge of basics of quantum chemistry, knowledge of terminology and nomenclature used in quantum chemistry, ability to describe the geometry of chemical molecules, the basics of statistical mechanics and molecular mechanics.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	presentation	51.0%	100.0%
Recommended reading	Basic literature	L. Piela, Ideas of Quantum Chemistry, Elsevier, 2013	
		A. Leach, Molecular Modelling: Principles and Applications, Prentice Hall, 2001	
	Supplementary literature	C.J. Cramer, Essentials of Computational Chemistry, Wiley, 2004	
	eResources addresses		
Example issues/ example questions/ tasks being completed			
Work placement	Not applicable		

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