

Subject card

Subject name and code	Computer instead of chemistry laboratory, PG_00080799						
Field of study	Chemical Business						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2026/2027		
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	3	Language of instruction			Polish Polish		
Semester of study	5	ECTS credits			1.0		
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. Piotr Skurski				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	0.0	0.0	15
	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	15	2.0	8.0	25		
Subject objectives	Acquainting students with the possibilities of using quantum chemistry software to solve chemical problems						
Learning outcomes	Course outcome	Subject outcome		Method of verification			
	[BCHINŻ_U09] Using the acquired knowledge, skills and various sources of scientific information independently prepares written papers and oral presentations.	Student interprets the results using own knowledge		[SU1] oral statement/conversation/discussion [SU4] test/exam - oral or written			
	[BCHINŻ_W03] Describes the techniques of higher mathematics and IT tools necessary to describe and model chemical phenomena and technological processes.	Student solves advanced problems related to computational chemistry methods.		[SW4] test/exam - oral or written [SW1] oral statement/conversation/discussion			
	[BCHINŻ_K02] Works individually demonstrating initiative and independence in actions, and effectively cooperates in a team, performing various roles in it.	Student works as a team member, respects the lecturer and other team members.		[SK1] oral statement/conversation/discussion			
	[BCHINŻ_W04] Describes the role of experiment and computer simulation in the design process of engineering issues.	Student selects and chooses proper algorithms and software packages which enable performing the calculations and solve a given problem.		[SW1] oral statement/conversation/discussion [SW5] implementation of a problem task			
	[BCHINŻ_U04] In the course of carrying out engineering tasks, s/he uses basic statistical methods, IT techniques and uses application software packages to describe chemical processes and experimental data.	Student performs calculations using computational quantum chemistry methods.		[SU5] implementation of a problem task			

Subject contents	Basic knowledge concerning various types of chemical problems that might be solved using quantum chemistry methods and software, the use of software designed to evaluating physicochemical properties of molecules, defining the problem that is to be solved, the ability to perform desired calculations using computers, the ability to properly interpret the results and formulate conclusions.		
Prerequisites and co-requisites	The ability of using PC computer		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	final exam (test)	51.0%	100.0%
Recommended reading	Basic literature	Molecular Quantum Mechanics (P. Atkins, R. Friedman)	
	Supplementary literature	Ideas of Quantum Chemistry (L. Piela)	
	eResources addresses		
Example issues/ example questions/ tasks being completed	<p>Choose the most accurate method from the list:</p> <p>A. Hartree-Fock method</p> <p>B. Second order Moller-Plesset method</p> <p>C. DFT method with B3LYP functional</p> <p>D. Coupled cluster method (CCSD(T)).</p>		
Work placement	Not applicable		

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