

Subject card

Subject name and code	Computer instead of chemistry laboratory, PG_00080800						
Field of study	Chemical Business						
Date of commencement of studies	October 2023		Academic year of realisation of subject		2025/2026		
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		
Semester of study	5		ECTS credits		2.0		
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		dr hab. Sylwia Freza				
			Natalia Wiszowska				
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						
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	Acquainting students with the possibilities of using quantum chemistry software to solve chemical problems						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[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_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 [SU5] implementation of a problem task		
	[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_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.		[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	Preparing input data files, graphical interpretation of the results, determining the equilibrium structures of molecules, simulating IR, NMR, and UV spectra, evaluating physicochemical parameters (energy, Gibbs free energy, entropy, heat capacity, dipole and quadrupole moments, polarizability and hyperpolarizability), chemical reaction modeling (determining reaction mechanism, estimating activation barriers, calculating the reaction rate). Knowledge acquainted by the students after attending the lectures: basic knowledge concerning the types of problems that could be solved by using quantum chemistry methods and software, the ability of choosing proper theoretical approach to given problems, the ability of interpreting the results that come from quantum chemistry calculations. Knowledge acquainted by the students after attending the seminars: the knowledge concerning input data preparation (for quantum chemistry software packages), the ability of performing calculations resulting with obtaining molecular structure, simulated IR, NMR and UV spectra, multipole moments, polarizabilities and hyperpolarizabilities, energy, Gibbs free energy, and entropy; the ability of chemical reaction modeling by locating the transition state structures, intermediate products and reaction products, estimating the height of the activation barriers, calculating the rate of the overall process.		
Prerequisites and co-requisites	Ability to use a PC computer (basic level).		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Reports documenting solved problems	51.0%	75.0%
	Activity during classes	51.0%	25.0%
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	Propose a path (series of steps) aiming to determine the ionization potential and electron affinity of a given molecule (using any chosen quantum chemistry method).		
Work placement	Not applicable		

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