

Subject card

Subject name and code	Quantum chemistry in practice, PG_00054865						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject		2026/2027		
Education level	Master's studies		Subject group		Obligatory subject group in the field of study Subject group related to scientific research 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	1		ECTS credits		3.0		
Learning profile	academic		Assessment form		exam		
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	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	Acquainting students with the possibilities of using quantum chemistry methods and quantum chemistry software to solve chemical problems						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.		Student demonstrates in-depth knowledge of the ability of solving various chemical problems by using quantum chemistry tools		[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion		
	[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.		Student applies acquired knowledge of the structure and properties of molecules, general chemistry and related scientific disciplines		[SU4] test/exam - oral or written		
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.		Student knows the limitations of her/his own knowledge; understands the need for further education		[SK4] test/exam - oral or written		
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.		Student has extended knowledge in the field of quantum chemistry tools and techniques		[SW4] test/exam - oral or written		
	[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.		Student selects suitable computational tools to the extent necessary to study various types of chemical problems		[SW4] test/exam - oral or written		

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, preparing input data files for QM software, 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), determining stationary points on the potential energy surface.		
Prerequisites and co-requisites	Basic knowledge in chemistry and physics		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Written final exam	51.0%	100.0%
Recommended reading	Basic literature	An Introduction to Theoretical Chemistry, Jack Simons, Cambridge University Press, 2003 Molecular Quantum Mechanics, P. W. Atkins, R. S. Friedman, Oxford University Press Inc., New York (2011) Energetic Principles of Chemical Reactions, J. Simons, Jones and Bartlett Publishers, Inc., 1983.	
	Supplementary literature	Quantum Mechanics in Chemistry, J. Simons, J. Nichols, Oxford University Press (1997) Geometrical Derivative of Energy Surfaces and Molecular Properties, P. Jorgensen, J. Simons, D. Reidel Publ. Company, 1985	
	eResources addresses		
	Example issues/ example questions/ tasks being completed	Describe the computational steps which must be undertaken to determine the Gibbs free reaction energy of the Gly-Ala dipeptide formation (using Gly and Ala substrates) at T=297 K and p=1 atm.	
Work placement	Not applicable		

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