

Subject card

Subject name and code	Quantum chemistry in practice, PG_00054866						
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 English		
Semester of study	1	ECTS credits			3.0		
Learning profile	academic	Assessment form					
Conducting unit	Katedra Chemii Teoretycznej -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Piotr Skurski				
	Teachers		prof. dr hab. Iwona Anusiewicz dr Jakub Brzeski				
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	Acquainting students with the use of using quantum chemistry methods and quantum chemistry software in practice to solve chemical problems						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[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	[SW1] oral statement/ conversation/discussion [SW3] text preparation/written work
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	Student critically assesses the results of performed theoretical calculations and discusses them in the context of predicted properties of molecules	[SU1] oral statement/conversation/discussion [SU6] demonstration of practical skills
	[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	[SK1] oral statement/conversation/discussion [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.	Student selects suitable computational tools to the extent necessary to study various types of chemical problems	[SW5] implementation of a problem task
	[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	[SU3] text preparation/written work [SU6] demonstration of practical skills
[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	[SW3] text preparation/written work [SW5] implementation of a problem task	
Subject contents	Practical skills 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 reports documenting all exercises	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	Adresy na platformie eNauczanie:	
Example issues/ example questions/ tasks being completed	Evaluate the stability of dichloroethylene isomers, identify the most stable isomer, and determine the proportion (percentage content) of the lowest-energy isomers in a mixture at a temperature of 298 K and a pressure of 1 atm.		
Work placement	Not applicable		

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