Subject card

Subject name and code	Introduction to computational quantum chemistry, PG_00179624						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject		2027/2028		
Education level	Master's studies		Subject group		Optional subject group		
Mode of study	full-time studies		Mode of delivery		at the university		
Year of study	2		Language of instruction		English		
Semester of study	4		ECTS credits		4.0		
Learning profile	academic		Assessment form		credit		
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Janusz Rak				
	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		30.0	40.0		100
Subject objectives	Preparation for selecting the appropriate computational chemistry method for analyzing a specific chemical problem, designing a computational algorithm to ensure the fastest possible solution to the problem, and evaluating the accuracy of the obtained numerical result.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_K03] Understands the need for systematic work on various projects of a long-term nature and knows how to set priorities for the implementation of undertaken tasks.	Works systematically and with priorities in mind to understand the theories used in computational chemistry.	[SK4] test/exam - oral or written
	[CHEMMU2_W04] Applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis.	Can characterize the properties of the studied compounds using the knowledge conveyed during the lecture.	[SW4] test/exam - oral or written
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	Can critically assess the results of quantum chemical calculations and evaluate their accuracy.	[SU4] test/exam - oral or written
	[CHEMMU2_U03] Finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry.	Finds information in journals such as: the Journal of Physical Chemisgry, Physical Chemistry Chemical Physics, the Journal of Chemical Physics etc.	[SU4] test/exam - oral or written
	[CHEMMU2_K05] Understands the need for independent search of information in scientific literature and popular science magazines.	Understands the need for independent study of papers published in specialist journals such as The Journal of Physical Chemistry, International Journal of Quantum Chemistry, etc.	[SK4] test/exam - oral or written
	[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	Possesses knowledge about the directions of development in computational chemistry methods, particularly density functional theory (DFT).	[SW4] 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.	Is aware of the continuous development of computational chemistry and the resulting limitations of their own knowledge. They understand the need for ongoing education.	[SK4] test/exam - oral or written
	[CHEMMU2_U10] Reads with understanding scientific and popular science chemical texts in English.	Understands scientific works on the applications of computational chemistry.	[SU4] test/exam - oral or written
	[CHEMMU2_U11] Communicates in English in accordance with the requirements specified for level B2 of the Common European Framework of Reference for Languages.	Discusses quantum chemistry topics in English. In particular, they are proficient in the terminology of computational chemistry.	[SU4] test/exam - oral or written
	[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	Utilizes knowledge from general, inorganic, organic, and physical chemistry.	[SU4] test/exam - oral or written
	[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	Knows methods, particularly in the field of linear algebra, used to solve the Schrödinger equation.	[SW4] test/exam - oral or written

Subject contents	Born-Oppenheimer approximation, time-independent Schrödinger equation, single-electron approximation, Slater determinant, Hartree-Fock (HF) and Hartree-Fock-Roothaan (HFR) methods, semi-empirical schemes of the HFR method: CNDO, INDO, NDDO, modified NDDO methods: MNDO, AM1, PM3, PM5, RM1, PM6, MNDO/d, SAM1, SAM1d. Basis functions. Electron correlation: configuration interaction (CI) method, Møller-Plesset perturbation theory (MPn), coupled cluster (CC) method. Density functional theory (DFT) methods. Applications of the HFR method and correlated methods: selection of basis functions, molecular geometry optimization, determination of reaction enthalpy, harmonic normal modes (IR spectrum), NMR shifts, and electronic spectra of molecular systems.
Prerequisites and co-requisites	Physical chemistry, quantum chemistry, the ability to describe a chemical reaction in thermodynamic and kinetic terms, knowledge of the fundamentals of molecular spectroscopy.

Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
		51.0%	100.0%

Recommended reading	Basic literature	1. Frank Jensen, "Introduction to Computational Chemistry", Wiley, 2017. 2.. Christopher J. Cramer, "Essentials of Computational Chemistry: Theories and Models", Wiley, 2004
	Supplementary literature	Attila Szabo, Neil S. Ostlund, "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", Dover Publications, 1996.
	eResources addresses	
Example issues/ example questions/ tasks being completed	1. Assumptions and approximations of the HF methods. 2. Types of basis functions used in quantum chemical calculations, their advantages and limitations. 3. What are diffuse functions? What is their mechanism of action, and when are they used? 4. What is the ZDO approximation, and what is its significance for semi-empirical methods? 5. Briefly describe the ideas behind DFT methods.	
Work placement	Not applicable	

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