University of Gdańsk

Subject card

Subject name and code	Quantum chemistry, PG_00080828			
Field of study	Chemical Business			
Date of commencement of studies	October 2024	Academic year of realisation of subject		2024/2025
Education level	undergraduate 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		Polish
Semester of study	2	ECTS credits		1.0
Learning profile	academic	Assessment form		
Conducting unit	Faculty of Chemistry			
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Iwona Anusiewicz		
	Teachers			

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	15.0	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 basics of quantum mechanics and quantum chemistryacquainting students with the most important quantum chemistry methods allowing the prediction of their molecular structure, physicochemical properties, and reactivity.

Learning outcomes		Course outcome	Subject outcome	Method of verification
		[BCHINŻ_U02] Uses basic methods, techniques and tools in formulating and solving engineering tasks in the field of chemistry.	After the course, the students are capable of: choosing the most suitable computational method for solving the Schrödinger equation for a given molecular system.	[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.	After the course, the students are capable of: explaining the most important quantum chemistry methods.	[SW4] test/exam - oral or written
		[BCHINŻ_U08] Uses the chemical nomenclature and engineering terminology properly.	After the course, the students are capable of: formulating the basics of quantum mechanics, explaining simple physical problems solved by quantum mechanics, identifying the symmetry of the wave-function, formulating Pauli exclusion principle and Hund rules, explaining the most fundamental approximations utilized in quantum chemistry, determining the multiplicity of a given molecular system	[SU4] test/exam - oral or written
		[BCHINŻ_W02] Enumerates basic laws and theories in chemistry, physics and mathematics necessary to formulate and solve simple engineering tasks.	After the course, the students are capable of: formulating the basics of quantum mechanics, explaining simple physical problems solved by quantum mechanics, identifying the symmetry of the wave-function, formulating Pauli exclusion principle and Hund rules, explaining the most fundamental approximations utilized in quantum chemistry,	[SW4] test/exam - oral or written

Subject contents	operators, eigenvectors and eigenvalues in Hilbert space, quantum numbers, orbitals, spin operators, symmetry of the wave-function, Slater determinants, evaluating electronic energy in Hartree-Fock method.
Prerequisites and co-requisites	basic knowledge concerning physics, linear algebra, infinitesimal and integral calculus

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

Recommended reading	Basic literature	Molecular Quantum Mechanics (P. Atkins, R. Friedman), An Introduction to Theoretical Chemistry (J. Simons),Quantum Mechanics in Chemistry (J. Simons, J. Nicols).
	Supplementary literature	Quantum Mechanics (A. Messiah), Ideas of Quantum Chemistry (L. Piela), Modern Quantum Chemistry (A. Szabo, N. Ostlund).
	eResources addresses	Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed	Is it possible to simultaneously measure the p(y) of the electron's momentum and the y of the position? Give an appropriate calculation.
Work placement	Not applicable

Document generated electronically. Does not require a seal or signature.