University of Gdańsk

Subject card

Subject name and code	Quantum chemistry, PG_00080827		
Field of study	Chemical Business		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2026/2027
Education level	Bachelor'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	Polish
Semester of study	2	ECTS credits	3.0
Learning profile	academic	Assessment form	exam
Conducting unit	Laboratory of Quantum Chemistry -> Department of Theoretical Chemistry -> Faculty of Chemistry -> Rector		
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	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 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_W03] Describes the techniques of higher mathematics and IT tools necessary to describe and model chemical phenomena and technological processes.	After completing the course, the students are capable of: explaining the most important quantum chemistry methods	[SW4] test/exam - oral or written
[BCHINŻ_U02] Uses basic methods, techniques and tools in formulating and solving engineering tasks in the field of chemistry.	After completing the course, the students are capable of: solving eigenproblems, predicting the possibility of accurate measuring certain observables, writing the proper single-determinant wave-function for a given configuration, calculating electronic energy in Hartree-Fock method, choosing the most suitable computational method for solving the Schrödinger equation for a given molecular system.	[SU4] 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,	[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 Pauli exclusion principle and Hund rules, explaining the most fundamental approximations utilized in quantum chemistry, determining the multiplicity of a given molecular system, explaining the most important quantum chemistry methods.	[SW4] test/exam - oral or written

Subject contents

Lectures: waveparticle duality; Heisenbergs principle of uncertainty; mathematical formulations of quantum mechanics (postulates of quantum mechanics); solving Schrödinger equation for a free particle, particle in a box, rigid rotor, harmonic oscillator, tunneling effect, and hydrogen atom; spin angular momentum, atomic terms, Pauli exclusion principle, and LS coupling; Born-Oppenheimer and one-electron approximations, perturbational methods; variational methods; electron correlation; MO theory; approximate quantum chemistry methods (Hartree-Fock method, Configuration-Interaction method, Multi-configurational self-consistent field method, Complete Active Space self-consistent field method, Møller-Plesset perturbational method, Coupled-cluster 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
	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	

Example issues/ example questions/ tasks being completed

Explain the terms: Born-Oppenheimer approximation; orbital; observable; independent electron approximation; spin.

Work placement

Not applicable

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