University of Gdańsk

Subject card

Subject name and code	Monographic lecture - Introduction into quantum computer chemistry, PG_00080897						
Field of study	Chemical Business						
Date of commencement of studies	February 2025		Academic year of realisation of subject	2025/2026			
Education level	Master's studies		Subject group	Obligatory subject group in the field of study Optional subject group			
Mode of study	full-time studies		Mode of delivery	at the university			
Year of study	2		Language of instruction	Polish			
Semester of study	3		ECTS credits	3.0			
Learning profile	academic		Assessment form				
Conducting unit	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		5.0		40.0	75
Subject objectives	Preparing students to choose the appropriate method of computational chemistry for analyzing a specific chemical problem, designing an algorithm that ensures a fast solution to the problem, and evaluating the accuracy of the obtained numerical result.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[BCHMU2_W01] Knows and understands complex physicochemical processes and is able to analyse their course in connection with other fields of science.	Has knowledge about the directions of development and applications of computational chemistry.	[SW4] test/exam - oral or written
[BCHMU2_U02] Is able to define her/his interests, develop them within the chosen direction and in connection with the subject of her/his master's thesis by implementing the process of self-education and planning her/his professional career.	Has awareness of their knowledge and skills, understands the need for continuous professional development and personal growth, conducts self-assessment of their competencies, improves skills, and sets directions for their own educational development.	[SU4] test/exam - oral or written
[BCHMU2_U01] Is able to, on the basis of her/his knowledge, propose a solution to problems in chemistry, taking into account the economic aspect by using advanced measurement techniques.	Proposing solutions to photochemical problems with the knowledge acquired during the lecture.	[SU4] test/exam - oral or written
[BCHMU2_K04] Is willing to properly assess the acquired knowledge, respect and disseminate it in order to solve specific cognitive and practical issues.	Shows caution and criticism in expressing opinions.	[SK4] test/exam - oral or written
[BCHMU2_W05] Knows and understands the main trends in the development of chemistry combined with economics as two interpenetrating scientific disciplines.	Has knowledge about the directions of development and applications of computational chemistry.	[SW4] test/exam - oral or written

Subject contents

The Born-Oppenheimer approximation, time-independent Schrödinger equation. Single-electron approximation, Slater determinant, Hartree-Fock method (HF) and Hartree-Fock-Roothaan method (HFR), semi-empirical schemes of HFR method: CNDO, INDO, ND-DO, modified NDDO methods: MNDO, AM1, PM3, PM5, RM1, PM6, MNDO/d, SAM1, SAM1d. Basis sets. Electron correlation: Configuration interaction (CI) method, Møller-Plesset perturbation theory (MPn), Coupled-cluster method (CC). Density functional theory (DFT) methods. Applications of HFR method and correlated methods: basis set selection, geometry optimization of molecules, determination of reaction enthalpies, harmonic vibrational modes (IR spectrum), NMR shifts, and electronic spectra of molecular systems.

Prerequisites and co-requisites

Physical chemistry, quantum chemistry, the ability to describe chemical reactions in terms of thermodynamics and kinetics, knowledge of the basics of molecular spectroscopy.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
test	51.0%	100.0%

Recommended reading

Basic literature	1. Lucjan Piela Idee chemii kwantowej, PWN 2003. 2. Frank Jensen Introduction to Computational Chemistry, Wiley, 2006. 3. Christopher J. Cramer Essentials of Computational Chemistry: Theories and Models, Wiley, 2004.
Supplementary literature	1. 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 method.
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 of DFT methods.

Work placement

Not applicable

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