University of Gdańsk

Subject card

Subject name and code	Monographic lecture - Introduction into quantum computer chemistry, PG_00080897		
Field of study	Chemistry		
Date of commencement of studies	October 2024	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	4	ECTS credits	3.0
Learning profile	academic	Assessment form	credit
Conducting unit	Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Janusz Rak	
	Teachers	prof. dr hab. Janusz Rak	

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
[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	Understands and can explain the regularities, phenomena, and processes correctly, especially able to independently reproduce basic laws and theorems.	[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 knowledge and skills, understands the need for continuous professional development and personal growth, conducts self-assessment of competencies, and strives for improvement.	[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.	Has knowledge about the directions of development and applications of computational chemistry.	[SW4] test/exam - oral or written
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Has profound knowledge of the basic concepts, principles, and theories used in computational chemistry.	[SW4] test/exam - oral or written

<table>
<tr><td>Subject contents</td><td colspan="3">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.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td colspan="3">Physical chemistry, quantum chemistry, the ability to describe chemical reactions in terms of thermodynamics and kinetics, knowledge of the basics of molecular spectroscopy.</td></tr>
<tr><td>Assessment methods and criteria</td><td colspan="3"><table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>test</td><td>51.0%</td><td>100.0%</td></tr></table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td colspan="2">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.</td></tr>
<tr><td>Supplementary literature</td><td colspan="2">1. Attila Szabo, Neil S. Ostlund Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, 1996.</td></tr>
<tr><td>eResources addresses</td><td colspan="2"></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="3">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.</td></tr>
<tr><td>Work placement</td><td colspan="3">Not applicable</td></tr>
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