University of Gdańsk

Subject card

Subject name and code	Monographic lecture - Modern quantum chemistry in use, PG_00051258						
Field of study	Chemistry						
Date of commencement of studies	October 2024		Academic year of realisation of subject	2025/2026			
Education level	postgraduate 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	English			
Semester of study	3		ECTS credits	3.0			
Learning profile	academic		Assessment form				
Conducting unit	Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		dr Jakub Brzeski				
	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	Acquiring knowledge about the possibility of using various theoretical methods to solve chemical problems. Teaching students about the areas of chemistry which may benefit from the use of computational chemistry tools.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	K_U02: critically assesses the results of performed theoretical calculations and discusses them in the context of predicted properties of the molecules studied	[SU4] test/exam - oral or written
[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	K_U04: applies acquired knowledge of the possibility of designing novel molecules having desired properties, general chemistry and related scientific disciplines	[SU4] test/exam - oral or written
[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	K_W07: selects suitable computational tools to the extent necessary to solve various chemical problems	[SW4] test/exam - oral or written
[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	K_W05: has extended knowledge in the field of computational chemistry	[SW4] test/exam - oral or written
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	K_W08: demonstrates in-depth knowledge of types of chemical problems whose solutions could be supported by the use of computational chemistry tools	[SW4] test/exam - oral or written
[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.	K_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	[SK4] 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.	K_K01: knows the limitations of her/his own knowledge; understands the need for further education	[SK4] test/exam - oral or written

Subject contents

Mathematical tools used in modern quantum chemistry methods, equation of motion methods (EOM), advanced coupled-cluster methods (CC), relativistic quantum chemistry, novel DFT methods, SAPT methods, quantum Monte Carlo methods, QM/MM methods, designing novel systems of desired properties.

Prerequisites and co-requisites

basic knowledge of chemistry and physics

Assessment methods and criteria

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

Recommended reading

Basic literature	Molecular Quantum Mechanics, P. W. Atkins, R. S. Friedman, Oxford University Press Inc., New York (2011)
Supplementary literature	Quantum Mechanics in Chemistry, J. Simons, J. Nichols, Oxford University Press (1997)
eResources addresses	Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed

selection of an appropriate DFT functional for the examined problem, selection of the coupled cluster method for the examined problem, design of nanoparticles with the desired properties, etc.

Work placement

Not applicable

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