


KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

 Projekt współfinansowany przez
Unię Europejską w ramach
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Społecznego

UNIA EUROPEJSKA
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Course title		ECTS code	
Diploma lecture - Disputes about molecular structure: From electron clouds to biological macromolecules		13.3.0470	
Name of unit administrating study			
null			
Studies			
faculty	field of study	type	pierwszego stopnia
Wydział Chemii	Chemia	form	stacjonarne
		specjalty	chemia biomedyczna, chemia kosmetyków, analityka i diagnostyka chemiczna, chemia żywności
		specialization	wszystkie
Teaching staff			
dr hab. Iwona Anusiewicz, profesor uczelni			
Forms of classes, the realization and number of hours		ECTS credits	
Forms of classes		2	
Lecture		classes 30 h	
The realization of activities		tutorial classes 5 h	
classroom instruction		student's own work 15 h	
Number of hours		TOTAL: 50 h - 2 ECTS	
Lecture: 30 hours			
The academic cycle			
2024/2025 summer semester			
Type of course		Language of instruction	
obligatory		polish	
Teaching methods		Form and method of assessment and basic criteria for evaluation or examination requirements	
		Final evaluation	
		Graded credit	
		Assessment methods	
		(mid-term / end-term) test	
		The basic criteria for evaluation	
		Passing the final oral exam (by answering open questions covering the issues presented during the lecture).	
Method of verifying required learning outcomes			
Required courses and introductory requirements			
A. Formal requirements			
mathematics, physics, quantum chemistry			
B. Prerequisites			
basic knowledge concerning physics, linear algebra, infinitesimal and integral calculus			
Aims of education			
acquainting students with the basics of quantum mechanics and quantum chemistry			
acquainting students with the most important quantum chemistry methods allowing the prediction of structures, physicochemical properties, and reactivity of chemical compounds.			
Course contents			
Solving problems by using theoretical chemistry tools, most frequently used ab initio methods, determining the equilibrium structures, dipole moments, physicochemical parameters, and other basic properties of molecules. Investigation of reaction mechanisms.			

Bibliography of literature	
Literature required to pass the course Either one of the following textbooks: Molecular Quantum Mechanics (P. Atkins, R. Friedman), An Introduction to Theoretical Chemistry (J. Simons), Quantum Mechanics in Chemistry (J. Simons, J. Nicols). Lucjan Piela „Idee chemii kwantowej” P.W. Atkins „Molekularna mechanika kwantowa” Extracurricular readings Quantum Mechanics (A. Messiah), Modern Quantum Chemistry (A. Szabo, N. Ostlund).	
The learning outcomes (for the field of study and specialization)	Knowledge
	After the course, the students are capable of: explaining simple physical problems solved by quantum mechanics, identifying the symmetry of the wave-function, explaining the most fundamental approximations utilized in quantum chemistry, determining the multiplicity of a given molecular system, explaining the most important quantum chemistry methods
	Skills
	After completing the course, the students are capable of choosing the most suitable computational method for solving the Schrödinger equation for a given molecular system and performing the calculations using standard quantum chemistry program package.
	Social competence
	After the course, the students are expected to understand the necessity of further learning, they are also taught to approach the problems and formulate their opinions with caution and criticism. In addition, the students are expected to remain open-minded for new ideas.
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