


KAPITAŁ LUDZKI
 NARODOWA STRATEGIA SPÓJNOŚCI

 Projekt współfinansowany przez
 Unię Europejską w ramach
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UNIA EUROPEJSKA
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Course title		ECTS code	
Quantum chemistry		13.3.1002	
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			
prof. dr hab. Piotr Skurski; dr Marcin Czapla; dr Sylwia Freza; dr Jakub Brzeski; mgr Marzena Marchaj; dr hab. Iwona Anusiewicz, profesor uczelni			
Forms of classes, the realization and number of hours		ECTS credits	
Forms of classes		5	
Auditorium classes, Lecture		classes - 60 h	
The realization of activities		tutorial classes – 20 h	
classroom instruction		student's own work – 45 h	
Number of hours		Total: 125 h - 5 ECTS	
Lecture: 30 hours, Auditorium classes: 30 hours			
The academic cycle			
2022/2023 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	
- discussion		Final evaluation	
- multimedia-based lecture		- Graded credit	
- problem solving		- Examination	
		Assessment methods	
		- (mid-term / end-term) test	
		- oral exam	
		The basic criteria for evaluation	
		Passing written tests and evaluation during seminars throughout the semester. The attendance and active participation in seminars is obligatory.	
		Passing the final oral exam (by answering open questions covering the issues presented during the lecture). The final exam may be taken only by students who passed earlier tests during the seminars.	
Method of verifying required learning outcomes			
Required courses and introductory requirements			
A. Formal requirements			
none			
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			

<ul style="list-style-type: none"> acquainting students with the most important quantum chemistry methods allowing the prediction of their molecular structure, physicochemical properties, and reactivity. 	
Course contents <p>A. Lectures: wave-particle duality; Heisenberg's 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).</p> <p>B. Seminars: operators, eigenvectors and eigenvalues in Hilbert space, quantum numbers, orbitals, spin operators, symmetry of the wave-function, Slater determinants, evaluating electronic energy in Hartree-Fock method.</p>	
Bibliography of literature <p>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). Extracurricular readings Quantum Mechanics (A. Messiah), Ideas of Quantum Chemistry (L. Piela), Modern Quantum Chemistry (A. Szabo, N. Ostlund).</p>	
The learning outcomes (for the field of study and specialization)	Knowledge <p>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, 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.</p>
	Skills <p>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.</p>
	Social competence <p>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.</p>
Contact <p>piotr.skurski@ug.edu.pl</p>	