



Subject card

Subject name and code	, PG_00058691						
Field of study	Materials Engineering, Materials Engineering, Materials Engineering						
Date of commencement of studies	February 2023	Academic year of realisation of subject			2022/2023		
Education level	second-cycle studies	Subject group			Obligatory subject group in the field of study Subject group related to scientific research in the field of study		
Mode of study	Full-time studies	Mode of delivery			at the university		
Year of study	1	Language of instruction			Polish		
Semester of study	1	ECTS credits			3.0		
Learning profile	general academic profile	Assessment form			assessment		
Conducting unit	Zakład fizyki układów nieuporządkowanych -> Instytut Nanotechnologii i Inżynierii Materiałowej -> Faculty of Applied Physics and Mathematics						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. Maciej Bobrowski				
	Teachers		dr hab. Maciej Bobrowski				
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	45.0	0.0	0.0	60
	E-learning hours included: 0.0						
	Modelowanie materiałów metodami kwantowymi - Moodle ID: 27970 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=27970						
Additional information: stationary classes, lectures + laboratories. In case of pandemic threat the classes could be held in online mode too.							
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	60		5.0		10.0	75
Subject objectives	Teaching of: ideas of quantum methods, those based on wave functions for systems from hydrogen atom (exact solution) up to many-atom systems, application of quantum methods for molecules in any electronic states, prediction and investigation of mechanisms of chemical reactions, practical application of quantum methods for problems from among the materials engineering. The laboratories should be realised in this way that each group should focus on the same main problem while each individual tasks of the students should be at the end gathered and compared.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	K7_U07	Student can plan realization of his tasks in the field of materials engineering by utilization of computing server: build the structure and coordinates, assign spins, charges, build input files, do the computations, copy files between the computing server and his PC, analyze graphically the results and compare them to the results of his mates from the same group.	[SU4] Assessment of ability to use methods and tools [SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject
	K7_U01	Student can: compare his own results with literature data and data achieved by his mates from the same group: description of the reaction mechanisms, basic properties: electron affinities, kinetic energy barriers, occupation numbers (of orbitals), influence of structures (and substituents) on the reactivity and stability of the molecular systems.	[SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU1] Assessment of task fulfilment
	K7_W02	Student can: derive formulas for total energies of given electronic configurations, derive formulas for matrix form of the Ritz method, normalize wave functions, justify choice of selected basis sets, build molecular structures, impose spins and charges, do the computations of the given mechanism of chemical reaction, locate saddle points, analyse processes from their physico-chemical point of view (rate constants, energies, vibrations, influence of change of the structures), use advanced software for quantum computations, analyze electronic structure.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects
	K7_K01	Student can independently build investigated models of molecular systems and on this basis do the scientific investigations by means of quantum ideas and tools in materials engineering. Student see that there is a direct connection between the simulations and their results and the experimental data from literature.	[SK1] Assessment of group work skills [SK2] Assessment of progress of work [SK3] Assessment of ability to organize work [SK4] Assessment of communication skills, including language correctness [SK5] Assessment of ability to solve problems that arise in practice
Subject contents	<p>Below it was split into hours of lectures:</p> <p>1--2. Examples of applications of quantum methods in realization of scientific projects dedicated to novel materials for applications in electrochemistry, optics, energetics, electronics.</p> <p>2--6. Two exact solutions of Schrodinger equation: rigid rotor and hydrogen atom: spherical harmonics and atomic orbitals, eigenvalues, properties.</p> <p>7--11 Variational methods: nonlinear and linear parameters, matrix equations.</p> <p>12--14. Many-electron systems: Slater determinant, Hartree-Fock method, SCF algorithm.</p> <p>15. Configuration interaction and basis functions. When it is necessary to apply more accurate methods.</p>		
Prerequisites and co-requisites	Basics from: physics, chemistry, quantum methods, mathematics, working under Linux operating system.		

Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	exam from lecture.	51.0%	50.0%
	report from laboratory.	51.0%	50.0%
Recommended reading	Basic literature	1. Lucjan Piela, Idee Chemii Kwantowej, wydawnictwo PWN, 2. Frank Jensen, Introduction to Computational Chemistry, Wiley	
	Supplementary literature	1. C.J. Ballhausen, H. B. Gray, Molecular Orbital Theory, W. A. BENJAMIN, INC., 1965 2. W. Kotos, Chemia Kwantowa, PWN, Warszawa 1978,	
	eResources addresses	Uzupełniająca https://enauczenie.pg.edu.pl/moodle/course/view.php?id=27970 - Course for both lectures and laboratories.	
Example issues/ example questions/ tasks being completed	<p>1. Draw energy diagram as a function of distance between atoms of reagents for dissociation process of water into two radicals: OH and H. Indicate spins, characteristic points, especially those which correspond to local minimas.</p> <p>2. Enumerate characteristic points at energy curve of a reaction, in which the total spin doesn't change during the reaction. Indicate basic mathematical properties of those points.</p> <p>3. Normalize the function $e^{-c \cdot x}$</p> <p>4. Calculate electron and total energies of given electronic configuration of hydrogen molecule.</p> <p>5. Calculate electronic energy of the given electron configuration of a system consisting of 5 electrons. In the next step draw an electron configuration which reveals from one-electron reduction reaction of that state and also calculate the new state's electronic configuration.</p> <p>6. Derive system of secular equations in the Ritz method for a system of 3 molecular orbitals $\{f_1, f_2, f_3\}$, from which each is normalized while the whole set is not orthogonal.</p>		
Work placement	Not applicable		