GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Modeling of materials using quantum methods, PG_00063526					
Field of study	Materials Engineering					
Date of commencement of studies	October 2024		Academic year of realisation of subject		2024/2025	
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	2		ECTS credits		2.0	
Learning profile	general academic profile		Assessment form		assessment	
Conducting unit	Division of Physics of Disordered Systems -> Institute of Nanotechnology and Materials Engineering -> 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	15.0	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	3.0	17.0	50	
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, parctical 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_U01] Can obtain information from literature, databases and other properly selected sources, also in English; can integrate the obtained information, interpret and draw conclusions, formulate and justify opinions	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_U07] Can plan and organize individual and team work.	Student can plan realization of his tasks in the field of materials engineering by utilization of computing server: build the structure and coocrdinates, 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_K01] Understands the need for lifelong learning, can inspire and organize the learning process of others. Is aware of own limitations and knows when to turn to experts, can accurately determine priorities helping to achieve the tasks specified by themselves or others.	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
	[K7_W02] Knows experimental, observatory and numerical techniques, as well as methods of building mathematical models relevant to materials engineering; can independently recreate basic theorems and laws, and their proofs.	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

Subject contents

Below it was split into hours of lectures:

1--2. Examples of applications of quantum methods in realization of scientific projects dedicated to novel materials for applications in electrochemistry, optics, energetics, electronics.

2--6. Two exact solutions of Schrodinger equation: rigid rotor and hydrogen atom: spherical harmonics and atomic orbitals, eigenvalues, properties.

7--11 Variational methods: nonlinear and linear parameters, matrix equations.

12--14. Many-electron systems: Slater determinant, Hartree-Fock method, SCF algorithm.

15. Configuration interaction and basis functions. When it is necessary to apply more accurate methods.

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
report from laboratory.	51.0%	100.0%

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. Kołos, Chemia Kwantowa, PWN, Warszawa 1978,
	eResources addresses	Adresy na platformie eNauczanie: Modelowanie materiałów metodami kwantowymi - Moodle ID: 44634 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=44634
Example issues/ example questions/ tasks being completed	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, chracteristic points, especially those which correspond to local minimas. 2.Enumerate characteristic points at energy curve of a reaction, in which the total spin doesn't change during the reaction. Indicate basic mathematical propertoies of those points. 3. Normalize the function e^{-c*x} 4. Calculate electron and total energies of given electronic configuration of hydrogen molecule. 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 electonic configuration. 6. Derive system of secular equations in the Ritz method for a system of 3 molecular orbitals {fi1, fi2, fi3}, from which each is normalized while the while set is not orthogonal.	
Work placement	Not applicable	