GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Computer modeling of materials II, PG_00048739		
Field of study	Materials Engineering, Materials Engineering, Materials Engineering		
Date of commencement of studies	February 2022	Academic year of realisation of subject	2021/2022
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 polish
Semester of study	1	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Solid State Physics -> 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	0.0	0.0	45.0	0.0	0.0	45

E-learning hours included: 0.0

Additional information:
Traditional classes. If necessary - online course.

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	45	5.0	5.0	55

Subject objectives

In given examples and withing introducing materials:

1. demonstration of dependencies between properties of materials and their structure,
2. demonstration of necessity of application of theoretical methods for investigation of properties of materials,
3. teachning of abilities of creation of structures utilizing different type of coordinate systems,
4. teaching of basics of quantum methods and basic equations,
5. teaching of utilization of specialized software for graphical results' analysis and visualization in independent course examples.

Learning outcomes

Course outcome	Subject outcome	Method of verification
K7_K01	Experiencing of limitation of the methods used and applied in students' tasks. Comparison of the results and results taken from experiment and literature.	[SK1] Assessment of group work skills [SK5] Assessment of ability to solve problems that arise in practice
K7_U07	Group can altogether divide the tasks and at the end of classes, share the results and draw conclusions.	[SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task [SU1] Assessment of task fulfilment
K7_W02	Ability of recognition of application of basic of physics: conservation of energy, angular momentum, etc. Ability of recognition and imposition of electronic structure of atoms and molecules. Ability of recognition of path (even experimental) of achieving a better material.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation
K7_U01	1. Transformation of the troblem into a model and an algorithm of solution, on the basis of physics and chemistry. 2. Transformation of the problem in order to improve the the material, in particular examples, also those requested by the students. 3. Analysis and intrepretation of the results.	[SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task

Subject contents

1. Reminding of basic tools of operating systems of computers, working in computer network, with emphasis on the software used further in the computations.
2. Theory introductions, basic algorithms: operators, wave functions, eigen problems, Schrödinger equation, variational methods, Hartree-Fock method.
3. Self-managed buidling of structures and systems for further computations,
4. Discussion of rules of using specialized software for quantum computing and graophical visualization.
5. Sel-managed performing computations, by means of quantum software.

Prerequisites and co-requisites

Chemistry and basics of physics and mathematics.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Practical test	50.0%	100.0%

Recommended reading

Basic literature	1. Lucjan Piela, Idee Chemii Kwantowej, PWN, Warsaw, 2003 i nowsze, 2. Włodzimierz Kołos. Chemia kwantowa. PWN, Warsaw, 1978, 3. Włodzimierz Kołos, Joanna Sadlej. Atom i cząsteczka. WNT, Warsaw, 2007. 4. Frank Jensen, Introduction to Computational Chemistry, Wiley, England, 2007. 5. PDF materials of teacher. 6. Gamess US, documentation: http://wild.life.nctu.edu.tw/~jsyu/gamess2k/index.html
Supplementary literature	Scientific papers (Elsevier, AIP, ACS, etc.) given after suitable selection of problem for self-managing realization.
eResources addresses	

Example issues/ example questions/ tasks being completed

Show that eigenvalues of hermitian operators are real.
For given function calculate energy by means of variational method.
What atomic and molecular orbitals will be taken into account within a given basis
Calculate electron energy for the given electron configuration. Assign the total spoin and multiplicity.
How to improve elasticity if a material and how to determine it by means of the quantum methods?
How to get increase redox potentials of metal oxide nanopatrticles?

Work placement