GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Materials Science - quantum particle approach, PG_00071217
Field of study	Nanotechnology, Nanotechnology

Date of commencement of studies	February 2027	**Academic year of realisation of subject**	2027/2028
Education level	second-cycle studies	**Subject group**	Specialty subject group 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**	English
Semester of study	2	**ECTS credits**	6.0
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 -> Faculties of Gdańsk University of Technology

Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Maciej Bobrowski
	Teachers	dr hab. Maciej Bobrowski

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	45.0	0.0	0.0	75

E-learning hours included: 0.0

eNauczanie source address: https://enauczanie.pg.edu.pl/2025/course/view.php?id=3649

Moodle ID: 3649 Materials Science - quantum particle approach 2027
https://enauczanie.pg.edu.pl/2025/course/view.php?id=3649

Additional information:

In-person.

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	75	2.0	73.0	150

Subject objectives	Course Objectives: 1. To provide knowledge on the application of quantum computational methods to solving problems involving electronic structure changes in material systems based on molecules and crystals: polymers, rubbers, metal oxides, chemical reactions, and galvanic cells (using examples from specific research projects implemented as part of research grants). 2. To teach the application of quantum mechanical axioms to small and multi-atomic systems. 3. To teach commonly used quantum methods based on calculated wave functions: HF, CI, MCSCF, MPn, CC. 4. To teach the use of commonly used basis functions in quantum computations. 5. To teach the interpretation of results for obtained quantum states in the process of researching the properties of materials, including the interpretation of properties based on the resulting spin of the system.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[K7_W05] has in-depth knowledge of mathematical, numerical, and simulation methods - both classical and quantum - used in the modeling of nanostructures	Students will gain in-depth knowledge of the representation of quantum states for multi-electron systems, including polyatomic systems, how to obtain quantum states for molecules, and how to account for spin in systems, both analytically (when deriving energy formulas) and practically, i.e., when performing computations using computers. Students will be able to construct molecular systems using atomic coordinates and then perform complex quantum calculations for them, imposing spin. Students will be able to investigate chemical reaction mechanisms using quantum methods.	[SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects
	[K7_U03] has enhanced abilities of using advanced specialist software packages	The student is able to operate a quantum computing program on a multiprocessor computer together with advanced programs for visualizing calculation results and building structures.	[SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools [SU3] Assessment of ability to use knowledge gained from the subject
	[K7_W02] has in-depth, theoretically grounded and detailed knowledge of phenomena, methods, and theories related to nanotechnology, as well as of related and allied fields of science or engineering	The student has in-depth knowledge of quantum methods used in calculations to change the electronic structure of chemical systems that build also nanosystems as well as the possibilities and limitations of such methods.	[SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects
	[K7_U05] is able to plan and carry out theoretical and numerical calculations as well as simulations of phenomena and processes, critically analyze their results, draw conclusions, and formulate well-founded opinions in nanotechnology and related physical and natural sciences	The student is able to solve a problem given by the instructor using a quantum computing program: a group of complex molecular systems, e.g. metal oxides, polymers, including chemical reactions of formation and decomposition.	[SU4] Assessment of ability to use methods and tools [SU2] Assessment of ability to analyse information [SU5] Assessment of ability to present the results of task [SU3] Assessment of ability to use knowledge gained from the subject

| Subject contents | Course content – lecture
The lecture hours are divided below:

1--2. Examples of the application of quantum methods in research projects focused on: the search for and characterization of new, complex materials for applications in electrochemistry, optics, energy, and electronics.

3--6. Schrodinger solutions for a rigid rotor and the hydrogen atom: spherical harmonics, atomic orbitals (including their graphical representation and orbital properties), eigenvalues, properties, and the method of molecular orbital formation.

7--11. Variational methods: nonlinear and linear parameters. Matrix representation.

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

15. Configuration interaction methods and basis functions. |
| | Course content – laboratory
The labs are divided as follows (by week):
1. Information about the Linux operating system, network organization, including access to the computational server and external data access, and setting up accounts on the computational server.
2. Molecular geometry and molecular coordinates: Cartesian and internal, and (at the end) assistance from the Molden program.Calculations using the advanced Gamess program.
3. Sample calculations on the computational server for cases assigned by the instructor: relatively small systems, e.g., ethyl alcohol, water radicals, the use of internal coordinates in chemical reaction calculations, and calculations on multiple processors.
4. Discussion of a common project problem and division of tasks (a different task for each student), e.g.,
(1) structure of isomers of iron(III), cobalt(III), etc. oxides in alternating and non-alternating configurations, taking into account all possible spin configurations and analysis (including within the entire group) of the probability of occurrence of given spatial configurations and quantum states of all obtained stable possibilities, and based on this, estimation of the magnetic properties of selected metal oxides, along with analysis of the causes and magnitude of such properties,
(2) construction of models of functionalized rubbers and their curing reactions to rubber using reactions with sulfur/oxygen, etc.
(3) termination reactions of selected polymers in the CVD polymerization process via combustion in oxygen (chemical reactions), along with the possibility of polymer functionalization.
5-15. Individual calculations conducted independently by each student on a given problem.

Prześlij opinię |

| Prerequisites and co-requisites | Base knowledge on physics, mathematics, chemistry and quantum mechanics. |

Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	exam	51.0%	50.0%
	sprawozdanie	51.0%	50.0%

Recommended reading	Basic literature	1. Frank Jensen, Introduction to Computational Chemistry, Wydawnictwo Wiley, 2007, 2. C. J. Ballhausen, H. B. Gray, Molecular Orbital Theory, Wydawnictwo W. A. Benjamin Inc. 1964,
	Supplementary literature	Yung-Kuo Lim, Problems and Solutions on Quantum Mechanics, Wydawnictwo World Scientific, 2005,
	eResources addresses	

Example issues/ example questions/ tasks being completed	Lectures: 1. Calculate the given commutators in Cartesian and spherical coordinates. 2. Normalize the given wave functions. 3. Orthogonalize the given basis functions. 4. Draw the electronic configurations and calculate the spins of: the nitrogen atom, the oxygen atom anion, the iron(III) cation, the oxygen molecule, the oxygen radical anion, and the nitrogen radical cation. 5. Calculate the electronic energies of the given electronic configurations. 6. Calculate the electronic states and energies for the wave function represented as a linear combination of the ground state and the doubly excited hydrogen molecule. 7. What molecular and atomic orbitals would be present in the NaCl molecule in the DZ basis? How many Slater determinants can be constructed using the full CI method? What can be done to reduce the number of possible electronic configurations? 8. When and why are relativistic methods used in quantum calculations?What about the influence of relativistic electrons on the entire pool of orbitals, especially those describing valence electrons? Labs: 1. Calculate the polymerization reaction mechanism for a given polymer. 2. Compare the energies of the electronic states of ferromagnetic iron(III) oxides.
Practical activites within the subject	Not applicable

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