GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

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|---|---|---|---|
| Subject name and code | THEORETICAL CHEMISTRY, PG_00037381 | | |
| Field of study | Chemistry | | |
| Date of commencement of studies | October 2023 | Academic year of realisation of subject | 2024/2025 |
| Education level | first-cycle studies | Subject group | Obligatory subject group in the field of study<br>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 | 2 | Language of instruction | Polish |
| Semester of study | 4 | ECTS credits | 3.0 |
| Learning profile | general academic profile | Assessment form | assessment |
| Conducting unit | Department of Inorganic Chemistry -> Faculty of Chemistry | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | dr inż. Andrzej Okuniewski | |
| | Teachers | | |

**Lesson types and methods of instruction**

| Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
|---|---|---|---|---|---|---|
| Number of study hours | 15.0 | 0.0 | 30.0 | 0.0 | 0.0 | 45 |

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 | 45 | 5.0 | 25.0 | 75 |

**Subject objectives**

The aim of the course is to acquaint students with the basics of theoretical chemistry and quantum mechanics.

**Learning outcomes**

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [K6_W05] knows and understands the chemical processes and algorithms of mathematical models which are necessary for the design of technological processes, knows chemical structure of contemporary materials and its relation to their properties, enabling the selection of the materials for sustainable development technology and material-efficient and energy-efficient methods | uses computer software to determine selected properties of atoms, interprets the obtained results and confronts them with literature experimental results | [SW3] Assessment of knowledge contained in written work and projects |
| K6_W03 | understands and is able to use the terminology and designations used in theoretical chemistry, knows the history and modern ideas in the field of quantum chemistry, analyzes the model quantum-mechanical problems and can qualitatively discuss their applications in chemistry, is prepared to continue learning of theoretical methods in chemistry | [SW1] Assessment of factual knowledge |
| [K6_U05] can, on the basis of the collected experimental or source material, prepare an oral communication with a multimedia presentation | N/A | [SU5] Assessment of ability to present the results of task |

<table>
<tr><td>Subject contents</td><td>Lecture: History of quantum mechanics. Wave-particle duality. The postulates of quantum mechanics. Uncertainty. Functions of many variables. Differential equations. Particle in a one-dimensional potential well. Quantum tunnelling. Harmonic oscillator. Particle in a ring. Particle in a two-dimensional potential well. Rigid rotor. Hydrogen atom and hydrogen-like ions. Multielectronic systems.<br><br>Computer labs: Verification of the validity of Aufbau principle. Determining the energy of the electronic excitation. Determination of ionization energy. Determination of Mulliken electronegativity and Pearson's hardness. Study of electronegativity and hardness variability in the periodic table. The charge of the nucleus and its shielding.<br><br>A detailed program of the course as well as the project and seminar topics are regularly updated and posted on the Department of Inorganic Chemistry webpage: chem.pg.edu.pl/kchn/ch-chemia-teoretyczna</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>The student must have mastered the following courses at the undergraduate level: mathematics, physics, general chemistry, physical chemistry.</td></tr>
<tr><td>Assessment methods and criteria</td><td><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Computer labs</td><td>60.0%</td><td>50.0%</td></tr>
<tr><td>Final test</td><td>60.0%</td><td>50.0%</td></tr>
</table></td></tr>
<tr><td>Recommended reading</td><td><table>
<tr><td>Basic literature</td><td>D. O. Hayward: Mechanika kwantowa dla chemików, PWN, Warszawa 2007.</td></tr>
<tr><td>Supplementary literature</td><td>R. F. Nalewajski: Podstawy i metody chemii kwantowej, PWN, Warszawa 2001.<br><br>L. Piela: Idee chemii kwantowej. PWN, Warszawa 2011.<br><br>W. Kołos, J. Sadlej: Atom i cząsteczka, WNT, Warszawa 1998.<br><br>H. Haken, H. Ch. Wolf: Fizyka molekularna z elementami chemii kwantowej, PWN, Warszawa 1998.</td></tr>
<tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:</td></tr>
</table></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td>chem.pg.edu.pl/kchn/ch-chemia-teoretyczna</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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