GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

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|---|---|---|---|
| Subject name and code | Introduction to Biological Modelling Systems, PG_00049378 | | |
| Field of study | Biomedical Engineering | | |
| Date of commencement of studies | October 2023 | Academic year of realisation of subject | 2025/2026 |
| Education level | first-cycle studies | Subject group | Optional subject group<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 | 3 | Language of instruction | Polish |
| Semester of study | 6 | ECTS credits | 4.0 |
| Learning profile | general academic profile | Assessment form | assessment |
| Conducting unit | Division of Theoretical Physics and Quantum Informaton -> Institute of Physics and Applied Computer Science -> Faculty of Applied Physics and Mathematics | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | dr hab. inż. Marta Łabuda | |
| | Teachers | | |

**Lesson types and methods of instruction**

| Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
|---|---|---|---|---|---|---|
| Number of study hours | 15.0 | 0.0 | 15.0 | 15.0 | 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 | 4.0 | 51.0 | 100 |

**Subject objectives**

Introduce the students to the basics of computational and theoretical methods necessary to perform simulations to illustrate the properties of molecules. Students will gain the knowledge on the quantum chemistry methods and techniques allowing to use them in practice in simple atomic systems as well as complex biological systems.

**Learning outcomes**

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [K6_W02] knows and understands, to an advanced extent, selected laws of physics and physical phenomena as well as methods and theories explaining the complex relationships between them, constituting the basic general knowledge in the field of technical sciences related to the field of study | The student knows the basics of theory necessary for performing calculations in atomic and molecular systems. | [SW3] Assessment of knowledge contained in written work and projects |
| [K6_U05] can plan and conduct experiments related to the field of study, including computer simulations and measurements; interpret obtained results and draw conclusions | The student can self perform simple calculations and computer simulations by using given tools for modeling of molecular systems. | [SU4] Assessment of ability to use methods and tools<br>[SU2] Assessment of ability to analyse information |
| [K6_U07] can apply methods of process and function support, specific to the field of study | The student knows the basic concepts and definitions of molecular physics and quantum-mechanical computations.<br>The student knows and distinguishes basic ab initio quantum chemistry methods. | [SU4] Assessment of ability to use methods and tools<br>[SU1] Assessment of task fulfilment |

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| Subject contents | Introduction. Theoretical background of quantum mechanics. Schroedinger equation. An electron and nuclei movements. Adiabatic approximation. Energy of the excitation. Potential energy curves. Introduction to the quantum chemistry methods. The Self-Consistent Field method and LCAO method. Atomic orbital basis sets. Calculation technique. Ab initio methods.Hartree-Fock method, multi-configurational and multi-reference methods. CI, CC and MP2 methods. Application of the methods to diatomic molecules. Quantum chemistry packages: description, structure and characteristics, advantages and disadvantages of the packages. An interpretation and visualisation of the results. Simple dynamics simulation in the chemical reactions. Simulation of the collisions and interactions between atoms in molecules. | |
| Prerequisites and co-requisites | Introduction to spectroscopy, basics of informatics. | |
| Assessment methods and criteria | | |

| Subject passing criteria | Passing threshold | Percentage of the final grade |
|---|---|---|
| Lecture-writting exam | 50.0% | 40.0% |
| Labs-raports | 50.0% | 60.0% |

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| Recommended reading | Basic literature | Review of the subject in the form of the e-booklet<br><br>Distance learning materials<br><br>Piela L., Idee chemii kwantowej, PWN 2005<br><br>Leach A. ,Molecular Modelling: Principles and applications Longman 1996<br><br>Szabo A., Ostlund N. S. Modern Quantum Chemistry McMillan, New York 1982<br><br>Schlick T. ,Molecular Modeling and Simulation Springer 2002<br><br>Jensen F. ,Introduction to Computational Chemistry, Academic Press 2007 |
| | Supplementary literature | User manual : www.molpro.net<br><br>Graphical user interfaces, for example: Gabedit (main page of the developer)<br><br>Instructions how to use the computational packages |
| | eResources addresses | Adresy na platformie eNauczanie: |
| Example issues/ example questions/ tasks being completed | | |
| Work placement | Not applicable | |

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