**SYLLABUS**

**regarding the qualification cycle FROM ………TO…..**

1. Basic Course/Module Information

|  |  |
| --- | --- |
| Course/Module title | *Atomic and molecular physics in biological and chemical research* |
| Course/Module code \* |  |
| Faculty (name of the unit offering the field of study) | *College of Natural Sciences* |
| Name of the unit running the course | *Institute of Physics* |
| Field of study | *Diagnostic systems in medicine* |
| Qualification level | *First-cycle studies* |
| Profile |  |
| Study mode | *Full-time* |
| Year and semester of studies | *2nd year, summer semester* |
| Course type |  |
| Language of instruction | *English* |
| Coordinator | *Dr Przemysław Kolek* |
| Course instructor | *Dr Izabela Piotrowska* |

\* - as agreed at the faculty

1.1.Learning format – number of hours and ECTS credits

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Semester  (n0.) | Lectures | Classes | Colloquia | Lab classes | Seminars | Practical classes | Internships | others | **ECTS credits** |
| summer |  | 30 |  |  |  |  |  |  | 5 |

1.2. Course delivery methods

☒ conducted in a traditional way

☒ involving distance education methods and techniques

1.3. Course/Module assessment (exam, pass with a grade, pass without a grade)

Pass with a grade

2. Prerequisites

|  |
| --- |
| *Thorough knowledge of the basics of physics and mathematics at the bachelor level and basic knowledge and skills in the field of physical measurements and the uncertainty analysis.* |

3. Objectives, Learning Outcomes, Course Content, and Instructional Methods

3.1. Course/Module objectives

|  |  |
| --- | --- |
| O1 | *mastering by the student issues in atomic and molecular physics, applicable in biological and chemical research and medicine* |
| O2 | *showing the student the inseparable connection between atomic and molecular physics and biology and chemistry* |

3.2. Course/Module Learning Outcomes (to be completed by the coordinator)

|  |  |  |
| --- | --- | --- |
| Learning Outcome | The description of the learning outcome  defined for the course/module | Relation to the degree programme outcomes |
| LO\_01 | the student knows and understands the basic concepts and laws in the field of atomic and molecular physics, in particular: physical theories regarding the structure of atoms and molecules and their interaction with electromagnetic radiation | K\_W02 |
| LO\_02 | the student is able to analyse problems in the field of atomic and molecular physics and find their solutions based on the known laws and methods | K\_U01 |
| LO\_03 | the student is able to create a study presenting a specific problem in the field of applications of atomic and molecular physics in biological and chemical sciences and medicine and provide ways to solve it, taking into account the initial economic assessment of the proposed solutions | K\_U05 |
| LO\_04 | the student is able to plan and perform simple experimental research, observations or computer simulations in the field of atomic and molecular physics and interpret the results obtained and formulate conclusions on this basis | K\_U06 |
| LO\_05 | the student is able to present in an accessible way the basic facts in the application of atomic and molecular physics in medicine and technology | K\_U10 |
| LO\_06 | the student is ready to recognize the limitations of his own knowledge and the need to consult experts in the event of difficulties in solving a problem on his own | K\_K01 |

**3.3. Course content (to be completed by the coordinator)**

1. Lectures

|  |
| --- |
| Content outline |
| **Introduction to the quantum theory of matter** Experimental foundations of quantum theory, atomic structure of matter, rise of quantum theory, successes and failures of Bohr's theory. Fundamentals of atomic spectroscopy: Rydberg's formula for hydrogen-like atoms, Ritz's combination principle. The hydrogen atom and hydrogen-like ions, wave-particle duality, de Broglie's hypothesis, basic concepts of quantum mechanics, Heisenberg's uncertainty principle. |
| **Quantum-mechanical foundations of the theory of one-electron systems**  The wave function and the Schrödinger equation. Schrödinger equation for hydrogen atom, quantum numbers for hydrogen atom, energy levels and emission spectrum of hydrogen atom, wave functions for hydrogen atom. Quantum numbers of the electron in one-electron atoms and the physical quantities quantized by them. Geometric properties of orbitals in hydrogen-like atoms and ions, probability density of finding an electron at a specific point in an atom. Spin of the electron, the concept of spinorbital. |
| **Fundamentals of the theory of many-electron systems**  Structure of multi-electron atoms. Multiplicity of a multi-electron system, indistinguishability of particles, principle of indistinguishability of identical particles, fermions and bosons, one-electron approximation, Pauli exclusion principle. Multi-electron function, Slater determinants. Effective orbital energies, self-consistent field method, Hartree-Fock equations. Electronic configurations of multi-electron atoms, concept of closed- and open-shell electron configuration, Hund's rule. Energy states of multi-electron atoms, definition of an atomic term, state of a multi-electron atom, fine structure of the emission spectrum, selection rules for optical transitions, determination of terms, magnetic field effect, correlation of electrons in atoms, configuration interaction method, other methods of taking electron correlation into account. |
| **Rotational states of molecules**  Separation of the motion of atomic nuclei and the motion of electrons in molecules, adiabatic and Born-Oppenheimer approximation. Separation of rotation and oscillation of a molecule. Diatomic molecule and linear molecule in rigid rotator approximation. Rotator level quantization, rotational constant. Rotation term of the molecule in the rigid rotator approximation vs. the frequency of the lines in the rotational spectrum. Thermal occupancy of rotational levels. Selection rules for rotation transitions. Moments of rotational transitions and intensity of transitions (influence of thermal occupancy). Isotopic effects in rotational spectra: influence of isotopic substitution on the values ​​of rotational constants. Molecule as non-rigid rotator - first correction of non-rigid rotator. The rotational term of the molecule in the non-rigid rotator approximation and the frequency of the lines in the rotational spectrum. |
| **Vibrational states of molecules**  Model potentials for vibrations in a diatomic molecule, Morse potential. A diatomic molecule in the harmonic oscillator approximation. Quantization of vibrational energy levels and transition rules. The influence of isotopic substitutions on the vibration frequency of a molecule. The molecule as an anharmonic oscillator - the first anharmonic correction. Dissociation energy and zero level energy. Molecule vibrational term in harmonic and anharmonic approximation and wavenumbers for transitions in progressions and sequences. The vibration-rotation spectrum of molecules. |
| **Electronic structure of molecules**  Methods of molecular orbitals, symmetry of molecular orbitals, electron densities, orbital model vs. electron excitation scheme, correlation energy of electrons in molecules, application of the molecular orbital method to diatomic homonuclear molecules, one-electron approximation, energy levels within a simple description of molecular orbitals, principle of building electron configurations . Multi-electron approximation for linear molecules: symbols of molecular terms, electron spectrum of homonuclear molecules, application of the molecular orbital method to simple heteronuclear molecules, simple molecular description, principle of building electron configurations. |

1. Classes, tutorials/seminars, colloquia, laboratories, practical classes

|  |
| --- |
| Content outline |
| Introduction to the quantum theory of matter: wave-particle duality, calculation of de Broglie wavelength, calculation of energy, velocity and radius of orbits in the Bohr model. |
| Fundamentals of the theory of one- and many-electron systems. Quantum numbers and calculation of total energy, angular momentum, projection of angular momentum on the distinguished axis, and the value of electron spin and its projection for an electron in various quantum states in an atom. Determining the orbital form of the wave function and notation of shells, subshells and orbitals for given values ​​of quantum numbers. Real orbitals and complex orbitals. |
| Structure of multi-electron atoms. Configurations of multi-electron atoms and atomic terms in L-S coupling for closed-shell configurations, and p2, p4, d2 and d8. |
| Rotational states of molecules. Calculation of the rotational constants of the rotator and the frequency of rotation lines in the spectrum. |
| Vibrational states of molecules. Calculation of the force constant, reduced mass and frequency in the vibrational spectrum of molecules in harmonic approximation. Calculations of frequencies in progressions and sequences of oscillatory transitions, as well as the vibrational constants and dissociation energy of diatomic molecules. |
| Electronic structure of molecules. Molecular orbital theory, molecular orbital diagrams, configurations and terms of diatomic molecules. |
| Interaction of atoms and molecules with electrostatic and magnetic fields, splitting energy levels. Ion movement in electrostatic and magnetic fields: calculating the trajectory and acceleration, velocity and time-of-flight of molecular ions in these fields and determining the mass-to-charge ratio for these ions. |
| Investigation of the emission spectrum of the hydrogen atom. Determination of the Rydberg constant. |
| Analysis of the vibration-rotation spectrum of a diatomic molecule. |
| Qualitative spectral analysis - identification of elements present in fluorescent lamps, neon lamps and sodium lamps based on emission spectrum measurement. |

3.4. Methods of Instruction

e.g.

*Lecture: a problem-solving lecture/a lecture supported by a multimedia presentation/ distance learning*

*Classes: text analysis and discussion/project work (research project, implementation project, practical project)/ group work (problem solving, case study, discussion)/didactic games/ distance learning*

*Laboratory classes: designing and conducting experiments*

Lecture: distance learning

Classes: group work (problem solving)

Laboratories: conducting experiments

4. Assessment techniques and criteria

4.1 Methods of evaluating learning outcomes

|  |  |  |
| --- | --- | --- |
| Learning outcome | Methods of assessment of learning outcomes (e.g. test, oral exam, written exam, project, report, observation during classes) | Learning format (lectures, classes,…) |
| LO-01 | tests, exam | lectures, classes |
| LO-o2 | observation during classes, tests, reports, exam | lectures, classes, laboratories |
| LO-03 | observation during classes, tests, reports | lectures, classes |
| LO-04 | observation during classes, tests, reports | laboratories, classes |
| LO-05 | observation during classes, tests, exam | lectures, classes |
| LO-06 | observation during classes, tests, exam | classes |

4.2 Course assessment criteria

|  |
| --- |
| Passing the course takes place through tests, reports, active participation in classes and participation in discussions. It will confirm the degree to which the student has achieved the assumed learning outcomes. Verification of the achieved learning outcomes is controlled on an ongoing basis during the course. The grade obtained from completing the course will allow you to assess the degree of achieved effects.  Lecture: written exam; passed after the student has scored at least 50% of the points  Classes: the final grade is the grade obtained in the written colloquium. Student activity in class is also taken into account.  Laboratories: the final assessment is the arithmetic average of the assessments from individual exercises. |

5. Total student workload needed to achieve the intended learning outcomes

– number of hours and ECTS credits

|  |  |
| --- | --- |
| Activity | Number of hours |
| Scheduled course contact hours | 30 |
| Other contact hours involving the teacher (consultation hours, examinations) | 5 |
| Non-contact hours - student's own work (preparation for classes or examinations, projects, etc.) | 65 |
| Total number of hours | 100 |
| Total number of ECTS credits | 5 |

\* One ECTS point corresponds to 25-30 hours of total student workload

6. Internships related to the course/module

|  |  |
| --- | --- |
| Number of hours | *Not applicable* |
| Internship regulations and procedures | *Not applicable* |

7. Instructional materials

|  |
| --- |
| Compulsory literature:   1. Robert L. Brooks “The Fundamentals of Atomic and Molecular Physics”, Springer, New York, 2013 (manual available from the instructor) 2. Samuel J. Ling, Jeff Sanny, William Moebs “University Physics Volume 3”, OpenStax, 2021 |
| Complementary literature:   1. David Bates “Advances in atomic and molecular physics”, Boston: Academic Press, 1988 2. Gordon M. Barrow “Introduction to molecular spectroscopy”, McGraw-Hill Book Company, Inc., Tokyo, 1962 (available from the instructor) |

Approved by the Head of the Department or an authorised person