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| Course title Chemia kwantowa / Quantum chemistry | | ECTS code 13.3.1002 | |
| Name of unit administrating study Faculty of Chemistry | | | |
| Studies | | | |
| Field of study | Type | Form | |
| Chemistry | Bachelor | Full-time studies | |
| Teaching staff Prof. dr hab. Piotr Skurski | | | |
| Forms of classes, the realization and number of hours | | ECTS credits 5 | |
| A. Forms of classes, in accordance with the UG Rector's regulations lecture, auditorium classes | | classes - 60 h tutorial classes – 20 h student's own work – 45 h | |
| B. The realization of activities in-class learning | | Total: 125 h - 5 ECTS | |
| C. Number of hours 60 h (30 h lecture, 30 h auditorium classes) | | | |
| The academic cycle First year, summer semester | | | |
| Type of course obligatory | | Language of instruction Polish | |
| Teaching methods Solving problems Discussions Lectures supported by multimedia presentations | | Form and method of assessment and basic criteria for evaluation or examination requirements | |
| | | A. Final evaluation, in accordance with the UG study regulations lecture – exam auditorium classes – course completion (with a grade) | |
| | | B. Assessment methods Oral exam Written tests | |
| | | C. The basic criteria for evaluation or exam requirements Passing written tests and evaluation during seminars throughout the semester. The attendance and active participation in seminars is obligatory. Passing the final oral exam (by answering open questions covering the issues presented during the lecture). The final exam may be taken only by students who passed earlier tests during the seminars. | |
| Required courses and introductory requirements basic knowledge concerning physics, linear algebra, infinitesimal and integral calculus | | | |
| Aims of education <ul style="list-style-type: none"> • acquainting students with the basics of quantum mechanics and quantum chemistry • acquainting students with the most important quantum chemistry methods allowing the prediction of their molecular structure, physicochemical properties, and reactivity. | | | |
| Course contents A. Lectures: wave-particle duality; Heisenberg's principle of uncertainty; mathematical formulations of quantum mechanics (postulates of quantum mechanics); solving Schrödinger equation for a free particle, particle in a box, rigid rotor, harmonic oscillator, tunneling effect, and hydrogen atom; spin angular momentum, atomic terms, Pauli exclusion principle, and LS coupling; Born-Oppenheimer and one-electron approximations, perturbational methods; variational methods; electron correlation; MO theory; approximate quantum chemistry methods (Hartree-Fock method, Configuration-Interaction method, Multi-configurational self-consistent field method, Complete Active Space self-consistent field method, Møller-Plesset perturbational method, Coupled-cluster method). | | | |

B. Seminars: operators, eigenvectors and eigenvalues in Hilbert space, quantum numbers, orbitals, spin operators, symmetry of the wave-function, Slater determinants, evaluating electronic energy in Hartree-Fock method.

Bibliography of literature

A. Literature required to pass the course

Either one of the following textbooks: Molecular Quantum Mechanics (P. Atkins, R. Friedman), An Introduction to Theoretical Chemistry (J. Simons), Quantum Mechanics in Chemistry (J. Simons, J. Nicols).

B. Extracurricular readings

Quantum Mechanics (A. Messiah), Ideas of Quantum Chemistry (L. Piela), Modern Quantum Chemistry (A. Szabo, N. Ostlund).

Knowledge

After the course, the students are capable of: formulating the basics of quantum mechanics, explaining simple physical problems solved by quantum mechanics, identifying the symmetry of the wave-function, formulating Pauli exclusion principle and Hund rules, explaining the most fundamental approximations utilized in quantum chemistry, determining the multiplicity of a given molecular system, explaining the most important quantum chemistry methods.

Skills

After completing the course, the students are capable of: solving eigenproblems, predicting the possibility of accurate measuring certain observables, writing the proper single-determinant wave-function for a given configuration, calculating electronic energy in Hartree-Fock method, choosing the most suitable computational method for solving the Schrödinger equation for a given molecular system.

Social competence

After the course, the students are expected to understand the necessity of further learning, they are also taught to approach the problems and formulate their opinions with caution and criticism. In addition, the students are expected to remain open-minded for new ideas.