UNIWERSYTET GDAŃSKI

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

A. **Forms of classes, in accordance with the UG Rector's regulations**
lecture, auditorium classes

B. **The realization of activities**
in-class learning

C. **Number of hours**
60 h (30 h lecture, 30 h auditorium classes)

ECTS credits 5

classes - 60 h
tutorial classes – 20 h
student's own work – 45 h

Total: 125 h - 5 ECTS

The academic cycle
2019/20 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
• 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.