Uniwersytet Gdański

KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title

Quantum chemistry

ECTS code

13.3.1002

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	pierwszego stopnia
		form	stacjonarne
		specialty	chemia biomedyczna, chemia kosmetyków, analityka i diagnostyka chemiczna, chemia żywności
		specialization	wszystkie

Teaching staff

prof. dr hab. Piotr Skurski; dr hab. Iwona Anusiewicz, profesor uczelni; dr Marcin Czapla; dr Sylwia Freza; dr Jakub Brzeski; mgr Marzena Marchaj

Forms of classes, the realization and number of hours

Forms of classes

Auditorium classes, Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours, Auditorium classes: 30 hours

ECTS credits

5

classes - 60 h

tutorial classes – 20 h

student's own work – 45 h

Total: 125 h - 5 ECTS

The academic cycle

2022/2023 summer semester

Type of course

obligatory

Language of instruction

polish

Teaching methods

- discussion
- multimedia-based lecture
- problem solving

Form and method of assessment and basic criteria for eveluation or examination requirements

Final evaluation

- Graded credit
- Examination

Assessment methods

- (mid-term / end-term) test
- oral exam

The basic criteria for evaluation

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.

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements

none

B. Prerequisites

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

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

The learning outcomes (for the field of study and specialization)

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.

Contact

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