KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI
FUNDUSZ SPOŁECZNY

Course title	ECTS code
Diploma lecture - Disputes about molecular structure: From electron clouds to biological macromolekules	13.3.0470

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

dr hab. Iwona Anusiewicz, profesor uczelni

Forms of classes, the realization and number of hours

Forms of classes

Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours

ECTS credits

2
classes 30 h
tutorial classes 5 h
student's own work 15 h
TOTAL: 50 h - 2 ECTS

The academic cycle

2024/2025 summer semester

Type of course

obligatory

Language of instruction

polish

Teaching methods

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

Final evaluation

Graded credit

Assessment methods

(mid-term / end-term) test

The basic criteria for evaluation

Passing the final oral exam (by answering open questions covering the issues presented during the lecture).

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements
mathematics, physics, quantum chemistry

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 structures, physicochemical properties, and reactivity of chemical compounds.

Course contents

Solving problems by using theoretical chemistry tools, most frequently used ab initio methods, determining the equilibrium structures, dipole moments, physicochemical parameters, and other basic properties of molecules. Investigation of reaction mechanisms.

Bibliography of literature

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).
Lucjan Piela „Idee chemii kwantowej”
P.W. Atkins „Molekularna mechanika kwantowa”

Extracurricular readings
Quantum Mechanics (A. Messiah), 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: explaining simple physical problems solved by quantum mechanics, identifying the symmetry of the wave-function, 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 choosing the most suitable computational method for solving the Schrödinger equation for a given molecular system and performing the calculations using standard quantum chemistry program package.

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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