UNIWERSYTET GDAŃSKI

Course title
Wykład dyplomowy - Rozmowy o strukturze molekuł: od chmur elektronowych do makrocząsteczek biologicznych/Diploma lecture - Disputes about molecular structure: From electron clouds to biological macromolecules

ECTS code
13.3.0916

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

B. The realization of activities
In-class learning

C. Number of hours
lecture 30 h

ECTS credits

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

The academic cycle
2021/2022 summer semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods

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
Course completion (with a grade)

B. Assessment methods

oral exam

The basic criteria for evaluation

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

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

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).**

Lucjan Piela „Idee chemii kwantowej"

P.W. Atkins „Molekularna mechanika kwantowa"

B. Extracurricular readings

Quantum Mechanics (A. Messiah), Modern Quantum Chemistry (A. Szabo, N. Ostlund).

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.