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 - Physicochemistry of molecules | 13.3.0500 |

**Name of unit administrating study**

Faculty of Chemistry

**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. Karol Krzymiński, profesor uczelni; dr Lidia Chomicz-Mańka; dr hab. Artur Sikorski, profesor uczelni; dr hab. Piotr Storoniak, profesor uczelni; dr inż. Beata Zadykowicz

**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
consultations 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**

multimedia-based lecture

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

**Final evaluation**

Graded credit

**Assessment methods**

- written exam (test)
- oral exam

**The basic criteria for evaluation**

• exam consists of 20 questions (each teacher prepares 10 questions);
• scale of grades in accordance with study regulations of UG.
• To pass the course the student must attend at least 50% lectures.

**Method of verifying required learning outcomes**

**Required courses and introductory requirements**

**A. Formal requirements**
passed subjects: general chemistry and physical chemistry

**B. Prerequisites**
none

**Aims of education**

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• To familiarize students with the theoretical foundations of luminescence phenomena of organic compounds (with particular emphasis on fluorescence, phosphorescence, chemiluminescence, bioluminescence) and using the above-mentioned phenomena in modern science
• Introduction to computational methods used to describe chemical systems at the molecular level.

• To familiarize students with thermochemical techniques (TA, DSC, TG) and the possibility of their applications in the determination of chemical substances
• To acquaint students with the issue of the impact of low- and high-energy radiation on genetic material with particular emphasis on the interaction between low-energy electrons and DNA components
• To acquaint students with the methodology and results of experimental and theoretical research on DNA damage by low-energy electrons
• To acquaint students with the applications of thermodynamic theory to describe processes in nature with particular emphasis on the phenomenon of substance migration as processes associated with chemical analytics

## Course contents

• Physico-chemical basics of fluorescence, phosphorescence, chemiluminescence and bioluminescence; Measurements of radiation emissions from solutions; Luminescence spectra analysis; Examples of the use of chemiluminescence and bioluminescence in medical analytics
• Internal coordinates and Cartesian coordinates; Introduction to ab initio and semi-empirical methods and the theory of electron density functionals; Applications of quantum chemistry to optimize geometry, determination of physicochemical properties and characteristics of atoms and molecules; Determination of solvation effects; Thermodynamics and kinetics of chemical reactions based on quantum chemistry; Predicting spectral characteristics by quantum mechanics methods
• Physicochemical foundations of thermochemical techniques (thermal analysis, thermogravimetric analysis, differential scanning calorimetry); Parameters affecting the quality of measurements; Analysis of the results of thermochemical measurements; Application of techniques in modern analysis
• The effect of high energy radiation and UV on DNA; Low-energy electrons (LEE) as a genotoxic factor.
• Theoretical modeling of DNA damage mechanisms involving anionic states located on nucleic bases
• Thermodynamic quantities characterizing the formation and stability of anion radicals (vertical and adiabatic electron affinity, vertical detachment energy)
• Thermodynamics of separation processes; equilibria in open and closed systems, factors controlling equilibrium between phases

## Bibliography of literature

Literature required to pass the course Podstawowa:
1. Electronic materials provided by the lecturers.
2. A. Kumar, M.D. Sevilla, J. Leszczynski et al. (eds.), Handbook of Computational Chemistry, 2017
Extracurricular readings Uzupełniająca:
1. Atkins, P.W., Chemia fizyczna, PWN, Warszawa 2001.
2. Suppan, P.: Chemia i światło, PWN, Warszawa 1997.
3. Frisch, E. Frisch M.J.: Gaussian 98 User's Reference, Manual Version: 6.1, January, 1999.

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

### Knowledge

Knowledge

• The student knows the basic physicochemical processes responsible for the functioning of nature
• The student knows and understands the causes of photo-chemiluminescence phenomena; knows how to determine luminescence spectra parameters
• The student knows and understands the theoretical basis of computational methods in chemistry - ab initio, semi-empirical and the theory of electron density functionals (DFT); knows calculation methods of geometry optimization, determination of physicochemical parameters and prediction of spectral characteristics of organic molecules
• The student knows and understands the physicochemical foundations of thermochemical techniques and their application; Student is able to determine the quality of thermochemical results obtained
• The student knows what are the processes of DNA strand damage under induced by the radiation of different energies
• The student characterizes the types of anion radicals that may appear in the biological system as a result of interaction with water radiolysis products
• The student understands the methodology of experimental and computational research related to the subject of DNA damage under the influence of radiation
• The student understands the importance of thermodynamic theory for the description of phenomena that can be encountered in research and in everyday life

### Skills

Based on the acquired knowledge, the student is able to analyze and solve problems in the field of chemistry

| | |
|---|---|
| | **Social competence** |
| | understands the importance of computational methods in chemistry, aimed at reducing the amount of generated waste by predicting the theoretical behavior of chemical systems<br>• the student shows inquisitiveness and creativity in obtaining information and acquiring knowledge<br>• student understands the need for continuous education related to the rapid progress in science<br>• student is involved in solving scientific problems |
| **Contact** | |
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