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

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

Aims of education

• 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 • the student shows inquisitiveness and creativity in obtaining information and acquiring knowledge • student understands the need for continuous education related to the rapid progress in science • student is involved in solving scientific problems
Contact	
karol.krzyminski@ug.edu.pl	