


**KAPITAŁ LUDZKI**  
 NARODOWA STRATEGIA SPÓJNOŚCI

 Projekt współfinansowany przez  
 Unię Europejską w ramach  
 Europejskiego Funduszu  
 Społecznego

**UNIA EUROPEJSKA**  
 EUROPEJSKI  
 FUNDUSZ SPOŁECZNY


<b>Course title</b>		<b>ECTS code</b>	
Diploma lecture - Physicochemistry of molecules		13.3.0500	
<b>Name of unit administrating study</b>			
Faculty of Chemistry			
<b>Studies</b>			
<b>faculty</b>	<b>field of study</b>	<b>type</b>	pierwszego stopnia
Wydział Chemii	Chemia	<b>form</b>	stacjonarne
		<b>specjalty</b>	chemia biomedyczna, chemia kosmetyków, analityka i diagnostyka chemiczna, chemia żywności
		<b>specialization</b>	wszystkie
<b>Teaching staff</b>			
dr hab. Karol Krzywiński, profesor uczelni; dr hab. Piotr Storoniak, profesor uczelni; dr hab. Artur Sikorski, profesor uczelni; dr Lidia Chomicz-Mańka; dr inż. Beata Zadykowicz			
<b>Forms of classes, the realization and number of hours</b>		<b>ECTS credits</b>	
<b>Forms of classes</b>		2	
Lecture		classes 30 h	
<b>The realization of activities</b>		consultations 5 h	
classroom instruction		student's own work 15 h	
<b>Number of hours</b>		total: 50 h - 2 ECTS	
Lecture: 30 hours			
<b>The academic cycle</b>			
2024/2025 summer semester			
<b>Type of course</b>		<b>Language of instruction</b>	
obligatory		polish	
<b>Teaching methods</b>		<b>Form and method of assessment and basic criteria for evaluation or examination requirements</b>	
multimedia-based lecture		<b>Final evaluation</b>	
		Graded credit	
		<b>Assessment methods</b>	
		- written exam (test)	
		- oral exam	
		<b>The basic criteria for evaluation</b>	
		• 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.	
<b>Method of verifying required learning outcomes</b>			
<b>Required courses and introductory requirements</b>			
<b>A. Formal requirements</b>			
passed subjects: general chemistry and physical chemistry			
<b>B. Prerequisites</b>			
none			
<b>Aims of education</b>			
Aims of education			
<ul style="list-style-type: none"> <li>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</li> <li>Introduction to computational methods used to describe chemical systems at the molecular level.</li> </ul>			

- 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

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