UNIWERSYTET GDAŃSKI

Course title
Wykład dyplomowy - Fizykochemia moleküł/Diploma lecture - Physicochemistry of molecules

ECTS code
13.3.0500

Name of unit administrating study

Faculty of Chemistry

Studies

Field of study	Type	Form	
Chemistry	Bachelor	Full-time studies	

Teaching staff
dr hab. Piotr Storoniak, Associate Professor; dr Beata Zadykowicz

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
classes in the classroom

C. Number of hours
lecture 30 h

ECTS credits

classes 30 h
consultations 5 h
student's own work 15 h
total: 50 h - 2 ECTS

The academic cycle
2019/2020 summer semester

Type of course
optional subject

Language of instruction
polish

Teaching methods

Lecture with multimedia presentation

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

A. Final evaluation, in accordance with the UG study regulations
credit for a grade

B. Assessment methods
test including open questions
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.

Required courses and introductory requirements

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

B. Prerequisites none

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

A. **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

B. **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.

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