University of Gdańsk

Subject card

Subject name and code	Diploma lecture - Physicochemistry of molecules, PG_00081850		
Field of study	Chemistry		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2028/2029
Education level	Bachelor's studies	Subject group	Obligatory subject group in the field of study Optional subject group
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	3	Language of instruction	Polish
Semester of study	6	ECTS credits	2.0
Learning profile	academic	Assessment form	credit
Conducting unit	Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Piotr Storoniak	
	Teachers		

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	0.0	0.0	0.0	30
	E-learning hours included: 0.0						

Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
	Number of study hours	30	5.0	15.0	50

Subject objectives	To familiarize students with thermochemical techniques (TA, DSC, TG). Introduction to computational methods used to describe chemical systems. To familiarize students with the theoretical foundations of luminescence phenomena in organic compounds (fluorescence, phosphorescence, chemiluminescence, bioluminescence) and with the application of these phenomena in modern science. To familiarize students with the applications of thermodynamic theory to describe processes in nature. To familiarize students with the impact of radiation on genetic material and research on DNA damage by radiation.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEML3_W02] Describes the properties of elements and the most important chemical compounds, enumerates the methods of their preparation and methods of analysis.	the student knows and understands the theoretical basis of computational methods in chemistry: ab initio, semi-empirical and electron density functional theory (DFT); knows computational methods for optimizing geometry, determining physicochemical parameters and predicting spectral characteristics of organic molecules; the student knows and understands the physicochemical basis of thermochemical techniques and their applications; the student is able to determine the quality of the obtained thermochemical results; the student characterizes the types of anion radicals that may appear in biological systems as a result of interaction with water radiolysis products; the student understands the methodology of experimental and computational research related to DNA damage under the influence of radiation	[SW4] test/exam - oral or written
	[CHEML3_K01] Identifies the level of her/his own knowledge and skills and the need for continuous learning and personal development.	demonstrates inquisitiveness and creativity in independently obtaining information and knowledge; understands the importance of computational methods in chemistry aimed at reducing the amount of waste generated by theoretically predicting the behavior of chemical systems	[SK4] test/exam - oral or written
	[CHEML3_W03] Explains the relationship between the structure of matter and its observed properties.	the student knows the basic physicochemical processes responsible for the functioning of nature; the student knows and understands the causes of photo- and chemiluminescence phenomena, knows how to determine the parameters of luminescence spectra; the student understands the importance of thermodynamic theory for describing phenomena that may be encountered in research work and in everyday life; the student knows what the processes of damaging DNA strands under the influence of radiation of various energies involve	[SW4] test/exam - oral or written
	[CHEML3_U08] Presents in an understandable way the basic facts about chemistry using a scientific language typical of chemical sciences.	Based on the acquired knowledge, the student is able to analyze and solve problems in the field of chemistry	[SU4] test/exam - oral or written

Subject contents	1. **Thermoanalytical methods**: temperature - physicochemical description, basic methods and temperature measuring instruments; thermal analysis - definition and characteristics of methods (TGA, DTA, DSC); factors influencing the signal of thermoanalytical methods. 2. **Computational chemistry**: internal and Cartesian coordinates; introduction to ab initio, semi-empirical methods and density functional theory; basis set; applications of quantum chemistry to optimize geometry, determine physicochemical properties and characteristics of atoms and molecules; computational determination of solvation effects; thermodynamics and kinetics of chemical reactions in quantum chemistry; predicting spectral characteristics using quantum mechanics methods. 3. **Luminescence methods**: luminescence - definition, division, spectral range; physicochemical basis of the fluorescence, phosphorescence and chemiluminescence; measurements of radiation emissions from solutions; analysis of luminescence spectra; luminophores - characteristic features; fluorescence microscopy; examples of applications of photoluminescence and chemiluminescence in chemical, medical and environmental analytics. 4. **Thermodynamics**: principles of thermodynamics, direction of spontaneous transformations, how thermodynamics describes interactions at the atomic level, equilibria in open and closed systems, factors controlling the equilibria between phases, thermodynamic description of separation processes 5. **The impact of high-energy and UV radiation on DNA**: low-energy electrons (LEE) as a genotoxic factor, theoretical modeling of DNA damage mechanisms involving anionic states located on nucleobases, thermodynamic quantities characterizing the formation and stability of nucleobase anionradicals (vertical and adiabatic electron affinity, vertical electron detachment energy)
Prerequisites and co-requisites	Completed courses: general chemistry and physical chemistry.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
written exam, test and open questions	51.0%	100.0%

Recommended reading

Basic literature	1. Electronic materials provided by the lecturers 2. A. Kumar, M.D. Sevilla, J. Leszczynski et al. (eds.), Handbook of Computational Chemistry, 2017
Supplementary literature	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.
eResources addresses	

Example issues/ example questions/ tasks being completed

1. Thermodynamic criterion of spontaneous transformations
2. The concept of entropy, what phenomena are accompanied by a decrease in the entropy of the system
3. In the light of thermodynamic theory, what is the equilibrium for a separation system containing two phases and a solute?
4. What is the difference between dispersion (van der Waals) and polar interactions?
5. As a result of the interaction between an electron (with energy above 4 eV) and a chemical molecule, a phenomenon called "excited core resonance" may occur. What is this phenomenon?
6. What does vertical electron affinity (VEA) describe?
7. What are the characteristics of dipole anions and how are they created?
8. Which DFT functionals would be the best choice to calculate the activation energy of breaking phosphodiester bonds in DNA due to the addition of an excess electron?
9. In what spectral range does electronic excitation occur in organic molecules?
10. What transition is fluorescence emission associated with?
11. What relationship is determined in thermogravimetric (TG) analysis?
12. What is the multiplicity of an ion created by removing an electron from a neutral molecule of an organic compound?

Work placement	Not applicable

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