Subject card

Subject name and code	Theoretical chemistry, PG_00054401		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2024/2025
Education level	postgraduate studies	Subject group	Obligatory subject group in the field of study
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish no comments
Semester of study	1	ECTS credits	3.0
Learning profile	academic	Assessment form	
Conducting unit	Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Józef Liwo	
	Teachers	prof. dr hab. Józef Liwo	

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	40.0	75

Subject objectives	Acquiring by the student the knowledge of theoretical basis of molecular modeling, including molecular mechanics, dynamics, and Monte Carlo methods, Boltzmann law and its applications, and the basics of statistical mechanics and its applications in chemistry.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student applies the methods of analytical geometry, linear algebra, and calculus in basic molecular modeling and statistical mechanics in chemistry.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
	[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	The student selects methodology which is appropriate ot solve the posed problems of molecular modeling and applications of statistical mechanics in chemistry.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	The student identifies her/his defficiencies in the knowledge of chemistry, physics, and mathematics and learns the ways of deeper understanding chemical phenomena on atomistic basis.	[SK1] oral statement/conversation/ discussion [SK4] test/exam - oral or written
	[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	The student learns the basics of numerical determination of minima and saddle points in potential-energy surfaces and numerical methods of integrating equations of motion.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
	[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	The student applies the knowledge of quantum chemistry and mathematics in the analysis of the energy surfaces of molecules, the knowledge of chemistry, physics and mathematics in molecular modeling, and applications of the Boltzmann law to chemical systems.	[SU1] oral statement/conversation/ discussion [SU4] test/exam - oral or written

Subject contents	Description of molecular geometry. Cartesian and internal coordinates. Description of potential-energy hypersurface. Minima, maxima first-order saddle points and their physical meaning. Higher-order saddle points. Empirical force fields and their applications. Methods of local energy minimization. Normal modes of molecules. Molecular dynamics. Equations of motion and methods of their numerical solution. Monte Carlo methods. Statistical mechanics: Elements of probability theory, random-variable distributions, averages, fluctuations. Density of states. Microcanonical, canonical, grand canonical, isothermal-isobaric ensemble. Boltzmann law. Energy equipartition principle. Partition functions of ensembles, thier derivatives and their connection to thermodynamic quantities. Molecular interpretation of energy, entropy, thermodynamic potentials and chemical potentials and its connection with phenomenological interpretation. Entropy and information theory. The Bose-Einstein and Fermi-Dirac statistics. Partition functions of systems of non-interacting particles and two- and polyatomic molecules in the gas phase given the harmonic approximation. Calculation of equilibrium constants of chemical reactions in the has phase from first principles. Calculation of partition functions of non-ideal gases.
Prerequisites and co-requisites	Knowledge of basic arithmetic functions, basics of calculus, basics of linear algebra, ordinary differential equations, kinematics and dynamics of a point particle and a rigid body, harmonic motion, postulates of quantum mechanics, solution of Schroedinger equation (free particle in a box, rigid rotator, harmonic oscillator), atomic terms, applying thermodynamic functions (Gibbs diagram).

Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	partial exams before lectures	51.0%	10.0%
	exam	51.0%	90.0%

Recommended reading		
	Basic literature	N.A. Smirnowa: Metody termodynamiki statystycznej w chemii fizycznej.
	Supplementary literature	1. D. McQuarrie: Statistical Mechanics 2. K. Gumiński, P. Petelenz, Elementy chemii teoretycznej 3. R. Leach: Molecular Modeling: Principles and Applications 4. H. Buchowski, Elementy termodynamiki statystycznej 5. K. Huang, Mechanika statystyczna 6. F. Reif, Mechanika statystyczna 7. R.P. Feynman, Wykłady z mechaniki statystycznej
	eResources addresses	Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed	1. How many Cartesian and how many internal coordinates are needed to determine the aminobenzene (aninlin) geometry? Explain why the number of coordinates of either kind is different. 2. What ocntribution to the energy of the following systems occur in the force-field approximation (a) methane molecule (CH_4), (b) ethanol molecule. Justify the answers. 3. How many normal modes occur in the following molecules: H_2O, HCN, CH_4, C_3O_2 (carbon suboxide; O=C=C=O)? Justify the anwers. 4. Based on the Boltzmann law explain why raising temperature increases the solubiliy of most of the salts in water and why the solubility decreases with temperature for some salts (e.g., calcium acetate). We consider the following isotope-exchange reaction (D denotes deuterium, ^{2}H): CD_4 + HCl = CD_3H + DCl Which contributions to energy of this reaction (translational, rotational, vibrational, electronic) are non-zero? Which contribiution must be taken into account to compute its equilibrium constant? Justify the answers. It is assumed that high-temperature approximation (the Boltzmann statistics) applies.
Work placement	Not applicable

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