


KAPITAŁ LUDZKI
 NARODOWA STRATEGIA SPÓJNOŚCI

 Projekt współfinansowany przez
 Unię Europejską w ramach
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 Społecznego

UNIA EUROPEJSKA
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Course title		ECTS code	
Theoretical chemistry		13.3.0456	
Name of unit administrating study			
null			
Studies			
faculty	field of study	type	drugiego stopnia
Wydział Chemii	Chemia	form	stacjonarne
		specjalty	chemia biomedyczna, analityka i diagnostyka chemiczna, chemia i technologia środowiska, chemia obliczeniowa
		specialization	wszystkie
Teaching staff			
prof. dr hab. Józef Liwo; dr hab. Artur Giełdoń; mgr Krzysztof Bojarski; prof. dr hab. Cezary Czaplewski, profesor uczelni			
Forms of classes, the realization and number of hours		ECTS credits	
Forms of classes		6	
Auditorium classes, Lecture		classes 75 h	
The realization of activities		tutorial classes 10 h	
classroom instruction		student's own work 65 h	
Number of hours		TOTAL: 150 h - 6 ECTS	
Lecture: 30 hours, Auditorium classes: 45 hours			
The academic cycle			
2022/2023 winter semester			
Type of course		Language of instruction	
obligatory		polish	
Teaching methods		Form and method of assessment and basic criteria for evaluation or examination requirements	
- multimedia-based lecture		Final evaluation	
- problem solving		- Graded credit	
		- Examination	
		Assessment methods	
		- written exam with open questions	
		- (mid-term / end-term) test	
		- oral exam	
		The basic criteria for evaluation	
		Recitation classes: passing two partial exams („colloquia”) understood as achieving no less than 50% of the maximum score. The final score is the arithmetic mean of the partial-exam scores; it can be increased based on the activity during the classes.	
		Lecures: passing the final exam understood as achieving no less than 50% of the maximum score or between 40% and 50% maximum score and successful answering an additional round of exam questions. Students who achieved the „very good” (5.0) score in recitation classes are exempt from the exam with “very good” (5.0) score.	
Method of verifying required learning outcomes			
Required courses and introductory requirements			
A. Formal requirements			
Mathematics, Physics, Introductory Chemistry, Quantum Chemistry, Physical Chemistry.			
B. Prerequisites			
Knowledge of basic arithmetic functions, calculus, matrix algebra, ordinary differential equations, point-mass and rigid-body kinematic and dynamics, harmonic motion, postulates of quantum mechanics, solutions of Schrodinger equations for simple systems (particle in a box, rigid rotator, harmonic			

oscillator), atomic terms, handling thermodynamic functions (Gibbs diagram).	
Aims of education	
<ul style="list-style-type: none"> Familiarizing the students with the basics of molecular modeling. Conveying the knowledge of basic statistical mechanics to the students and teaching the students of the application of this knowledge in solving chemical problems. 	
Course contents	
<p>Description of molecule geometry. Cartesian and internal coordinates. Description of potential-energy surface. Minima, maxima, first-order saddle points and their physical meaning. Higher-order saddle points. Empirical force fields and their applications. Algorithms for 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 calculus, random-variable distributions, averages and fluctuations. Density of states. The microcanonical, canonical, grand-canonical, and isothermic-isobaric statistical ensembles. Boltzmann distribution law. Energy equipartition principle. Partition functions of statistical ensembles and their derivatives, and their connection to thermodynamic quantities. Molecular interpretation of energy, entropy, thermodynamic potentials, and chemical potentials and their connection to phenomenological interpretation. Entropy and information theory. Bose-Einstein and Fermi-Dirac statistics. Partition functions of non-interacting particles di- and polyatomic molecules. Calculation of thermodynamic corrections to the thermodynamic functions of chemical compounds in the gas phase in the harmonic approximation. Calculation of chemical-equilibrium constants in the gas phase from first principles. Calculation of the partition functions of non-ideal gases</p>	
Bibliography of literature	
<p>A. Literature required to pass the course</p> <p>A.1. used during the course: N. A. Smirnowa, Methods of Statistical Thermodynamics in Physical Chemistry. 2nd ed. Moscow, Visshaya shkola, 1982, 456p. (in Russian). Translated in Japan: Tokyo, Kenkutosoe, Kenkukai, 1989; in Poland: Warszawa. Państwowe Wydawnictwo Naukowe, 1980.</p> <p>A.2. for self-study: Gumiński K., Petelenz P. 1989. Elements of Theoretical Chemistry. Warsaw: Państwowe Wydawnictwo Naukowe, 1989. ISBN 83-01-08109-0; H. Buchowski, Elementary Statistical Thermodynamics, WNT, Warsaw 1998</p> <p>Extracurricular readings</p> <p>A.R. Leach: Molecular Modeling: Principles and Applications, Pearson Education EMA, 2001.</p> <p>K.Gumiński, Thermodynamics, PWN, Warszawa 1976.</p> <p>R.P. Feynman, Statistical Mechanics: A Set Of Lectures, CRC Press</p> <p>K. Huang, Statistical mechanics, Wiley</p> <p>F. Reif, Fundamentals of Statistical and Thermal Physics, Waveland Press Inc..</p> <p>D. McQuarrie, Statistical Mechanics, University Science Books, 2000.</p>	
The learning outcomes (for the field of study and specialization)	Knowledge
	Skills
	Social competence
	<p>The student describes the geometry of a molecule by using the Cartesian and internal coordinates, explains the term „potential energy hypersurface” and describes potential-energy hypersurface topology, defines the energy of a molecular system in the molecular-mechanics approximation, identifies basic terms of molecular dynamics, describes the Boltzmann distribution law, defines the partition function and describes its connection with thermodynamic functions, describes the Bose-Einstein and Fermi-Dirac statistics, explains the applications of statistical mechanics to calculating the thermodynamic functions of atomic and molecular gases and and to calculating equilibrium constants of chemical reactions in the gas phase.</p> <p>The student calculates internal coordinates from Cartesian coordinates and vice versa, calculates Energy minima and transition points on potential-energy hypersurface, calculates energy and forces acting on a system in the molecular-mechanics approximation, solves the equations of harmonic motion, calculates normal frequencies of the diatomic molecules and their force constants and moments of inertia from spectroscopic data, calculates thermodynamic quantities of atomic and molecular gases and calculates gas-phase-reaction equilibrium constants from the first principles.</p> <p>The student develops the ability of logical and precise thinking and inference and carrying out calculations accurately</p>
Contact	
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