University of Gdańsk

Subject card

Subject name and code	Theoretical chemistry, PG_00054402		
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	Katedra Chemii Teoretycznej -> 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	0.0	45.0	0.0	0.0	0.0	45
	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	45	8.0	22.0	75

Subject objectives	Acquring by the students abilities of calculation of geometric parameters of molecules, finding critical points in the potential energy surface, conducting simple molecular-mechanics calculations, calculating normal frequencies of molecules, determining the average energy, heat capacity, pressure and other physical quantities based on the Boltzmann law, calculating the thermodynamic functons of atomic gases and gases of resilient molecules, calculating the equilibrium constants of chemical reactions in the gas phase.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	The student calculates internal coordinates from Cartesian coordinates and vice versa, calculates energy minima and transition states in the potential-energy hypersurface of the molecule, calculates the energy and forces in the molecular mechanics approximation, solves the harmonic-motion equations, calculates characteristic frequencies of diatomic molecules and bond force constants and monents of inertia from spectroscopic data, calculates thermodynamic quantites of atomic and molecular gases, calculates equilibrium constants of gas-phase reactions from the first principles.	[SU1] oral statement/conversation/ discussion [SU4] test/exam - oral or written [SU8] observation of student's independent or team work
[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 realizes that performing calculations for molecular systems requires combination and connecting knowledge in organic, inorganic, physical, and quantum chemistry and ability to apply the linear algebra and calculus methodolgy at least at the basic level. The student indefifies the leaks in her/ his knowledge and knows how to complete and extend the knowlege.	[SK1] oral statement/conversation/ discussion [SK8] observation of student's independent or team work
[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student applies the methods of analyticla geometry, linear algebra and calculus applied in molecular modeling and statistical mechanics.	[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 correctly selects mathematical method(s) which should be applied in solving a particular problem of theoretical chemistry.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	The student gets to know the methods of analytical geometry, linear algebra and calculus applied in molecular modeling and statistical mechanics.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion

Subject contents

Description of molecular geometry. Cartesian and internal coordinates. Description of potential-energy hypersurfaces. Minima, maxima, saddle points. Higher-order saddle points. Empirical force fields and their applications. Normal modes of molecules. Statistical mechanics: averages and fluctuations. Density of states. Statistical ensembles: microcaninical, canonical, grand canonical, isothermal-isobaric. Boltzmann law. Energy equipartition principle. Parition functons, their derivatives and their connection to thermodynamic quantities. Molecular interpretation of energy,entropy, thermodynamic potentials, chemical potentials and its connection with phenomenological interpretation. Calculation of thermodynamic correction to the thermodynamic functions of chemical compounds from first principles in the harmonic approximation. Calculation of equilibrium constants of chemical reactions from first principles.

Prerequisites and co-requisites

Knowledge of basic arithmetic functions, calculus, linear algebra, ordinary differential equations, kinematics and dynamics of a point particle and rigid body, harmonic motion, postulates of quantum mechanics, solving the Schroedinger equation for simple systems (a free particle in a box, rigid rotator, harmonic oscillator), atomic terms, application of thermodynamic functions (the Gibbs diagram).

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
partial tests, every week (10)	51.0%	20.0%
activity during recitation classes	51.0%	5.0%
extended partial tests (kolokwia) (2)	51.0%	75.0%

Recommended reading

Basic literature	N. A. Smirnowa, Elementy termodynamiki statystycznej w chemii fizycznej, PWN.

	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. The potential energy of the biphenyl (Ph-Ph) molecule as a function of the C-C bond length (d) expressed in angstroms and the dihedral angle for the rotation about this bond () can approximately be expressed by the following equation: $E(d,t) = 317(d - 1{,}45)^2 + 1{,}5[1 - \cos(2t)]$ Find the critical points in this energy surface and determine their characters treating d and as variables. The angle is in the [-180°,180°] interval. 2. Calculate the force acting on each atom of the bromine molecule and determine the direction of these forces with respect to the H-Br bond axis given the Br-Br bond length of 2,33 Å. The equilibrium Br-Br bond length is d^o = 2,28 Å and the wavenumber of thei $^{79}Br_2$ molecule is 322 cm^{-1}. 3. As a result of chlorobenzene nitration at t=101°C equal amounts of p-nitrochlorobenzena (p) and o-nitrochlorobenzene (o) were obtained. No other reaction products were detected. Assuming thermodynamic control of the reaction, calculate the energy difference between the ortho and para isomer ($e = e_o\ e_p$) and derive the formula for the dependence of the amount of the ortho form on temperature. 4. Determine the contributions to the heat capacity of 1 mol of atomic gold (Au) in the gas phase, derive the formulas for these contributions as functions of temperatures (if they are dependent on temperature) and calculate their values at t t=2927°C (above the boiling point of this metal). The degeneracy of the ground state is w_0=2 (the $^2S_{1/2}$ term) and the degeneracy and energy of the first excited state are w_1=6, e_1=109,6 kJ/mol (the $^2D_{5/2}$ term) respectively. The energies of higher excited states are too high for those states to contribute remarkably to the electronic partition function. 5. Given the reaction of the formation of 1 mol of gaseous chlorine bromide from 1/2 mol of chlorine molecules and 1/2 mol of bromine molecules in the gas phase: $1/2\ ^{79}Br_2 + 1/2\ ^{35}Cl_2 = {}^{79}Br^{35}Cl$ Derive the expression for the change of the translational, rotational, vibrational, and electronic energy resulting from this reaction.	
Work placement	Not applicable	

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