Subject card

Subject name and code	Specialization lecture: Statistical mechanics in chemistry, PG_00117810					
Field of study	Chemistry					
Date of commencement of studies	October 2025		Academic year of realisation of subject		2025/2026	
Education level	Master'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	1		Language of instruction		English	
Semester of study	2		ECTS credits		3.0	
Learning profile	academic		Assessment form		credit	
Conducting unit	Faculty of Chemistry -> Rector					
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 basics of statistical mechanics and its application in chemistry.

Learning outcomes			
	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.	The student applies methods of statistical mechanics to solve chemical problems.	[SK5] implementation of a problem task
	[CHEMMU2_U11] Communicates in English in accordance with the requirements specified for level B2 of the Common European Framework of Reference for Languages.	The student acquires the English-language terminology of statistical mechanics.	[SU5] implementation of a problem task
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	The student learns applications of statistical mechanics to describing chemical systems and phenomena at the upper-intermediate level and applies the methods of calculus and linear algebra.	[SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	The student applies methods of statistical mechanics to solve chemical problems.	[SU5] implementation of a problem task
	[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student applies appropriate methods of calculus and linear algebra.	[SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
	[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 Chemistry, Physics, and Mathematics and learns the ways of extending the understanding of chemical phenomena on atomistic baiss.	[SK1] oral statement/conversation/ discussion [SK5] implementation of a problem task

Subject contents	Geometry and energy surfaces of molecules, probability, random variables, averages, fluctuations. Density of states. Ensembles. Boltzmanns law. Energy equipartition. Partition function and its relation with system properties. Energy, entropy, free energy and their molecular interpretation. Entropy and information theory. Simple applications of statistical mechanics: blackbody, crystals. Multi-particle systems: the Bose-Einstein and Fermi-Dirac statistics Partition functions of gases of non-interaction atoms, diatomic, and polyatomic molecules. Calculation of thermodynamics properties of gaseous substances. Calculations of equilibrium constants of chemical reactions in the gas phase. Non-ideal gases: the Mayer diagrams. Liquids: radial distribution functions and potentials of mean force. Statistical-mechanical theory of coarse graining. Statistical mechanics and molecular simulations.
Prerequisites and co-requisites	Quatum Mechanics, Physical Chemistry, Linear Algebra, Calculus.

Assessment methods and criteria			
	Subject passing criteria	Passing threshold	Percentage of the final grade
	Assignment of problem sets	51.0%	100.0%

Recommended reading		
	Basic literature	1. D. McQuarrie: Statistical Mechanics 2. R. Leach: Molecular Modeling: Principles and Applications
	Supplementary literature	1. K. Huang, Statistical Mechanics 2. F. Reif, Statistical Mechanics 3. R.P. Feynman, Lecutres in Statisticlal Mechanics
	eResources addresses	

Example issues/ example questions/ tasks being completed	1. There are two apples and two oranges in a box. Somebody took a fruit from that box at random. What is the probability that we get an orange when taking another fruit at random? 2. To what temperature would gaseous oxygen in the ground triplet state (^{3} $_{g}$, degenercy 3) have to be heated to get 0.1 % of it excited to the singlet (1g, degenercy 1) state? Singlet oxygen has energy by 21 kcal/mol higher than triplet oxygen 3. The partition coefficient of terminally-blocked L-methionine (Ac-L-Met-NHMe) between n-octanol (n-oct) and water (wat) at t = 25 C is equal to P = x_{noct}/x_{wat} = 0.25, where x_{noct} and x_{wat} denote the molar fractions of L-methionine in the n-octanol and water phase, respectively (data from Fauch`ere and Pliska, Eur. J. Med. Chem., 18, 369-375, 1983). Determine the difference of the chemical potentials of L-methionine in the two phases ($_{noct}$ $_{wat}$) at t = 25 C. 4. Demonstrate that the grand partition function of a system of non- interacting fermions with two energy levels with energies e1 and e2 can be epxressed as = [1 + exp (e $_{1}$)] [1 + exp (e $_{2}$)] 5. Calculate the mole fractions of lithium (Li) atoms in the first and in the second excited state at its boiling temperature (t = 1330 C). The degeneracy of the ground electronic state (term $^{2}S_{1/2}$) is = 2, while the degeneracies and the excitation energies of the first and the second excited states (terms $^{2}P_{1/2}$ and $^{2}P_{3/2}$, respectively), are $_{1}$ = 2, $_{1}$ = 1.85 eV and $_{2}$ = 4, $_{2}$ = 1.85 eV, respectively.
Work placement	Not applicable

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