KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI
Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego
UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title

Specialization lecture: Statistical mechanics in chemistry

ECTS code

13.3.1296

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	drugiego stopnia
		form	stacjonarne
		specialty	Digital Chemistry
		specialization	wszystkie

Teaching staff

prof. dr hab. Józef Liwo; dr hab. Artur Giełdoń

Forms of classes, the realization and number of hours

Forms of classes

Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours

ECTS credits

3
classes – 30 h
tutorial classes – 20 h
student's own work – 25 h
TOTAL: 75 h – 3 ECTS

The academic cycle

2023/2024 summer semester

Type of course

obligatory

Language of instruction

English

Teaching methods

multimedia-based lecture

Form and method of assessment and basic criteria for eveluation or examination requirements

Final evaluation

Graded credit

Assessment methods

A set of written tests

The basic criteria for evaluation

according to "Rules and regulations for studies at the University of Gdansk"

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements

Math (including Calculus), Quantum Chemistry, Physics

B. Prerequisites

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Aims of education

Understanding the connection between the microscopic and macroscopic (ensemble-based) properties of the system studied, in particular acquiring the ability of computing its macroscopic properties from molecular properties and from molecular simulations.

Course contents

Probability, random variables, averages, fluctuations. Density of states. Ensembles. Boltzmann's 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 function of ideal atomic, diatomic, and polyatomic gases. 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.

Bibliography of literature

Literature required to pass the course

D. McQuarrie, Statistical Mechanics, University Science Books, 2000

Extracurricular readings

R.P. Feynman. Lectures in Statistical Mechanics.

The learning outcomes (for the field of study and specialization)

K_W05: has extended knowledge in the field of the specialisation studied

K_W06: applies mathematics to the extent necessary to understand, describe and model chemical processes of extended complexity.

K_U02: critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors

K_U11: communicates in a foreign language in accordance with the requirements specified for level B2 of the Common European Framework of Reference for Languages and can use specialist terminology

K_K01: knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so

K_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

Knowledge

The student correctly identifies the ensembles, knows and understands Boltzmann's law, defines the Bose-Einstein and Fermi-Dirac statistics, defines the partition functions of given systems and its derivatives.

Skills

The student applies the apparatus of statistical mechanics in solving chemical problems such as computing the properties of gaseous substances and computing the equilibrium constants of chemical reactions in the gas phase. The student applies statistical mechanics to process the results of molecular simulations.

Social competence

The student develops the skills of accurate and logical thinking and inference. Applies the formalism of statistical mechanics to solve chemical problems.

Contact

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