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

Course title

Theoretical chemistry

ECTS code

13.3.0456

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	drugiego stopnia
		form	stacjonarne
		specialty	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; prof. dr hab. Cezary Czaplewski, profesor uczelni; mgr Krzysztof Bojarski

Forms of classes, the realization and number of hours

Forms of classes

Auditorium classes, Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours, Auditorium classes: 45 hours

ECTS credits

6

classes 75 h

tutorial classes 10 h

student’s own work 65 h

TOTAL: 150 h - 6 ECTS

The academic cycle

2022/2023 winter semester

Type of course

obligatory

Language of instruction

polish

Teaching methods

- multimedia-based lecture
- problem solving

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

Final evaluation

- 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 Schroedinger equations for simple systems (particle in a box, rigid rotator, harmonic oscillator), atomic terms, handling thermodynamic functions (Gibbs diagram).

Aims of education

• Familiarizing the students with the basics of molecular modeling.
• Conveying the knowledge of basic statistical mechanmics to the students and teaching the students of the application of this knowledge in solving chemical problems.

Course contents

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 mechanic: Elements of probability calculus, random-variable distributions, averages and fluctuations. Density of states. The microcanonical, canonical, grand-canonical, and isothermic-isobaric statisrical ensembles. Boltzmann distribution law. Energy equipartition principle. Partition functions of statistical ensembles and their derivatives, and their connection to thermodynamic quantities. Molecular intepretation 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-equlibrium constants in the gas phase from first principles. Calculation of the partition functions of non-ideal gases

Bibliography of literature

A. Literature required to pass the course
A.1. used duiring the coarse: 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. Panstwowe Wydawnictwo Naukowe,1980.
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

Extracurricular readings
A.R. Leach: Molecular Modeling: Principles and Applications, Pearson Education EMA, 2001.
K.Gumiński, Thermodynamics, PWN, Warszawa 1976.
R.P. Feynman, Statistical Mechanics: A Set Of Lectures, CRC Press
K. Huang, Statistical mechanics, Wiley
F. Reif, Fundamentals of Statistical and Thermal Physics, Waveland Press Inc..
D. McQuarrie, Statistical Mechanics, University Science Books, 2000.

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

Knowledge

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.

Skills

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 spectroscopipc data, calculates thermodynamic quantities of atomic and molecular gases and calculates gas-phase-reaction equilibrium constants from the first principles.

Social competence

The student develops the ability of logical and precise thinking and inference and carrying out calculations accurately

Contact

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