UNIWERSYTET GDAŃSKI

Course title	ECTS code
Chemia teoretyczna/Theoretical chemistry	13.3.0456

Name of unit administrating study
Faculty of Chemistry

Studies

Field of study	Type	Form	
Chemistry	Master	Full-time studies	

Teaching staff
Prof. dr hab. Adam Liwo

Forms of classes, the realization and number of hours

A. **Forms of classes, in accordance with the UG Rector's regulations**
lecture, audytorium classes

B. **The realization of activities**
In-class learning

C. **Number of hours**
lecture 30 h, audytorium classes 45 h

ECTS credits 6

classes 75 h
tutorial classes 10 h
student's own work 65 h
TOTAL: 150 h - 6 ECTS

The academic cycle
2019/2020 winter semester

Type of course
obligatory

Language of instruction
Polish

VeTeaching methods

Lectures including multimodal presentation

Case studies

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

A. Final evaluation, in accordance with the UG study regulations
Course completion (with a grade), exam

B. Assessment methods
Determining the final scores based on partial scores achieved during the semester and partial exams ("colloquia").

C. The basic criteria for evaluation or exam requirements

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.

Required courses and introductory requirements
Mathematics, Physics, Introductory Chemistry, Quantum Chemistry, Physical Chemistry.
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

B. 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.

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.

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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.