GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

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| Subject name and code | Physical Chemistry , PG_00054877 | | |
| Field of study | Biotechnology | | |
| Date of commencement of studies | October 2023 | Academic year of realisation of subject | 2024/2025 |
| Education level | first-cycle studies | Subject group | Obligatory subject group in the field of study<br>Subject group related to scientific research in the field of study |
| Mode of study | Full-time studies | Mode of delivery | at the university |
| Year of study | 2 | Language of instruction | Polish |
| Semester of study | 3 | ECTS credits | 6.0 |
| Learning profile | general academic profile | Assessment form | exam |
| Conducting unit | Department of Physical Chemistry -> Faculty of Chemistry | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | prof. dr hab. inż. Jacek Czub | |
| | Teachers | prof. dr hab. inż. Jacek Czub | |

**Lesson types and methods of instruction**

| Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
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| Number of study hours | 45.0 | 15.0 | 0.0 | 0.0 | 15.0 | 75 |
| 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 |
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| Number of study hours | 75 | 8.0 | 67.0 | 150 |

**Subject objectives**

The aim of the course is to learn the physical laws governing (bio)chemical processes and to provide theoretical tools for describing and predicting these processes.

**Learning outcomes**

| Course outcome | Subject outcome | Method of verification |
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| K6_U02 | The student learns to apply the acquired theoretical knowledge of thermodynamics and chemical kinetics to the solution of practical tasks of a problematic nature. The student learns to create schemes for solving problems of varying degrees of difficulty. The student learns to solve computational tasks in the field of thermodynamics and kinetics of (bio)chemical systems. | [SU2] Assessment of ability to analyse information<br>[SU4] Assessment of ability to use methods and tools<br>[SU5] Assessment of ability to present the results of task<br>[SU1] Assessment of task fulfilment |
| K6_W02 | The student learns the laws of thermodynamics and kinetics governing the course of (bio)chemical reactions and processes and also the phase behavior of biological systems. The student learns to interpret the thermodynamic and kinetic properties of biomolecular systems in the context of intermolecular interactions. The student acquires theoretical knowledge of the most important experimental techniques used in molecular biotechnology. The student learns to communicate newly acquired knowledge and present the results of his/her work in an understandable and communicative manner | [SW3] Assessment of knowledge contained in written work and projects<br>[SW1] Assessment of factual knowledge |

| Subject contents | Lecture<br><br>• Fundamentals of chemical thermodynamics: characteristics of ideal gas; equipartition theorem; internal energy, work and heat; temperature and heat capacity; first law of thermodynamics, the Joule and Joule-Thompson experiments, enthalpy; thermochemistry: standard enthalpy of reaction, Hess and Kirchhoff laws; second law of thermodynamics; entropy and elements of statistical thermodynamics; Carnot cycle and the performance of heat engines; Boltzmann distribution; Gibbs and Helmholtz free energy; how to determine spontaneity; spontaneous (irreversible), non-spontaneous and reversible processes; fundamental equations of thermodynamics; third law of thermodynamics; standard entropy of reaction; chemical potential, Gibbs-Duhem equation; interpretation of thermodynamic parameters of reactions and processes from the intermolecular interactions viewpoint<br><br>• Phase equilibria: one-component systems, Clausius-Clapeyron equation, phase diagrams; thermodynamics mixing; ideal and real solutions, Raoult's and Henry's laws; activities, standard states, including biological standard state; colligative and osmotic properties of solutions; Gibbs phase rule; liquid-vapor and liquid-liquid equilibria for two-component systems, physicochemical foundations of distillation and rectification; thermodynamics of protein folding; ternary systems and the Gibbs triangle; phase equilibria within phospholipid membranes; partition coefficient, logP and extraction.<br><br>• Chemical equilibrium: Gibbs energy of reaction and equilibrium constant; elements of bioenergetics: ways of accumulating Gibbs energy in the cell, ATP and ion gradients, three types of cellular work; ways of driving non-spontaneous processes; effect of pressure and temperature on equilibrium<br><br>• Introductory electrochemistry: ionic conductivity; electrochemical cells: electrodes, types of half-cells, cell voltage and cell thermodynamics, Nernst equation, examples of cells, lithium-ion batteries; standard reduction potentials and their application: prediction of spontaneous direction of redox reactions, electron transport chain in respiration and photosynthesis, potentiometry<br><br>• Chemical kinetics: rate of reactions and processes, and how to measure it; rate equations and methods for determining the order of reactions and rate constants; integration of simple rate equations; elementary and complex (composite) reactions; reactions close to equilibrium and the relationship between kinetics and thermodynamics; dependenc of the rate on temperature; Gibbs energy profiles for reactions and processes; thermodynamic and kinetic control of reactions; basics of enzymatic catalysis, Michaelis-Menten model; chain reactions<br><br>• Transport phenomena: Brownian motion and diffusion; modes of transport across biological membranes; diffusion as discrete random walk; diffusion equation and its solutions; Einstein-Smoluchowski relation; Stokes equation; dynamic viscosity; ionic solvation, Grotthuss mechanism; diffusion in external potential and Smoluchowski's equation; rate theories for conformational changes and chemical reactions; theoretical description of electrophoresis<br><br>Practicals<br><br>• Thermodynamics and thermochemistry: the ideal gas equation; first law of thermodynamics; thermodynamic cycles; thermochemistry: Hess and Kirchhoff laws, the second law of thermodynamics; absolute entropy; Gibbs and Helmholtz free energy<br>• Phase equilibria: phase transitions in a one-component system; the Clausius-Clapeyron equation; liquid-vapor equilibrium in a two-component system<br>• Chemical equilibrium: reaction equilibrium constant; relationship between the equilibrium constant ant the standard Gibbs energy of reaction; van't Hoff's isotherm; dependence of reaction equilibrium constant on temperature, van Hoff's isobar.<br>• Kinetics of chemical reactions: determination of the order of the reaction, rate constant, activation energy, reaction half-lifes<br><br>Seminar<br><br>• Familiarizing students with good practices in scientific presentation.<br>• Discussion of elementary aspects of molecular interactions theory.<br>• Interpretation of models that introduce empirical corrections to fundamental physical chemical theories.<br>• Simple statistical and information-theoretic intepretation of entropy.<br>• Review of applications of modern spectro- and microscopic methods for the analysis of physicochemical properties of biological materials.<br>• Discussion of calorimetry methods that enable measurement of thermodynamics of processes involving biomacromolecules and their complexes.<br>• Description of physicochemical fundamentals of modern methods of structural biology.<br>• Physicochemical characterization of biological membrane systems.<br>• Applications of basic thermodynamic and kinetic models to solve complex research problems, including an analysis of metabolic processes. |
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<tr><td>Prerequisites and co-requisites</td><td>General chemistry: knowledge of basic concepts.<br><br>Mathematics: elements of differential and integral calculus, elements of probability theory<br><br>Physics: basic physical quantities, basic mechanics and electrostatics.</td></tr>
<tr><td>Assessment methods and criteria</td><td>
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<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Mid-term test (2, practicals)</td><td>50.0%</td><td>20.0%</td></tr>
<tr><td>Presentation of the solved problem (seminar)</td><td>50.0%</td><td>10.0%</td></tr>
<tr><td>Final written exam</td><td>50.0%</td><td>60.0%</td></tr>
<tr><td>Presentation on a given topic (seminar)</td><td>50.0%</td><td>10.0%</td></tr>
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<tr><td rowspan="3">Recommended reading</td><td>Basic literature<br>1. P. W. Atkins, J. De Paula. "Physical chemistry", PWN<br>2. I. N. Levine. "Physical Chemistry", McGraw-Hill<br>3. Uruska I. (redakcja), Zbiór zadań z chemii fizycznej, Wydawnictwo PG<br>4. Uruska I., Zbiór zadań testowych z chemii fizycznej, Wydawnictwo PG<br>5. Internet resources: wikipedia, lecture notes, etc.</td></tr>
<tr><td>Supplementary literature<br>1. G. Barrow. "Physical chemistry", PWN<br>2. D. W. Ball. "Physical Chemistry", Thompson / Brooks-Cole<br>3. K. Pigoń, Z. Ruziewicz, "Physical chemistry", PWN,<br>4. D. M. Zuckerman "Statistical physics of biomolecules", CRC Press</td></tr>
<tr><td>eResources addresses<br>Adresy na platformie eNauczanie:</td></tr>
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| Example issues/ example questions/ tasks being completed | (a) sample presentation topics<br><br>1. The van der Waals equation (gas compression isotherms, physical interpretation of coefficients in the vdW equation, phase transition curves predicted by this equation, Maxwell construction: a sample ad hoc solution<br>2. FRET (Forster resonance, efficiency of energy transfer vs chromophore distance and orientation, confocal microscopy, sample applications - conformational transitions in the ATP synthase or transcription initiation by DNAPol, smFRET)<br>3. Atomic force microscopy (working principle, anchoring biomacromolecules to the tip/surface, applications: protein unfolding, mechanical mapping)<br><br>(b) sample projects<br><br>1. Membrane proteins are crucial in the cell's response to the environment, e.g., through modulation of ion permissivity. Here, we will see how the amino acid sequence affects the protein's interaction with the bilayer.<br>2. By analyzing the effect of single amino acid mutations, we can gain indirect insight into the mechanisms of protein folding. In this case, we will investigate the impact of a single key residue on the folding and unfolding kinetics of an extremely stable protein.<br><br>Selected exam questions:<br><br>1. Substrate A can be converted to two products B and C. The standard Gibbs energy and Gibbs energy of activation for product B are -50 and 80 kJ/mol, respectively, and for product C, -15 and 20 kJ/mol, respectively. Which product will dominate when the reaction is carried out at a low temperature, and which when at a high temperature allowing for reaching equilibrium? Why? How can the concentration ratio of both products be determined at low temperatures?2. It is known that stretching a rubber band involves conformational ordering of polymer molecules in the rubber; the resulting entropy decrease accounts for the main force opposing the deformation. Is the force exerted by the rubber band greater or smaller after heating? Why?3. The folding process of a certain protein was studied in a calorimeter with a heat capacity of 0.4 kJ K. It was found that at 330 K, unfolding of 0.01 mole of this protein is accompanied by a 1 K decrease in calorimeter temperature. Knowing that the entropy change upon folding of this protein is -0.1 kJ/(mol K), determine which form of the protein, folded or unfolded, dominates in the cell in equilibrium (T = 300 K). Assume that for the folding process Cp = 0. How can the molar fractions of the folded and unfolded forms be determined from these data (do not calculate the final values, just indicate the formula and plug in the data)? |
| Work placement | Not applicable |