



## COURSE DESCRIPTION CARD - SYLLABUS

Course name

Computational exercises in physical chemistry [S1TOZ1>ĆOzCF]

### Course

Field of study

Circular System Technologies

Year/Semester

2/4

Area of study (specialization)

–

Profile of study

general academic

Level of study

first-cycle

Course offered in

Polish

Form of study

full-time

Requirements

compulsory

### Number of hours

Lecture

0

Laboratory classes

0

Other

0

Tutorials

15

Projects/seminars

0

### Number of credit points

1,00

### Coordinators

dr hab. inż. Agnieszka Świdorska-Mocek  
agnieszka.swiderska-mocek@put.poznan.pl

### Lecturers

### Prerequisites

Students: have knowledge in general chemistry (writing chemical reactions, converting concentrations, knowledge of laboratory glassware and basic laboratory equipment). have knowledge in mathematics and physics enabling the introduction of problems in physical chemistry (basic laws of physics, differential calculus). are able to prepare solutions of specific concentrations. are aware of further development of their competences.

### Course objective

To familiarise students with basic problems in physical chemistry and electrochemistry at the academic level in the field of: chemical kinetics, simple and complex reactions, surface phenomena, homo- and heterogeneous catalysis and electrolysis, type of half-cells and type of cells.

### Course-related learning outcomes

Knowledge:

students will be able to characterise, list and identify simple and complex reactions, define homo- and heterogeneous catalysis, define the causes of corrosion, define the causes of surface phenomena.

k\_w02, k\_w04

students will be able to define and explain the basic principles, theories in the field of chemical kinetics, such as: rate of chemical reaction, order and molecularity, half-life, activation energy, collision and activated-complex theory. k\_w02, k\_w04

students will be able to define and explain the basic principles, theories in the field of electrochemistry, such as: types of half-cells, types of cells, the concept of electrolysis or corrosion. k\_w02, k\_w04

#### Skills:

students will be able to obtain information from literature, databases and other sources; interpret it as well as draw conclusions and formulate and substantiate opinions. k\_u01

students will be able to work individually and as part of a team; estimate the time needed to complete the assigned task. k\_u08

students will have the self-study skills in the subject. k\_u04

students will be able to elaborate, describe and present results of an experiment or theoretical calculations. k\_u03

#### Social competences:

students will understand the need for further training and developing their professional competences.

k\_k05

students will be able to properly prioritise the task. k\_k03

### Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

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Exercises: grade on the basis of points obtained for activity during classes, writing test. Passing exercises above 50% . If the classes will be held remotely, the forms of course assessments will remain unchanged and will be carried out with the use of tools provided by the Poznań University of Technology (the e-courses platform).

### Programme content

Chemical kinetics, simple and complex reactions, surface phenomena, homo- and heterogeneous catalysis and electrolysis, half-cells, cells.

### Course topics

Physicochemical calculations in the field of:

Mathematical description of the rate of chemical reactions. Determination of rates, constant rates of simple chemical reactions. Calculation of the order of chemical reactions based on experimental data.

Methods for determining orders of chemical reactions. Complex reaction kinetics. Dependence of the reaction rate constant on temperature - calculation of the reaction activation energy from the Arrhenius equation. Eyring equation - determining the enthalpy and entropy of activation of the active complex.

Calculations regarding the electrical properties of electrolyte solutions: transfer numbers, conductivity, ion mobility. Electrolysis, Faraday's laws, electrochemical calculations. Electrode potentials, determination of standard half-cell potentials - Nernst's equation. Construction of galvanic cells, calculation of electromotive forces. The equation of the process is the source of electrical work.

Determination of the standard SEM. Calculation of standard thermodynamic functions of a chemical reaction based on SEM measurement of cells.

### Teaching methods

Exercises with discussion. Deductive method. The exercises involve solving partial tasks and solving detailed problems.

### Bibliography

Basic

1. K. Pigoń, Z. Ruziewicz, *Chemia Fizyczna*, PWN Warszawa 2007
2. P. Atkins, *Chemia Fizyczna*, PWN, Warszawa 2016
3. A. Molski, *Wprowadzenie do kinetyki chemicznej* WNT warszawa 2000
4. L. Sobczyk , *Eksperymentalna Chemia Fizyczna*, PWN Warszawa 1982

5. A. Kiswa, Elektrochemia I Jonika, WTN Warszawa 2000
6. A. Kiswa, Elektrochemia I Elektrodyka, WTN Warszawa 2001

Additional

1. P. Atkins, Podstawy Chemii Fizycznej, PWN, Warszawa 2009
2. L. Sobczyk, A. Kiswa, Chemia fizyczna dla przyrodników PWN Warszawa 1982
3. J. Minczewski, Chemia analityczna, PWN Warszawa 2005
4. H. Buchnowski, W. Ufnalski, Wykłady z chemii fizycznej WNT Warszawa 1998
6. Instrukcje do ćwiczeń laboratoryjnych z chemii fizycznej

### Breakdown of average student's workload

|   | Hours | ECTS |
|---|-------|------|
| Total workload  | 25    | 1,00 |
| Classes requiring direct contact with the teacher   | 16    | 0,50 |
| Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation) | 9     | 0,50 |