Universitat Autònoma de Barcelona

2023/2024

Thermodynamics, Kinetics and Phase Transformations

Code: 103285
ECTS Credits: 6

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OB	2	2

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Teachers

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Prerequisites

This subject requires prior knowledge of basic thermodynamics concepts given in the 1st year.

Objectives and Contextualisation

Regarding knowledge:

Students should acquire the knowledge required for the understanding of physical-chemical processes, from both thermodynamic and kinetic points of view.

Regarding skills and abilities:

- Apply the knowledge to problem solving, through the analysis and critical scrutinizing of the procedures used and the results obtained in the resolution of the problems.

- Prepare good quality reports on laboratory practices.

Regarding attitudes, values and rules:

- Be able to analyze and sum up the theoretical framework of the subject. This means students should be able to interpret and understand the issues involved and to reach a reliable result when facing a thermodynamics-based problem.

- Work in the laboratory in an organized and clean manner.

- Take care of the laboratory equipment, apparatus and instruments.

Competences

- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Apply the general standards for safety and operations in a laboratory and the specific regulations for the use of chemical and biological instruments, products and materials in consideration of their properties and the risks.
- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.
- Handle the standard instruments and materials of physical, chemical and biological testing laboratories for the study and analysis of phenomena on a nanoscale.
- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Recognise the terms used in the fields of physics, chemistry, biology, nanoscience and nanotechnology in the English language and use English effectively in writing and orally in all areas of work.
- Resolve problems and make decisions.
- Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Learning Outcomes

1. Analyse and resolve problems in the field of chemical kinetics.
2. Analyse and resolve problems of a thermodynamic nature.
3. Analyse and resolve thermodynamic and kinetic problems in molecules and solids.
4. Analyse situations and problems in the field of physics and propose answers or studies of an experimental nature using bibliographic sources.
5. Apply equations of state and determine the thermal properties of matter.
6. Apply the acquired theoretical contents to the explanation of experimental phenomena.
7. Be ethically committed.
8. Calculate the performance of a thermal machine and the efficiency of a cooling one.
9. Communicate orally and in writing in one's own language.
10. Correctly use computer tools to calculate, graphically represent and interpret the data obtained, as well as its quality.
11. Critically evaluate experimental results and deduce their meaning.
12. Describe and apply Maxwell-Boltzmann's statistic.
13. Describe the thermodynamics of equilibrium between phases.
14. Determine the kinetics of a phase transformation in accordance with the mechanisms that produce it.
15. Draw phase diagrams and predict the formation of new phases using equilibrium phase diagrams.
16. Employ information and communication technology in the documentation of cases and problems.

17. Enumerate the principles of thermodynamics and their consequences.
18. Explain the concepts of heat, work and temperature.
19. Explain transformations between phases using nanoscale concepts.
20. Identify and situate safety equipment in the laboratory.
21. Identify the phenomena of transport.
22. Learn autonomously.
23. Make adequate use of laboratory materials and instruments.
24. Manage the organisation and planning of tasks.
25. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
26. Perform bibliographic searches for scientific documents.
27. Perform calculations associated to the phenomena of transport involved in a change of phase.
28. Propose creative ideas and solutions.
29. Reason in a critical manner
30. Recognise in physical and chemical processes the phenomena of energy exchange and the laws that govern them.
31. Recognise one and two component phase diagrams.
32. Recognise the direct relationship between thermodynamic formalism and experiments.
33. Recognise the microscopic description of a system and the principles of statistical mechanics.
34. Recognise the terms for processes and devices for the generation, storage and transport of energy, as well as the applications and impact of nanomaterials on the environment.
35. Resolve problems and make decisions.
36. Resolve problems relative to the phenomena of transport
37. Resolve problems with the help of the provided complementary bibliography.
38. Safely handle laboratory materials and instruments.
39. Use data processors to produce reports.
40. Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Content

CLASSICAL THERMODYNAMICS

2nd and 3rd principles of thermodynamics

Spontaneity and equilibrium. Gibbs free energy

THERMODYNAMICS OF PHASE EQUILIBRIA

System stability and stability conditions

Equilibirum of phases in pure substances

Phase equilibria in multicomponent systems

TRANSPORT PHENOMENA

Kinetic theory of gases. Flow. Effusion. Thermal conductivity. viscosity

Transport in solution: diffusion, migration and convection. Laws of Fick, Ohm and Kohlraush. Principles of hydrodynamics

HOMOGENEOUS CHEMICAL KINETICS

Reaction rate. Rate equation. Order and molecularity. Integration of equations of integer order. Effect of temperature

Complex reactions. Reaction mechanism. Opposite, parallel and consecutive reactions. Approximate methods.

Homogeneous catalysis. Acid-base. Red-ox. Enzymatic

Methodology

This subject aims to furnish knowledge through lectures and problem solving sessions. Likewise, self-learning activities are also considered, wherein students prepare reports of laboratory practices and delivers exercises requested throughout the course.

The proposed teaching methodology and assessment may undergo some modification depending on the attendance restrictions imposed by the health authorities.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
In-class exercises	15	0.6	3, 2, 1, 5, 14, 15, 27
Laboratory practices	8	0.32	6, 22, 24, 20, 35, 40, 23
Lectures	30	1.2	5, 13, 15, 17, 18, 21, 31, 32
Type: Supervised			
Mentoring	5	0.2	9, 7
Type: Autonomous			
Problem solving	15	0.6	3, 2, 1, 5, 14, 15, 29, 27, 35
Self-study	30	1.2	5, 13, 14, 15, 17, 18, 21, 27, 31, 32
Writing lab practices reports	8	0.32	4, 6, 22, 11, 9, 7, 29, 39

Assessment

The evaluation of the subject comprises two parts:

(PART 1) FUNDAMENTALS OF CLASSICAL THERMODYNAMICS AND THERMODYNAMICS OF PHASE EQUILIBRIA
- Midterm exam (40% of the mark).
- In-class tests / Moodle questionaries (5% of the mark).
- Lab practices reports (5% of the mark).

(PART 2) TRANSPORT PHENOMENA AND HOMOGENEOUS CHEMICAL KINETICS
- Midterm exam (40% of the mark).
- In-class tests / Moodle questionaries (5% of the score).
- Lab practices reports (5% of the grade).

The weight of parts (1) and (2) on the overall scoring is the same (50%).

The realization of the "In-class tests" in part (1) and the laboratory practices (as well as the delivery of the corresponding reports) in parts (1) and (2) is mandatory, otherwise the student will not have the right to take the midterm exams.

Each midterm exam should be scored with a minimum of 4.0/10 for further averaging and, where appropriate, pass the subject. Otherwise, the student will have to take the final (reassessment) exam of the failed part(s). In this case, it will be necessary to have 4.0/10 in both reassessment exams for averaging and to reach at least 5.0 in the overall score. To be reassessed, the student must previously have submitted a minimum of two-thirds of the course-assessment items.

The reassessment exams can be used to improve the score. Attendance at this exam will mean that the student renounces the grade of the exams obtained previously, and it may be the case that the final grade obtained is lower.

Single evaluation:

The assessment of the subject consists of two parts:

(1) BLOCKS CLASSICAL THERMODYNAMICS AND PHASE EQUILIBRIUM THERMODYNAMICS

- Partial exam (45% of the mark).
- Laboratory practice reports (5% of the mark).

(2) BLOCKS TRANSPORT PHENOMENA AND HOMOGENEOUS CHEMICAL KINETICS

- Partial exam (45% of the mark).
- Laboratory practice reports (5% of the mark).

Students who have chosen the single evaluation modality will have to take a final test that will consist of an exam covering the entire theoretical content and problem-solving of the subject. This test will be held on the same day that students in the continuous assessment take the second partial exam. The student's grade will be calculated as follows:

Subject grade = (Final exam mark * 90 + Practices mark * 10)/100

If the final grade does not reach 5, the student has another opportunity to pass the subject through the resit exam, which will be held on the same day as the resit of the continuous assessment. In this exam, it will be possible to recover 90% of the grade corresponding to the theoretical part. The practice part is not recoverable.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Experimental laboratory	10%	17	0.68	6, 22, 11, 9, 16, 26, 24, 20, 38, 7, 25, 28, 29, 34, 32, 35, 40, 10, 23, 39
Problem solving	10%	10	0.4	3, 2, 1, 4, 5, 8, 14, 15, 26, 29, 27, 37, 36
Written exam of block 1	40%	6	0.24	5, 8, 13, 15, 17, 18, 19, 31, 30
Written exam of block 2	40%	6	0.24	3, 1, 12, 14, 21, 27, 33, 36

Bibliography

1. Química Física, Atkins, Peter; De Paula, Julio.8ª ed. 2008. Ed. Médica Panamericana.

https://cataleg.uab.cat/iii/encore/record/C__Rb2043130

2. Principios de Físicoquímica. Levine, Ira N. 6ª ed. 2014. Ed. McGraw-Hill.

https://cataleg.uab.cat/iii/encore/record/C__Rb2093346

3. Problemas de físico química. Levine, Ira N. McGraw-Hill, 2005.

Software

Spreadsheet

Wofram Demonstrations Project: https://demonstrations.wolfram.com/