Universitat Autònoma de Barcelona

2019/2020

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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Use of Languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

Teachers

Xavier Domènech Antúnez

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 ones 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 ones 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-Boltzmanns 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.

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 (45% of the mark).
- In-class tests (30% of the mark).
- Lab practices reports (25% of the mark).

(PART 2) TRANSPORT PHENOMENA AND HOMOGENEOUS CHEMICAL KINETICS
- Midterm exam (45% of the mark).
- In-class tests (45% of the overall score).
- Lab practices reports (10% 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 part should be scored with a minimum of 4/10 for further averaging and, where appropriate, pass the subject. If 5 is not reached in the overall grade, the student will have to take the final (reassessment) exam of the failed part(s). In this case, it will be necessary to have 4/10 in each part for averaging and reach at least 5 points. To be reassessed, the student must previously have submitted a minimum of two-thirds of the course-assessment items.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Experimental laboratory	17.5%	10	0.4	22, 9, 16, 26, 24, 20, 7, 25, 28, 29, 34, 35, 40, 10, 23, 39
Problem solving	27.5%	20	0.8	3, 2, 1, 4, 5, 11, 14, 15, 26, 38, 29, 27, 37

Written tests	55%	9	0.36	3, 2, 1, 6, 5, 8, 12, 13, 14, 15, 17, 18, 19, 21, 27, 31, 30, 33, 32, 36

Bibliography

ATKINS, P. W. (PETER WILLIAM), 1940- ; DE PAULA, JULIO.

Química física. 8a ed. Buenos Aires: Médica Panamericana, cop. 2008

LEVINE, IRA N., 1937-. *Fisicoquímica*. 5a ed.

Madrid: McGraw-Hill / Interamericana, cop. 2004. Vol. 1

LEVINE, IRA N., 1937-. *Problemas resueltos de fisico química : del texto de teoría.* Madrid: McGraw-Hill, 2005