

#### **Transport Phenomena and Surface Phenomena**

Code: 105040 ECTS Credits: 6

2024/2025

Degree	Туре	Year
2502444 Chemistry	ОВ	3

#### Contact

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### **Teachers**

Jose Peral Perez

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## **Teaching groups languages**

You can view this information at the <u>end</u> of this document.

#### **Prerequisites**

It is advisory to have completed "Fonaments de Química", "Química Quàntica" and "Termodinàmica i Cinètica"

## **Objectives and Contextualisation**

The student continues to advance in his/her training in Physical Chemistry with the aim of completing his/her training in this subject. After the microscopic approach in Quantum Chemistry and the macroscopic approach in Thermodynamics and Kinetics (with brief microscopic notes), in this subject - as its title indicates - Transport Phenomena and Surface Phenomena will be studied. The Kinetic Theory of Gases will serve as a basis for the study of transport phenomena in the gas phase. Next, the study of electrolyte solutions allows us to address transport phenomena in the liquid phase. Regarding surface phenomena, we will focus on those that take place at the liquid-gas, solid-liquid and solid-gas interfaces. Knowledge in Thermodynamics and Kinetics will be used to address them, with special emphasis on the study of adsorption, both in gas-solid and solution-solid interfaces, and Heterogeneous Catalysis. Electrochemistry, which can also be visualized as a surface phenomenon, will be studied from a thermodynamic and kinetic point of view. The course will end with the introduction of colloids and macromolecules from the point of view of Physical Chemistry.

#### Competences

- "Interpret data obtained by means of experimental measures, including the use of IT tools; identify their meaning and relate the data with appropriate chemistry, physics or biology theories."
- Adapt to new situations.
- Apply knowledge of chemistry to problem solving of a quantitative or qualitative nature in familiar and professional fields.
- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Have numerical calculation skills.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- Obtain information, including by digital means.
- Operate with a certain degree of autonomy and integrate quickly in the work setting.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show motivation for quality.
- Show sensitivity for environmental issues.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.

## **Learning Outcomes**

- 1. Adapt to new situations.
- 2. Analyse surface adsorption processes and adapt them to different isothermals.
- 3. Be ethically committed.
- 4. Classify and analyse the properties of colloids and macromolecules.
- 5. Communicate orally and in writing in one's own language.
- 6. Define colloids and macromolecules.
- 7. Define surface chemistry.
- 8. Describe the components of electrochemistry.
- 9. Have numerical calculation skills.
- 10. Identify the English names of fundamental physical and chemical variables.
- 11. Identify the phenomena of transport.
- 12. Interpret data referring to surface tension (surfactants), wetting (angles of contact) and detergence.
- 13. Interpret intensity/potential graphs (I/E) and their relation with the operation of batteries.
- 14. Learn autonomously.
- 15. Manage the organisation and planning of tasks.
- 16. Manage, analyse and synthesise information.
- 17. Obtain information, including by digital means.
- 18. Operate with a certain degree of autonomy and integrate quickly in the work setting.
- 19. Propose creative ideas and solutions.
- 20. Reason in a critical manner
- 21. Recognise and analyse problems related with surface chemistry (adherence and detergence).
- 22. Recognise, analyse and resolve electrochemical problems (batteries).
- 23. Relate macroscopic properties and the properties of individual atoms and molecules.
- 24. Resolve problems and make decisions.
- 25. Resolve qualitative problems related to transport phenomena, colloids and macromolecules.
- 26. Resolve quantitative problems in surface chemistry, chemical kinetics and electrochemistry.
- 27. Show initiative and an enterprising spirit.
- 28. Show motivation for quality.
- 29. Show sensitivity for environmental issues.
- 30. Use IT to treat and present information.
- 31. Use the English names for the different states of matter and their changes.

#### Content

Topic 1. Gases.

Real Gases: general characteristics and deviations from ideality. Compressibility factor. Virial and van der Waals equations of state. Fugacity and equilibrium constants for real gases.

Topic 2. Kinetic theory of gases

Molecular interpretation of the pressure of a gas. Maxwell-Boltzmann distribution of velocities Most probable velocity, mean velocity, and root mean square velocity. Collision frequency and mean free travel. Collisions with walls. Effusion.

Topic 3. Introduction to transportation. General aspects and transport in the gas phase.

Transport phenomena: flows and gradients. Gas phase transport: diffusion, thermal conductivity and viscosity.

Topic 4. Electrolyte solutions.

lon-solvent interactions. Enthalpy and entropy of solvation. Chemical potential of electrolytes. Average ionic activity coefficients. Ion-ion interactions: Debye-Hückel model. Ionic association.

Topic 5. Transport in solution.

Diffusion of dissolved species. Mean square displacement.

Conductivity and molar conductivity. Classification of electrolytes. Ionic mobility. Transport number. Diffusion and conductivity.

Topic 6. Interfaces. General features. Fluid/fluid interfaces.

Definition of interface. Curved interfaces: surface tension. Experimental measurement of surface tension. Contact angle. Wettability. Vapor pressure on curved surfaces: Kelvin equation. Gibbs isotherm.

Topic 7. Adsorption.

Physical adsorption and chemical adsorption. Adsorption isotherms. Adsorption enthalpy Langmuir isotherm. BET isotherm. Characterization of porous materials. Interfaces loaded. Double layer models.

Topic 8. Catalysis.

General mechanism of catalysis. Homogeneous catalysis. Acid-base catalysis.

General mechanism of heterogeneous catalysis. Characteristics of solid catalysts. Langmuir-Hinshelwood and Eley-Rideal mechanisms.

Topic 9. Electrochemical equilibrium.

Electrochemical potential. Nernst equation. Notation of galvanic cells. Normal electrode potentials. Types of galvanic cells. Obtaining thermodynamic data from measuring the EMF of a galvanic cell.

Topic 10. Electrochemical kinetics.

Overpotential. Exchange current density. Kinetics of charge transfer. Approximations of the Butler-Volmer equation. Polarizable and non-polarizable electrodes. Effect of matter transport.

Topic 11. Colligative properties.

Decrease in freezing point and increase in boiling point. Osmotic pressure.

Topic 12. Colloids and macromolecules.

Colloids: classification, structure and stability. Applications. Techniques for characterizing macromolecules and colloids in solution.

## **Activities and Methodology**

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Problems	12	0.48	2, 10, 13, 21, 22, 25, 26, 31
Theory Lectures	37	1.48	2, 4, 7, 8, 11, 12, 13, 23
Type: Supervised			
Study. Problem solving. Readings and Information Obtaining	87	3.48	1, 3, 5, 9, 14, 15, 16, 17, 18, 19, 20, 24, 27, 28, 29, 30

The acquisition of knowledge will be done through the use of theoretical classes and problems.

Theoretical classes (lectures with a blackboard and / or with the help of  $\epsilon$  Classes of problems (with more participation of the students) in which the

The lecturers will dedicate approximately 15 minutes of a class to allow the students to fill the "Teaching Activity a

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.

#### Assessment

## **Continous Assessment Activities**

Title	Weighting	Hours	ECTS	Learning Outcomes
Evidences	50%	6	0.24	1, 2, 3, 5, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31
Final Exam	50%	2	0.08	2, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15, 16, 18, 20, 21, 22, 23, 24, 25, 26, 27, 28, 31
Partial Exam 1	25%	3	0.12	2, 5, 7, 9, 10, 11, 12, 14, 15, 18, 19, 20, 21, 23, 24, 25, 26, 27, 29, 31
Partial Exam 2	25%	3	0.12	3, 4, 5, 6, 8, 9, 10, 13, 15, 16, 18, 19, 20, 22, 23, 24, 25, 26, 27, 28, 31

#### Continued avaluation

Exams: Two partial exams (P1 and P2) will be held throughout the course. All exams will be graded between 0 and 10.

Follow-up work: A series of follow-up tests will be carried out throughout the course. The set of tests corresponding to each partial S1 and S2 will have a grade between 0 and 10. The follow-up test will not be repeated due to the student's absence if this is not documented in a valid form (official medical report,...)

Qualifications: To pass the subject per course, you must obtain a final grade (NFC) greater than or equal to 5.0 and obtain a grade greater than or equal to 3.5 in each of the partial exams. Follow-up tests (S) will have a weight of 20% and the grade of the partial exam (P) 80%

NFC = (0.1 S1 + 0.4 P1) + (0.1 S2 + 0.4 P2) = 0.1 (S1 + S2) + 0.4 (P1 + P2)

Students who do not pass the course by course (continuous assessment) and students who want to improve their course grade

Students who do not pass the subject per course, in accordance with the previous continuous assessment scheme or who wish to improve their qualification, may sit the two remedial exams for partials P1 and P2. To take part in the recovery, students must have previously participated in the two written tests and 75% of the classroom work

When the student takes a make-up exam, the grade Pi will be that of the make-up exam, if this is higher than the one obtained in the corresponding exam during the course. If the mark obtained in the make-up exam is lower than the one obtained during the course, the grade Pi will be the average of the make-up grade and the exam grade taken during the course. S tracking notes are not refundable.

To pass the subject with recovery, the student must meet the same requirements as to pass the subject by course.

If the student has been evaluated on only 25% or less of the tests, the final grade will be NOT EVALUABLE.

#### Unique assessment

Exams: A final test that will consist of an examination of the entire syllabus of the subject to be carried out on the day on which the students of the continuous assessment take the second part exam, P2. The exam will be scored with a grade between 0 and 10.

Qualifications: The student's grade will be the grade of this test. To pass the subject per course, a grade greater than or equal to 5.0 must be obtained.

Students who do not pass the subject per year.

If the final grade does not reach 5.0 the student has another chance to pass the subject through the resit

exam.

The student's grade will be the grade of this test.

To pass the subject with recovery, the student must meet the same requirements as to pass the subject by course.

## **Bibliography**

Most relevant bibliography

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Interfacial Science: an introduction (2<sup>on</sup> ed.), G.T. Barnes, G.T.; Gentle, I.R. 2010 Oxford University Press, ISBN 978-0-19-657118-5

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Additional Bibliography

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

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Physics and Chemistry of Interfaces. Butt,H.-J. K.; Kappl Graf, M., , 2003 WILEY-VCH Verlag GmbH & Co. ISBN 3-527-40413-9.

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Fundamentals of chemical reaction engineering. Chapter 5 Davis, Mark E. and Davis, Robert J. -

Heterogeneous Catalysis-. McGraw-Hill Higher Education, New York. (2003).

https://authors.library.caltech.edu/records/arr0q-97509

#### Accessible online free

## Software

No special software is required

# Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Spanish	first semester	morning-mixed
(PAUL) Classroom practices	2	Spanish	first semester	afternoon
(TE) Theory	1	Catalan	first semester	morning-mixed
(TE) Theory	2	Spanish	first semester	afternoon