

#### 2021/2022

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

Code: 105040 ECTS Credits: 6

Degree	Туре	Year	Semester
2502444 Chemistry	ОВ	3	1

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

#### Contact

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### Teachers

José Peral Pérez

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### **Use of Languages**

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

#### **Prerequisites**

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

#### **Objectives and Contextualisation**

The student keeps progressing on its Physical Chemistry education with the goal of visiting the full extension of issues that make this subject total content, the Physical Chemistry. After the microscopic approximation involved in Quantum Chemistry, the macroscopic approximation to Thermodynamics and Kinetics (with minor microscopic hints), this subject will be dealing - as its title indicates- with Transport Phenomena and Surface Phenomena. Thus, gases kinetic theory, the different types of solution transport (diffusion, migration and convection), the existence and definition of interphases, and their application to kinetics (heterogeneous catalysis) and electrochemistry (double layers), will be studied. Electrochemistry, that can also be visualized as a surface phenomenon, will be treated from a thermodynamic and kinetic point of view. The course will end up with the study of some macromolecules: colloids and polymers, hence closing with all these contents the full view of the Physical Chemistry field.

#### 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 ones 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 ones 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

1. Introduction to transport phenomena.

Gases kinetic theory. Flux. Effusion. Thermal Conductivity. Viscosity.

2. Solution transport (I).

Solution structure: Ion-solvent interaction. Solvation. Ion-Ion interaction. Debye-Hückel model. Activity coefficient.

Solution transport:diffusion, migration and convection. Fick's laws. Diffusion microscopic issues.

3. Solution transport (II).

Conductivity and molar conductivity. Ionic mobility. Transport index. Onsager's equation. Diffusion and conductivity.

4. Surface phenomena. The interphase.

Surface tension. Surface thermodynamics. Surface excess. Electrified interphase: double layer models.

5. Surface phenomena. Heterogeneous catalysis.

Homogeneous catalysis. Surface adsorption: physisorption and chemisorption. Adsorption isotherms. General mechanisms on heterogeneous catalysis. Features of solid catalysts.

6. Electrochemical equilibrium.

Electrochemical potential. Nernst equation. Galvanic cells types. Transports batteries. Diffusion potential.

7. Electrochemical kinetics.

Basic concepts. Charge transfer kinetics at the electrodes: Butler-Volmer equation. Mass transport effect.

8. Macromolecules.

Colloids: types and stability. Polymers: general concepts, characterization and synthesis.

# Methodology

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  $\varepsilon$  Classes of problems (with more participation of the students) in which the

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

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			
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, 14, 5, 27, 28, 15, 16, 3, 29, 17, 18, 19, 20, 24, 9, 30

#### **Assessment**

In this half face-to-face year:

Classroom written exams (50% of the final mark). Accordingly to the academic calendar 2 exams will be carried out. A mark equal or above to 3,5 (out of 10) is required in order to be able to add it to the remaining 50% of the marks (classroom exercises). If the mark is below 3,5, the student will have to take the second-chance exam, that will include the whole course, in order to pass the subject.

Classroom exercises fulfillment (50% of the marks). The culmination of these exercises (problem solution, test,..) is mandatory and is not subjected second-chance attempts.

In order to participate in the second-chance exam the students have to sit for the two previous written exams and for 75% of the classroom exercises.

In case the Covid 19 situation forces the classroom written exams to change to on-line exams, the marks percentage distribution would change: 30 % for the on-line written exams, and 70% for the "classroom" exercises (either face-to-face or on-line).

### **Assessment Activities**

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

# **Bibliography**

ATKINS,P.W.; DE PAULA, J. *Atkins' Physical Chemistry*. 9<sup>a</sup> ed. Oxford University Press, 2009. (Traducció espanyola de la 8<sup>a</sup> ed., Ed. Pananmericana, 2008)

BERTRÁN, J.; NÚÑEZ, J. (coords.) Química Física, Ariel, 2002.

LEVINE, I.N. Physical Chemistry. 5ª ed. Mc Graw Hill, 2002. (Traducció espanyola, McGraw-Hill, 2004)

# **Software**

No special software is required