FACULTAD DE CIENCIAS QUÍMICAS

APPLIED PHYSICAL CHEMISTRY

COURSE GUIDE

BSc Chemistry

Academic Year 2023-2024

UNIVERSIDAD COMPLUTENSE MADRID

I.- IDENTIFICATION

COURSE NAME:	Applied Physical Chemistry
CREDITS (ECTS):	6
CHARACTER:	Optional
SUBJECT:	Advanced Physical Chemistry
MODULE:	Advanced
UNDERGRADUATE DEGREE:	Bachelor's Degree (BS) in Chemistry
SEMESTER/TERM:	Second semester (fourth year)
DEPARTMENT/S:	Physical Chemistry

LECTURERS:

Group E		
Theory Seminar Tutorial	**Lecturer:** **Departament:** **Office number:** **e-mail:**	ALBERTINA CABAÑAS PÓVEDA Physical Chemistry QA-276 a.cabanas@quim.ucm.es
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Laboratory QA238					
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II.- OBJECTIVES

■ GENERAL OBJECTIVE

The student will acquire the necessary concepts to understand and quantify systems, phenomena and chemical techniques of special technological relevance, such as:

- Mixtures and solutions.
- Polymeric materials.
- Colloidal and supramolecular systems.
- Heterogeneous catalysts.
- Corrosion, electrochemical energy conversion and electrokinetic phenomena.

In addition, the student will become familiar to the use of specialized bibliography and databases, and resources accessible through the Internet.

SPECIFIC OBJECTIVES

The specific objectives are to:

- Know the thermodynamic conditions that determine phase equilibrium.
- Understand the concept of the critical point and introduce the student to the use of supercritical fluids as extraction and reaction media.
- Become familiar with the technological implications of the appearance of metastable phases.
- Familiarize the student with the properties, phase transitions, characterization techniques and applications of polymeric materials.
- Understand the interactions between particles and the mechanisms of self-association.
- Become familiar with the basic principles and applications of supramolecular chemistry.
- Become familiar with solid surface structures, the general mechanisms of heterogeneous catalysis and its main industrial and environmental applications.
- Introduce the applications of electrochemistry to the treatment of materials and the generation of clean energy.
- Become familiar with the main applications based on electrokinetic phenomena.
- Know the principles of sustainable chemistry and be able to relate them to the remaining contents of the course.

III.- BACKGROUND KNOWLEDGE AND RECOMMENDATIONS

BACKGROUND KNOWLEDGE:

Those corresponding to the subjects Physical Chemistry I and Physical Chemistry II from the Chemistry degree or equivalent.

RECOMMENDATIONS:

It is recommended to have passed the subjects of the Basic Module in the Chemistry degree, or equivalent.

IV.- CONTENTS

BRIEF DESCRIPTION OF CONTENTS:

Mixtures and solutions. Supercritical states. Metastable states and nucleation phenomena. Industrial applications. Polymers. Mechanical and electrical properties.

Glass transition. Colloidal and supramolecular chemistry. Industrial use and technological applications of polymers and supramolecular systems. Heterogeneous catalysis. Mechanisms, types and characterization of heterogeneous catalysts. Industrial processes and environmental aspects. Electrochemistry Corrosion. Coatings. Electrochemical synthesis. Fuel cells. Electrokinetic phenomena. Sustainable chemistry.

SYLLABUS:

UNIT I: PHASE EQUILIBRIUM

- **Lesson 1:** Equilibrium conditions and spontaneity. Metastability. Nucleation.
- **Lesson 2:** Phase equilibrium in real systems. Critical point. Equilibria: vapour-liquid (LV), liquid-liquid (LL), solid-liquid (SL), three-phase equilibria. Phase diagrams at high pressure.
- **Lesson 3:** Fugacity and activity of gases and liquids. Activity coefficient models. Equations of state.
- **Lesson 4:** Calculation of phase equilibrium. Vapour-liquid equilibrium at low pressure. Vapour-liquid equilibrium at medium and high pressure. Solid-fluid equilibrium.
- **Lesson 5:** Properties and Applications of Supercritical Fluids. Supercritical extraction. Separation, reaction and preparation of materials. Industrial processes. Other sustainable solvents: ionic liquids and deep eutectic mixtures.

Programmed Tutorial I: *Phase diagrams in multicomponent systems.*

Seminar I*: The principles of sustainable chemistry.*

Laboratory 1: *Phase equilibrium calculation at high pressure with equations of state.*

UNIT II: POLYMERIC MATERIALS

- **Lesson 6:** Types of polymeric materials and their applications. Thermoplastics, thermosets, elastomers, fibres, composites.
- **Lesson 7:** Crystalline and amorphous state in polymers. Thermal transitions in polymers: melting and glass transition. Thermodynamics and kinetics of transitions. Factors affecting the crystallinity. Factors affecting the glass transition.
- **Lesson 8:** Mecanical behaviour of polymeric materials. Elastic modules. Stress-strain curves. Viscoelasticity. Elastomers.
- **Lesson 9:** Electrical behaviour of polymeric materials. Applications in the optoelectronic industry. Lithographic process. Conductive polymers.
- **Lesson 10:** Life cycle analysis of plastics. Degradation and stability of plastics. Chemical and mechanical recycling. Bioplastics. Microplastics.

Programmed Tutorial II: *Study by Differential Scanning Calorimetry (DSC) of thermal transitions in polymers.*

Programmed Tutorial III*: Composition-structure-properties relationship in polymeric materials: technological implications.*

UNIT III: COLOIDAL AND SUPRAMOLECULAR CHEMISTRY

- **Lesson 11:** Interparticle forces: van der Waals forces, electric double layer forces, hydrophobic interactions, steric forces. Colloidal stability: DLVO theory.
- **Lesson 12**: Colloids: basic concepts. Types of colloidal. Association colloids: spherical micelles, cylindrical micelles, bilayers, vesicles, bicontinuous structures. Emulsions. Gibbs and Langmuir monolayers.
- **Lesson 13:** Self-organization. Supramolecular chemistry. Static and dynamic self-assembly.
- **Lesson 14:** Nanoparticles: Methods of synthesis.

Seminar II: Technological applications of colloidal systems: emulsion polymerisation, liposomes and drug encapsulation, food industry, detergency and cosmetics, sensors,...

Laboratory 2: *Synthesis and characterization of nanoparticles.*

Laboratory 3: *Physicochemical Applications of Raman Spectroscopy.*

UNIT IV: HETEROGENEOUS CATALYSIS

- **Lesson 15:** Structure of solid surfaces. Chemisorption isotherms. General mechanisms of catalysis.
- **Lesson 16:** Application of kinetic models in heterogeneous catalysis: Langmuir-Hinselwod and Eley-Rideal. Promoters and inhibitors.
- **Lesson 17:** Catalyst design and synthesis.
- **Lesson 18:** Catalysis, one of the principles of sustainable chemistry. Catalytic processes of industrial and environmental interest. Cracking and reforming of petroleum. Sustainable biorefinery. Three-way catalyst in automobiles. Ammonia synthesis.

Seminar III: *Surface caracterización techniques.*

UNIT V: ELECTROCHEMISTRY

- **Lesson 19:** Thermodynamic, kinetic and transport aspects in electrochemistry. Electrokinetic phenomena and applications.
- **Lesson 20:** Electrosynthesis. The chloralkali process, metal extraction, H_2 generation by electrolysis, adiponitrile synthesis.
- **Lesson 21:** Electrochemistry of surfaces. Corrosion, passivation, surface protection methods. Electroplating.
- **Lesson 22:** Electrochemical energy conversion: Batteries, fuel cells, capacitors.

Seminar IV: Fundamentals of electroanalytical sensors and biosensors. Process monitoring and sustainable chemistry. Membrane potentials in biology.

Laboratory 4: *Polarisation curve of a direct methanol fuel cell.*

V.- COMPETENCES

GENERAL:

The general competences of the Advanced module of application in this subject are to:

- **CG1-MA1:** Recognise and value chemical processes in everyday life.
- **CG2-MA1:** Value the importance of Chemistry and its impact on industrial and technological society.
- **CG2-MA2:** Relate interdisciplinary areas in full expansion, and become aware of the importance of interdisciplinary research in the advancement of science.
- **CG3-MA1:** Demonstrate a base of knowledge and skills with which to continue their studies in specialised areas of chemistry or in multidisciplinary areas.
- **CG4-MA1:** Translate the specific knowledge of each subject into the universal scientific language, understood and shared interdisciplinarily.
- **CG7-MA1:** Apply theoretical and practical knowledge to the solution of problems in Chemistry and select the most appropriate method to solve them.
- **CG8-MA1:** Assess research and detailed studies in the field of Chemistry,
- **CG13-MA1:** Develop good scientific practice in measurement and experimentation.

SPECIFIC:

In addition to the general and generic competences of the module, the specific competences of the degree CE11, CE12 and CE13 are developed, for this subject, in the following Specific competences of the advanced module in the subject Advanced Physical Chemistry (CE-MAQF). The specific competence are to:

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- **CE11-MAQF2:** Explain and quantify systems, phenomena and chemical techniques of special technological relevance in terms of both their equilibrium and transport properties.
- **CE11-MAQF3:** Describe colloidal and supramolecular systems.
- **CE12-MAQF2:** Manage computer programs, both commercial and open access, for the modelling and simulation of molecules and chemical systems.
- **CE13-MAQF1:** Recognise and apply polymeric materials in technological and industrial applications.
- **CE13-MAQF2:** Formulate and use the concepts of heterogeneous catalysis, its industrial use and environmental implications.
- **CE13-MAQF3:** Describe and explain electrokinetic phenomena, corrosion and surface protection, and electrochemical synthesis.

GENERIC:

The generic competences of the advanced module that apply to this subject are to:

- **CT1-MA1:** Prepare and wrie scientifical and technical reports
- **CT2-MA1:** Work as a team.
- **CT3-MA1:** Learn to make decisions when faced with a real practical problem.
- **CT4-MA1:** Select the most appropriate method to solve a given problem.
- **CT5-MA1:** Consult, use and analyse any bibliographical source.
- **CT5-MA2:** Manage bibliography and specialised databases, and resources accessible through the Internet.
- **CT7-MA1:** Use computer programs that serve, in the world of chemistry, to calculate, design, simulate, approximate and predict.
- **CT11-MA1:** Develop autonomous work
- **CT12-MA1:** Develop sensitivity towards environmental issues and preservation of the environment.

VI.- LEARNING OUTCOMES

Upon successful completion of this course, the student should be able to:

UNIT I

1. Explain the phase diagrams of binary and ternary mixtures and the different phase changes.
2. Be able to propose separation processes from the phase diagrams of mixtures.
3. Recognise the technological implication of nucleation phenomena in separation processes.
4. Know the applications of supercritical fluids as sustainable solvents in extraction, reaction and preparation of materials, focusing on their industrial applications.
5. Critically compare processes in which supercritical fluids are used with other conventional processes and assess the advantages and disadvantages of each of them.
6. Know the different thermodynamic models and the systems in which they are applied depending on the characteristics of the system.
7. Calculate the thermodynamic properties of pure substances and mixtures and predict phase diagrams using simple equations of state.
8. Know the applications of ionic liquids and deep eutectic solvents in catalysis, separation, preparation of pharmaceuticals or CO_2 capture.

UNIT II

9. Classify the different types of polymeric materials according to their structure and properties.
10. Explain the technological importance of the different types of polymers.
11. Identify the different thermal transitions in polymers.
12. Interpret DSC curves of polymers.
13. Extract thermodynamic information about phase transitions from DSC curves.
14. Differentiate between the different types of polymers from their stress-strain curves.
15. Know the electrical and optical properties of polymeric materials and relate them to their structure.
16. Know the main methods of polymer recycling, both physical and chemical.
17. Apply the principles of sustainable chemistry when selecting polymeric materials for different applications considering not only the physical properties of the material, but also the life cycle of the polymer.

UNIT III

18. Identify the forces between particles in colloidal systems.
19. Describe the structure of electrified interfaces.
20. Apply thermodynamic knowledge to describe the various self-organised structures.
21. Explain the variations of the critical micellar concentration with the characteristics of the amphiphile and dispersing medium.
22. Predict the colloidal stability against different perturbations of the system.
23. Recognise the importance of colloidal systems in life.
24. Explain the importance of non-covalent interactions in the phenomena of molecular recognition.
25. Decide among the different methods of nanoparticle synthesis considering not only their properties but also sustainability criteria.
26. Apply spectroscopic characterization techniques to colloidal systems.
27. Recognise the importance of colloidal systems in technology.

UNIT IV

28. Describe the structure of solid surfaces.
29. Propose the most appropriate techniques to characterise different heterogeneous catalysts.
30. Propose the possible catalytic reaction mechanism on the basis of kinetic data.
31. Decide which model of chemisorption isotherms best describes a set of experimental data.
32. Design strategies for the synthesis of catalysts depending on the desired catalytic properties.
33. Describe the catalytic reaction mechanisms of industrial processes of interest and the catalysts that are used.
34. Compare catalytic and non-catalytic processes and quantify their sustainability using parameters such as atomic economy and E-factor.
35. Compare from the point of view of Sustainable Chemistry the different methods of preparation of catalysts.

UNIT V

36. Apply electrochemistry to problems of synthesis and electrocatalysis.
37. Describe industrial electrosynthesis processes.
38. Explain the phenomena of surface corrosion and passivation.
39. Decide the best method of surface protection for each system.
40. Describe the processes of surface treatment by electrochemical methods.
41. Distinguish between the different types of batteries, supercapacitors and fuel cells.
42. Recognise the importance of electrochemistry in biological systems.

VII. – WORKING HOURS DISTRIBUTED BY ACTIVITY

Activity	Attendance (hours)	Self-study (hours)	Credits
Lectures	30	55	3,4
Seminars	7,5	17,5	1,0
Tutorials/Guided work	3	4,5	0,3
Laboratory	12	9	0,84
Written assignments and exams	5	6,5	0,46
Total	**57,5**	**92,5**	**6**

VIII.- METHODOLOGY

The teaching practice will follow a mixed methodology based on cooperative learning, collaborative learning and self-learning. This methodology will be developed through **theory lectures, seminars and Programmed tutorials**.

The training activities for the acquisition of competences in "Applied Physical Chemistry" consist of theory lectures (3.4 credits), seminar classes (1 credit), preparation and presentation of work and/or programmed tutorials (0.3 credits) and laboratory (0.84 credits). In order to promote autonomous work, the presentation of work related to advanced contents and applications of the contents of the course will be assessed. The laboratory practicals will have contents directly related to those of the theory classes. The preparation and presentation of work and exams will account for a total of 0.46 credits.

During the theory lectures, the main objectives of the subject will be clearly stated, the content will be taught and all the materials necessary for its understanding will be made available to the students on the Virtual Campus. Whenever possible, a specialist in the subject will be invited to cover the more advanced aspects of the subject. In the Programmed tutorials, students will be asked questions to solve or discuss, individually or in groups.

The contents of the course are presented to students in face-to-face classes, divided into two types:

The so-called **theory lectures** will be given to the whole group and the student will be introduced to the fundamental contents of the subject. At the beginning of each topic, the syllabus and the main objectives of the subject will be clearly stated. At the end of the subject, a brief summary of the most relevant concepts will be made and new objectives will be proposed that will allow the interrelation of contents already studied with those of the rest of the subject and with other related subjects. During the presentation of contents, illustrative examples of the concepts developed or which serve as an introduction to new contents will be proposed. In order to make it easier for students to follow the lectures, they will be provided with the necessary teaching material on the Virtual Campus.

In the **face-to-face seminar classes**, questions related to the contents developed in the face-to-face theory classes will be raised. The procedure followed to solve them, the result obtained and its meaning will be discussed.

The theory and seminar classes and the work involved develop the general competences CG2-MA1, CG2-MA2, CG4-MA1, CG7-MA1 and CG8-MA1 and the generic competences CT1-MA1, CT2-MA1, CT3-MA1, CT4-MA1, CT5-MA1 and CT7-MA1. During the development of the syllabus, both in theory and seminar classes, the student will acquire the knowledge and experience necessary to satisfy all the specific competences to be covered, CE11-MAQF2, CE11-MAQF3, CE12-MAQF2, CE13-MAQF1, CE13-MAQF2 and CE13-MAQF3 and the generic CT11-MA1 In addition, during the development of the sessions, special emphasis will be placed on relating the aspects studied with other disciplines and chemical phenomena in daily life, as well as on their multidisciplinary nature, which will satisfy the general competences CG1-MA1, CG2-MA1, CG3-MA1, and CG4-MA1, and the generic competences CT8-MA1 and CT12-MA1.

Programmed tutorials will be held, both on topics directly related to the theoretical content, to broaden knowledge and develop skills, and on more cross-cutting topics that allow the contents of the subject to be interrelated with other aspects of interest to the chemist. As a complement to the personal work carried out by the student, and in order to promote the development of group work, **the preparation, presentation and defence of a group-work** will be proposed. All this will allow the student to put into practice their skills in obtaining information, developing skills related to the critical use of bibliographic information and databases and teamwork (CT1-MA1, CT5-MA1, CT5-MA2). In addition, each working group will be able to evaluate, anonymously, the topic developed by another group, in a similar way to peer review in scientific publications, which will develop a critical and self-critical sense. This process should be carried out prior to the presentation of each of the groups, so that the students involved can make the necessary corrections to the final version of the work. The evaluation process will help students to develop skills of critical analysis in scientific work and to be able to correct in their own elaborations the defects they find in the work they evaluate. Students will also be able to evaluate the oral presentations of their peers.

The lecturer may schedule additional **tutorials** on issues raised by the lecturer or by the students themselves. Tutorials will also be available for individual students who wish to resolve any doubts that may arise during their studies. These tutorials will be held in person at the times indicated by each lecturer or, exceptionally, virtually.

The Virtual Campus will be used to allow fluid communication between lecturers and students and as an instrument for making available to students the material to be used in both theory and problem classes. It can also be used as a forum in which to present some complementary topics whose content, although important for the subject as a whole, is not considered necessary to present in the face-to-face classes. Finally, this tool will allow self-assessment exercises to be carried out by means of multiple-choice objective tests that will show both the teacher and the student which concepts require more work for their learning.

A laboratory will be carried out throughout the course with topics directly related to the contents of the subject. This laboratory will consist of both experimental practices, where the general competence CG13-MA1 will be specifically developed, and calculation practices and the use of theoretical tools or computational simulation in which the specific competences (CE11-MAQF1, CE11-MAQF2, CE11-MAQF3, CE12-MAQF2, CE13-MAQF1, CE13-MAQF2 and CE13-MAQF3) will be developed. In some practicals, problems that require the simultaneous use of the theoretical knowledge acquired and the experimental and calculation tools available in the laboratory will be posed. Finally, the student will present, individual and/or in group, scientific reports of some of the practicals carried out (CT1-MA1, CT5-MA1, CT7-MA1). Although the subject is offered in English as part of the bilingual degree, the laboratory will be taught in Spanish.

IX.- BIBLIOGRAPHY

BASIC:

- Bertrán Rusca, J. y Núñez Delgado, J. (coord.), "*Química Física*", Volúmenes I y II., Ariel Ciencia, 2002.
- Freire Gómez, Juan José; Esteban Pacios, M. I.; García Baonza, V.; Ortega Gómez, F.; Monroy Muñoz, F. "*Química Física IV. Materia condensada*", UNED, 2017.
- Atkins, P. y de Paula J., "*Química Física*", 8ª Edición, Editorial Médica Panamericana, Buenos Aires, 2008.

COMPLEMENTARY:

- Prausnitz, J.M.; Lichtenthaler, R.N. y Gomes de Azevedo, E., "*Termodinámica Molecular de los Equilibrios de Fase*", 3ª Ed., Prentice Hall, 2001.
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- Areizaga J.,Cortázar M.M., Elorza J.M., Iruin J.J., "*Polímeros*", Síntesis S.A., 2002
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- Hamann C.H., Hamnett A. y Vielstich W., "Electrochemistry", Wiley-VCH, 2nd, Ed., 2007
- Anastas P.T. and Warner J.C., *"Green Chemistry. Theory and Practice"*, Oxford University press, Oxford, 1998.
- R. Mestres, *"Química Sostenible"*, Ed. Síntesis, Madrid, 2011.

X.- ASSESSMENT PROCEDURE

The student's academic performance and the final grade for the subject will be calculated according to the following percentages, which will be maintained in all the examinations:

- **WRITTEN EXAMS** **60 %**

Ordinary call: There will one final exam. In addition, mid-term exams may be held throughout the course to assess the learning outcomes. Students who pass the mid-term exams will not have to take the final exam, although the compensation between mid-term exams will require a minimum mark of 4 out of 10. In any case, the minimum mark of the written exam to pass the course is 4 out of 10. The exams will consist of questions and/or issues on the contents taught during the course, both in theory lectures and seminars as well as in tutorials and laboratories. In the extraordinary call, there will be a single final exam similar to the one taken in the ordinary call.

Competenes assessed: CG1-MA1, CG2-MA1, CG2-MA1, CG2-MA2, CG3-MA1, CG4-MA1, CG7-MA1, CG8-MA1, CT1-MA1, CT2-MA1, CT3-MA1, CT4-MA1, CT5-MA1, CT7-MA1, CT8-MA1, CT12-MA1,CE11-MAQF2, CE11-MAQF3, CE12-MAQF2, CE13-MAQF1, CE13-MAQF2, CE13-MAQF3.

- **PERSONAL WORK:** **20%**

The assessment of the individual learning work carried out by the student will be carried out by taking into account the following factors:

- Assessment of the work carried out during the Programmed group tutorials, attendance of which is compulsory.
- Assessment of practical exercises proposed by the lecturer as deliverables.
- Assessment of the work proposed and carried out individually or in groups by the students.

The grade obtained by the student in the ordinary call for this concept will be maintained in the extraordinary call.

Competences assessed: CG1-MA1, CG2-MA1, CG2-MA1, CG2-MA2, CG3-MA1, CG4-MA1, CG7-MA1, CG8-MA1, CT1-MA1, CT2-MA1, CT3-MA1, CT4-MA1, CT5-

MA1, CT7-MA1, CT8-MA1, CT12-MA1,CE11-MAQF2, CE11-MAQF3, CE12-MAQF2, CE13-MAQF1, CE13-MAQF2, CE13-MAQF3.

- **LABORATORY** **20%**

Students will develop in small groups throughout the course as a directed activity a series of laboratory practices, both experimental and calculation, and use of theoretical tools or computational simulation, with attendance at all practical sessions being **compulsory.** Students will be assessed on their theoretical and practical skills, as well as their skills in the use of experimental equipment and in the use of computer packages for data processing and the prediction of thermodynamic properties. Students will be required to produce a scientific report which will be subject to assessment. A minimum mark of 4 out of 10 will be required in each of the laboratory practicals and a mark of 5 out of 10 in the overall laboratory mark in order to average with the different activities. An exam about the contents of the laboratory may be taken if necessary.

The grade obtained by the student in the ordinary call in the lab will be maintained in the extraordinary call. In those cases, in which a student fails the subject, but has passed the laboratory activities, the grade of these will be maintained during the following academic year, being able to take, however, a written or oral exam on the methodology of the practices.

Competences assessed: CG1-MA1, CG2-MA1, CG2-MA2, CG3-MA1, CG4-MA1, CG7-MA1, CG8-MA1, CT1-MA1, CT2-MA1, CT3-MA1, CT4-MA1, CT5-MA1, CT7-MA1, CT8-MA1, CT12-MA1,CE11-MAQF2, CE11-MAQF3, CE12-MAQF2, CE13-MAQF1, CE13-MAQF2, CE13-MAQF3

- **ATTENDANCE AND ACTIVE PARTICIPATION IN CLASSES**

Attendance at all face-to-face activities is compulsory, and the student's active participation in all teaching activities will be positively valued in the final grade.

ACTIVITIES SCHEDULE

UNIT	ACTIVITY	HOURS	BEGGINIG	END	FIN
I. Phase equilibrium. Applications of supercritical fluids and other sustainable solvents.	Theory clases	6	1	1st Week	3rd Week
	Seminars	1,5	1		
	Programmed tutorial*	2	1		
	Laboratory	3	4		
II. Polymeric material and their applications	Theory clases	6	1	4th Week	7th Week
	Seminars	1,0	1		
	Programmed tutorial*	2	1		
	Laboratory	3	4		
III. Colloidal and Supramolecular chemistry	Theory clases	5	1	8th Week	10th Week
	Seminars	1,0	1		
	Programmed tutorial*	1	-		
	Laboratory	3	4		
IV. Heterogeneous catalysis	Theory clases	5	1	11th Week	13th Week
	Seminars	1,0	1		
	Programmed tutorial*	1	1		
	Laboratory	-	-		
V. Applied Electrochemistry	Theory clases	5	1	14th Week	15th Week
	Seminars	1,0	1		
	Programmed tutorial*	1	-		
	Laboratory	3	4		

* The scheduling of tutorials depends on the overall planning of all the subjects of the course.

SUMMARY OF THE ACTIVITIES

Teaching activity	Associated competences	Lecturer activity	Student activity	Assessment procedure	P	NP	Total	C
Theory lectures	CG1-MA1, CG2-MA1, CG2-MA2, , CG3-MA1, CG4-MA1, CG7-MA1 CG8-MA1, CT1-MA1, CT2-MA1, CT3-MA1, CT4-MA1, CT5-MA1, CT7-MA1, CT8-MA1, CT11-MA1, CT12-MA1, CE11-MAQF2, CT11-MA1, CE11-MAQF3, CE12-MAQF2, CE13-MAQF1, CE13-MAQF2, CE13-MAQF3	Presentation of theoretical concepts and raising questions and new objectives.	Note-taking. Resolution of questions. Development of new objectives. Formulation of questions and doubts.	Grading of the answers given to questions related to theoretical concepts.	30	55	85	20%
Seminars		Application of the theory to problem solving. Raising new questions.	Resolution of numerical exercises, problems and questions. Formulation of questions and doubts.	Grading of the answers (approach and result) given for the resolution of numerical exercises and problems.	7,5	17,5	25	
Tutoríal		Direction and supervision of the student's study and activities. Raising of questions. Resolution of doubts.	Discussion with the teacher on the conceptual and methodological difficulties encountered when studying the subject. Raising questions and answering those proposed by the teacher.	Not assessable				
Programmed tutorials		Proposal and critical evaluation of work. Presentation and proposal of new objectives.	Cooperation with classmates in the preparation of work. Critical analysis of the work of other groups. Oral presentation and discussion of work. Formulation of questions and doubts	Assessment of the work, the analyses carried out and the presentation.	3	4,5	7,5	

Teaching activity	Associated competences	Teacher activity	Student activty	Assessment procedure	P	NP	Total	C
Laboratory	CG1-MA1, CG2-MA1, CG2-MA2, CG3-MA1, CG4-MA1, CG7-MA1, CG8-MA1, CT1-MA1, CT2-MA1, CT3-MA1, CT4-MA1, CT5-MA1, CT7-MA1, CT8-MA1, CT12-MA1,CE11-MAQF2, CE11-MAQF3, CE12-MAQF2, CE13-MAQF1, CE13-MAQF2, CE13-MAQF3	Application of theoretical contents to practical problems. Development of experimental and numerical calculation skills. Obtaining and processing experimental data. Molecular modelling tools.	Preparation, completion and study of the proposed contents. Preparation of reports on some of the practicals carried out.	Assessment of the work carried out and the results obtained. Assessment of the practical reports presented. Assessment of the skills and knowledge acquired.	12	9	21	20%
Exams		Proposal, invigilation and correction of the exam. Grading of the student	Preparation and realization.	Correction and assessment of the exams.	5	6,5	11,5	60%
P : In-person; NP: Self-study; C: Evaluation								