COURSE DATA

Data Subject	
Code	44604
Name	Advanced physical chemistry
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2218 - Master's Degree in Chemistry	Faculty of Chemistry	1	First term

Subject-matter

Degree	Subject-matter	Character
2218 - Master's Degree in Chemistry	1 - Advanced chemistry	Obligatory

Coordination

Name	Department
PEREZ PLA, FRANCISCO	315 - Physical Chemistry

SUMMARY

The Advanced Physical Chemistry is part of the Advanced Chemistry matter, which aims to expand and complement the Physical Chemistry knowledge acquired in the Grade. Specifically, the course provides a deep insight into Molecular Spectroscopy introducing the basics of photochemistry. The subject also deepens in the thermodynamic study of real systems allowing a better understanding of these systems by reinforcing the knowledge of Statistical Thermodynamics of systems having intermolecular interactions. In this line, the basics of Chemical Kinetics seen in the Grade are extended to complex reactions, and the basic concepts of homogeneous and heterogeneous catalysis and biocatalysis are studied. Finally, the basics of electrochemistry are extended by means of the description of processes taking place on electrodes, in particular the kinetics of the processes that occur on them. The acquired skills are applied to study the problem of electrochemical corrosion.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

Previous knowledge of chemistry is required, at the level attained in the profiles recommended for admission of candidates to the Master Degree.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

2218 - Master's Degree in Chemistry

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Fomentar, en contextos académicos y profesionales del ámbito de la política económica, ?el avance tecnológico, social o cultural dentro de una sociedad basada en el conocimiento y en el respeto a: a) los derechos fundamentales y de igualdad de oportunidades entre hombres y mujeres, b) los principios de igualdad de oportunidades y accesibilidad universal de las personas con discapacidad y c) los valores propios de una cultura de paz y valores democrático.
- Be able to design, perform, analyse and interpret experiences and complex data in the environment of chemistry at a specialization level.
- Acquire advanced knowledge to assess the importance of chemistry in health, the environment, new materials and energy.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

(1) To know the physical bases of the different types of molecular spectroscopy and of the techniques derived from them, and the photophysical and photochemical processes.
(2) To Know how to relate intermolecular interactions and description of the different models of real systems (gases, liquids, electrolyte solutions and non-electrolytes), and use the concepts of transience and activity, radial distribution functions, partial molar properties and functions excess.
(3) To know the concepts of statistical thermodynamics, to systems and independent particles taking into account the intermolecular interactions and their application to obtaining state functions of real gases, liquids and solids behavior.

(4) To be able to obtain the relevant kinetic data of chemical reactions, from proposed mechanisms and know the basics of the homogeneous, heterogeneous catalysis and biocatalysis.
(5) To know the fundamentals of the electrode kinetics and its application to the study and corrosion inhibition.

DESCRIPTION OF CONTENTS

1. Molecular spectroscopy and photochemistry

General aspects of the interaction between light and matter. Models of electromagnetic radiation. Radiation and matter: absorption, emission, dispersion, diffusion and related spectroscopic techniques. Selection rules. The spectroscopic signal: position, width, intensity. Laser emission. Absorption coefficients.
Nuclear magnetic resonance spectroscopy. Basics of NMR technique in chemistry. Factors that determine the position of the NMR bands. Pulse techniques (NMR-TF). Free induction decay ("FID"). Spin Relaxation Time: longitudinal and transverse relaxation.
Electronic spectroscopy absorption and emission. Basics of the structure of the electronic spectra in diatomic molecules. Vibrational structure and the Franck-Condon principle. Different types of polyatomic molecule transitions. Photophysics and photochemistry: radiative and non-radiative transitions. Emission spectroscopy: fluorescence and phosphorescence.

2. Statistical thermodynamics of interacting systems

Intermolecular interactions. Multipolar moments, attractive forces, repulsive forces, models for intermolecular interactions and their limitations.
Statistical thermodynamics of real systems and condensed phases. Partition function of real systems and thermodynamic properties. Application of statistical thermodynamics to real gases. Heat capacity of crystalline solids. Radial distribution function and structure in liquids.
Simulation methods: Force fields, Strategies for simulations of realistic systems, Molecular Dynamics, Monte Carlo method.

3. Chemical Kinetics of complex reactions

Mechanism and rate law: Review of basic concepts. Complex reactions. Mechanism and rate law. Simplification of the rate law. Stationary linear equations.
Detection of reaction intermediates: Intermediate products and reaction centers. Techniques for the detection and characterization of intermediates. The technique of stopped-flow. Other techniques (SF-EXAFS, MS-ESI).
Data analysis Chemical Kinetics I: Monitoring of physical properties. Analysis of simple irreversible reactions. General analysis of simple reactions.
Data analysis Chemical Kinetics II: The response Model. Two-dimensional responses. Factorization of multi-channel responses. The chemical model. Systems of differential and algebraic-differential equations. The integration of model. Stiff systems. The least-squares technique. Objective functions. Minimization of the objective function.

4. Corrosion and electrodic processes

Electrochemistry of Molecules and and Materials.
Overview of Electrochemistry. Types of electrodes. Disturbance and electrical response in cells. Electrode processes. The interfacial region electrode / solution. Scales and units Electrochemical potential magnitudes.
Irreversibility Electrochemical Cells.
Faradaic and non-faradaic electrode processes. Transport in electrochemical cells. Nernst diffusion controlled processes. The electron transfer coefficient and the symmetry parameter.
Simulation and Data Processing in electrode Processes.
Current-potential curves. Voltammetry of electroactive films. Electro-synthesis and characterization of conductive polymers. Metal electro-deposits and electro-solutions. Equivalent electrical circuits. Simulation and multiparameter fitting of the electrode response.
Metallic Corrosion and Inhibition.
The phenomenon of corrosion. Corrosion types. Experimental techniques for measuring the corrosion rate. Predicting corrosion of technological materials. Methods for corrosion inhibition.

5. Catalysis

Basics. Interaction catalyst/substrate. Sabatiers principle. Catalyst deactivation: sintering and thermal degradation.
Homogeneous catalysis. Catalysis by metal complexes. Acid-base catalysis. Organocatalysis. Recovery and recycling of the homogeneous catalyst. hybrid catalysis. "Click Chemistry". Biocatalysis.
Heterogeneous catalysis. Stages of the catalytic process. Langmuir-Hinshelwood kinetics. Solid-gas catalysis. Solid catalyst types. Catalyst characterization. Catalytic solid / liquid and liquid / liquid systems. Phase-transfer catalysts.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	5,00	100
Seminars	5,00	100
Development of individual work	15,00	0
Study and independent work	30,00	0
Readings supplementary material	10,00	0
Preparation of evaluation activities	20,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

The subject will be taught through participatory lectures, seminars will be held where, among other training activities, applied practical problems, and tutored classes designed to assess understanding of the subject by students.

EVALUATION

First call:

The rating of the subject, on first call, will be obtained from the marks obtained in the final exam, continuous assessment activities conducted and the papers presented throughout the course. Exam, work and activities will be averaged according to the following percentages:

(A) Final exam: 60%.

(B) continuous assessment activities (b.1 + b.2): 40%.

(B.1) activities throughout the year: 20%.

(B.2) Work performed during the course: 20%.

Second call:

The rating of the subject, on second call, will be obtained from the exam grades obtained second call and the work presented throughout the course. Examination and averaged works according to the following percentages:

(A) Final exam: 80%.

(B) Work performed during the course: 20%.

REFERENCES

Basic

- ATKINS, P. W. Química Física, 6a ed. Ed. Omega, 1999. ISBN 8428211817
- ATKINS, P i DE PAULA, J. Química Física. 8a edició. Editorial Médica Panamericana, 2008. ISBN 9789500612487
- BANWELL, C. N. i McCASH, E.M. Fundamentals of Molecular Spectroscopy, 4a ed., McGraw-Hill, 1994. ISBN 9780077079765

- HORE, P. J. Nuclear Magnetic Resonance. Sèrie Oxford Chemistry Primers. Oxford University Press. Oxford. 1995 . ISBN 0198556829
- LEVINE, I. N. Physical Chemistry [6th edition], Mc Graw-Hill, Dubuque, IA, 2009
- CASTELLÁN, G. W. Físicoquímica, [2a ed., trad. M. Costas Basín i C. Amador Bedolla], Addison-Wesley, 1990.
- DÍAZ PEÑA, M. i MUNTANER, R. Química Física, [tom II], Alhambra, Madrid, 1975
- BERTÁN, J. i NÚÑEZ, J. (coords.) Química Física, Ariel, Barcelona 2002
- Mc.QUARRIE, D. A. Statistical Mechanics, University Sicence Books, Sausalito, 2000
- TUÑÓN, I. i SILLA, E. Química Molecular Estadística, Síntesis, Madrid, 2008
- STONE, A. The Theory of Intermolecular Forces, Oxford University Press, 2013
- ROTHENBERG, G. Catalysis. Concepts and Green Applications. Wiley-VCH, Weinheim. 2008
- PILLING, M. J. i SEAKINS, P. W. Reaction Kinetics, Oxford Science Publications, Oxford University Press, Oxford, 1999
- BARD, A.J. ; FAULKNER, L.R. Electrochemical Methods. Fundamentals and Applications. John Wiley &Sons, Inc. New York, 2001.
- MASEL, R.I. Chemical Kinetics and Catalysis. Wiley-Interscience, 2001.

Additional

- A. REQUENA, A. i ZÚÑIGA, J. Espectroscopia, Pearson Prentice Hall, Madrid, 2003. ISBN 8420536776
- PLANELLES, J., CLEMENTE, I. i GABRIEL, J. Espectroscòpia, Publicacions de la Universitat Jaume I. Castelló, 2002. ISBN 9788480213936
- HOLLAS, J. M. Modern Spectroscopy, 2a ed., John Wiley & Sons, 1992. ISBN 0471930776
- HARRIS, R. K. Nuclear Magnetic Resonance Spectroscopy. A Physico-chemical view, Pitman. Londres. 1983. ISBN 0273016849
- LEVINE, I. N. Espectroscopia Molecular, AC, 1980. ISBN 8472880389
- GRAYBEAL, J. D. Molecular Spectroscopy, McGraw-Hill, 1988
- BOCKRIS, J. O'M., REDDY, A., GAMBOA-ALDECO, M.E., Modern Electrochemistry 2A, Fundamentals of Electrodics. Springer-Verlag US, 2000.