UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2015/16
Subject (*)	Química Física Avanzada		Code	610G01020
Study programme	Grao en Química			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	1st four-month period	Fourth	Obligatoria	6
Language	SpanishEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química Física e Enxeñaría Química 1			
Coordinador	Iglesias Martinez, Emilia	E-mail	emilia.iglesias@udc.es	
Lecturers	Brandariz Lendoiro, Maria Isabel Iglesias Martinez, Emilia	E-mail	i.brandariz@udc.es emilia.iglesias@udc.es	
Web	campusvirtual.udc.es			
General description	KEY WORDS: ionic interactions and molecular transport phenomena. Rate equation and reaction mechanisms. Chemical Kinetic Theories. Homogeneous catalysis. Introduction to electrochemical kinetics. Macromolecules and colloids. DESCRIPTION: Advanced Physical Chemistry addresses the phenomenological study of the interactions between ions and molecules, which allow us to understand the configuration of macromolecules of chemical and biological interest. Transport phenomena in solution makes possible the characterization of macromolecules and are central to the application of certain techniques to kinetic study of reactions. Chemical kinetics introduces the time variable in the study of a chemical reaction, analyzing the factors that modify reaction rate in order to determine the rate equation, and finally to propose a reaction mechanism at the molecular level to interpret the observed macroscopic reaction.			

Study programme competences / results	
Code	Study programme competences / results
A1	Ability to use chemistry terminology, nomenclature, conventions and units
A3	Knowledge of characteristics of the different states of matter and theories used to describe them
A4	Knowledge of main types of chemical reaction and characteristics of each
A10	Knowledge of chemical kinetics, catalysis and reaction mechanisms
A14	Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry
A19	Ability to follow standard procedures and handle scientific equipment
A20	Ability to interpret data resulting from laboratory observation and measurement
A22	Ability to plan, design and develop projects and experiments
A23	Critical standards of excellence in experimental technique and analysis
A25	Ability to recognise and analyse link between chemistry and other disciplines, and presence of chemical processes in everyday life
A27	Ability to teach chemistry and related subjects at different academic levels
B1	Learning to learn
B3	Application of logical, critical, creative thinking
B4	Working independently on own initiative
C3	Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life
C6	Ability to assess critically the knowledge, technology and information available for problem solving

Learning outcomes	
Learning outcomes	Study programme competences / results

Methodology: · Be able to plan, design, and perform experiments related to the transport of matter and charge transport. · Be able to propose and design a kinetic study of a chemical reaction. · Simple software application to the quantitative analysis of kinetic data. · Interpretation of kinetic results on the basis of reaction mechanisms. · Simulation / prediction of unpublished data from the rate equation	A3 A19 A20 A22 A23 A27	B3	C3
Conceptual: · Knowledge of interionic interactions and inter-or intramolecular interactions and their relationship with association phenomena, self-aggregation or molecular conformation. · Mastering the own methods of chemical kinetics. Interpretation at molecular level (mechanistic) of chemical reactions. Understand and know the factors that can change the rate of a chemical reaction. · Understand the catalysis process and its relation to chemical-, photochemical- or electrochemical-activation	A1 A4 A10 A14	B3	
Attitudinal: · Provide appropriate reports of an experimental study · Analyze and critique published kinetic studies of low difficulty.	A23 A25 A27	B1 B3 B4	C3 C6

Contents	
Topic	**Sub-topic**
Ionic and molecular interactions	· Ionic interactions in the liquid phase: activity coefficient. Debye-Hucke's law. Ionic strength. · Molecular interactions. Dipole moment. Polarizability: equation of Clausius-Mossotti. Dipolar interactions. Hydrophobic interaction: self-aggregation and molecular conformation. ·Colloids: direct and reverse micelles, biological membranes. · Macromolecules
Transport phenomena	· Flux. Diffusion. Fick's first lay. Stokes-Einstein equation. · Thermal conductivity · Electric conductivity: the Deby-Huckel-Onsager theory. · Viscosity
Rate equation and reaction mechanism	· Integrated rate equation. Initial rates. Order of reaction. The method of flooding. Physical properties in kinetic studies. Experimental techniques. · Complex reaction schemes: parallel and concurrent reactions, reversible reactions, consecutive reactions. · The steady-state approximation. · Reaction mechanisms: elementary reactions. Deduction of reaction mechanisms.
Kinetic Theories and their applications	· Collisions theory: the frequency factor · Transition state theory. The activated complex. Statistical thermodynamics approach. Activation parameters. Potential energy surfaces. · Reactions in the gas phase: Lindeman mechanism · Reactions is solution. Diffusion controlled reactions · Electron transfer reactions: Marcus theory · Photochemical reactions
Catalysis	· Homogeneous, heterogeneous and microheterogeneous catalysis · General mechanism of catalysis: rate equations. · Homogeneous catalysis: nucleophilic catalysis, acid-base catalysis, ... · Linear free energy relations: the Swain-Scott equation, the Bronsted law, the Hammett correlation, the Taft equation. · Microheterogeneous catalysis; micellar catalysis, enzyme catalysis. Inhibition

Introduction to electrochemical kinetics	· Electrochemical reactions: special topics · Interface electrode-solution: the Gouy-Chapman model · Rate of charge transfer. The Butler-Volmer equation · Voltametry
Lab experiments	· Laboratory experiments relative to Transport phenomena, determination of rate equations and catalytic processes.

Planning				
Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A25 A27 B3	21	42	63
Seminar	A27 B1 C6	7	14	21
Laboratory practice	A19 A20 A22 A23 A27 B1 B4 C3	20	40	60
Mixed objective/subjective test	A1 A3 A4 A10 A14 A20	4	0	4
Personalized attention		2	0	2
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	Description
Guest lecture / keynote speech	? In the exposition classes the teacher introduces all concepts, models, methodologies and theories of the fundamental contents of the discipline program. Through the virtual campus, the student will can find the material that complements the class for his previous study and analysis. The previous reading of the subjects that expose in class, definitely, improves the academic yield and facilitates the interaction student-teacher.
Seminar	? Seminars: session to make the most important concepts and methods understandable to undergraduate students by means of the resolution of questions, problems and the criticism of practical studies. One of the important objectives of the seminars is to learn how to solve numerical problems, which help emphasize features in the underlying theory, and they illustrate practical applications.
Laboratory practice	?They will perform experiments related with the concepts treated in the discipline. The student will treat to reproduce simple laboratory experiments under the guidance of the instructor. Each student will have to elaborate a report of each experiment, following the indications of the professor, and /or the exposition / discussion of his results. It is required to pass the experimental probes to can pass the overall discipline.
Mixed objective/subjective test	? Proposal of questions and exercises, related with the concepts introduced in the classes of theory, seminar or in Lab experiments, to solve. The student alone will demonstrate, during a fixed time interval, the adquired knowledges and his capacity for solving exercices and/or developing conceptual questions.

Personalized attention	
Methodologies	Description
Laboratory practice	Previously to the experimental work, the student must understant the scientific article that summarizes the experiments to be make. For that he will be help by his instructor, as well as, during the experiments go on. After ending the Laboratory experiments, the instructor will help the student in the interpretation of the results on the basis of the models developed in class and in the Classroom of Computing for the quantitative treatment of results. It recommends to the students the use of tutorials to solve all kind of doubts, questions and concepts that have not remained sufficiently clear, and that refer, either to the development of material concepts or to find the answers to problems introduced in the seminars.

Assessment

Methodologies	Competencies / Results	Description	Qualification
Guest lecture / keynote speech	A25 A27 B3	? The participation of the student during the development of this activity, by means of the formulation of questions that help to understand concepts or by means of the proposal of alternative approaches, will be take into account in the final mark.	0
Seminar	A27 B1 C6	? Seminar sessions are supported on the personal work of each student. These sessions help emphasize topics and concepts introduced in the different parts of the course. They also serve of discussion scenary of the methodologies and procedures applied in each case. ? The evaluation of this activity will be based on the personal work in seminar sessions.	20
Laboratory practice	A19 A20 A22 A23 A27 B1 B4 C3	? Lab experiments reflect the abillity and capacity of the student in the planning, design and development of simple experiments. ? Essay of different techniques in the characterisation of systems or in monitoring reaction processes. ? Quantitative treatment of the experimental results following the models explained in the lectures. ? Explanation of the results on the basis of the theoretical models. ? Submitting a lab eport to reflect the previous concepts is required. ? For evaluating this activity it is taken into account the lab work, the obtained results, and the prepared report.	25
Mixed objective/subjective test	A1 A3 A4 A10 A14 A20	? Performance of written examination about theoretical and practical questions, regarding the contents treated in all parts of the course. ? It is required to surpass each of the activities to pass the course. The qualification of a surpassed activity will be kept in the remaining opportunities of the current academic year. ? Failure to pass the course, the final qualification shall correspond to the average of activities NON-exceeded. ? The maximum achievable quallification does not depend on the oppotunity in which the subject is surpass. ? The student will obtain the qualification of No Presented when he do not take part in the official examination (programming by the Faculty).	55

Assessment comments

Sources of information	
Basic	- P. W. Atkins, J. de Paula (2008). Química Física, 8ª Ed. . Panamericana - Espenson J. H. (1995). Chemical kinetics and reaction mechanisms 2ª ed.. McGraw-Hill, New York. - Laidler K. J. (1994). Chemical Kinetics . Harper and Row, New York. - Bockris, J.O.M., Reddy, A K.N. (1998). Modern Electrochemistry 1. Ionics. 2nd ed.. Plenum Press, New York

Complementary	- P. L. Brezonik (1994). Chemical Kinetics and Process Dynamic in Aquatic Systems.. Lewis Publishers - P. Sanz Pedredo (1992). Físicoquímica para Farmacia y Biología.. Masson-Salvat Medicina - R. A. Jackson (2004). Mechanism in Organic Reactions.. Royal Society of Chemistry (RSC) - LEVINE I. N. (2004). Fisicoquímica 5ª ed.. McGraw-Hill, Madrid - KORITA, J, DVORAK, J., KAVAN, L. (1987). Principles of Electrochemistry. 2nd ed.. Wiley, Chichester - BERRY R. S., RICE S. A., ROSS J. (2000). Physical Chemistry. 2ª ed.. Oxford University Press, New York - J. BERTRAN-RUSCA, J. NUÑEZ-DELGADO Eds , (2002). Química Física, vol. II. Ariel Ciencia - S. R. Logan (2000). Fundamentos de Cinética Química. Addison Wesley - BOCKRIS, J.O.M., REDDY, A.K.N., GAMBOA-ADELCO, M.E. (2000). Modern Electrochemistry 2A. Fundamentals of Electrodics.. Kluwer Academic/Plenum Press: New York

Recommendations
Subjects that it is recommended to have taken before
Química 1/610G01007 Química 2/610G01008 Química 3/610G01009 Química 4/610G01010 Química Física 1/610G01016 Química Física 2/610G01017 Química Física 3/610G01018 Experimentación en Química Física/610G01019
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments
They are necessary the knowledges of Chemistry and Physical Chemistry materias -To know draft,synthesize and correctly present a work. -To dominate the graphic representation, linear regression with basic knowledges of statistics. -To use at basic level tools of computing, such as Excel, Word, Power Point. -It recommends to know English of intermediate level (reading).