Teaching Guide					
Identifying Data					2014/15
Subject (*)	Química Física Aplicada			Code	610500005
Study programme	Mestrado Universitario en Ciencias. Tecnoloxías e Xestión Ambiental (plan 2012)				
Descriptors					
Cycle	Period	Year		Type	Credits
Official Master's Degree	1st four-month period	First		Optativa	6
Language	Spanish				
Prerequisites					
Department	Química Física e Enxeñaría Química 1				
Coordinador	Iglesias Martinez, Emilia		E-mail	emilia.iglesias@udc.es	
Lecturers	Brandariz Lendoiro, Maria Isabel Fernandez Perez, Maria Isabel Iglesias Martinez, Emilia Santaballa Lopez, Juan Arturo		E-mail	i.brandariz@udc.es isabel.fernandez.perez@udc.es emilia.iglesias@udc.es arturo.santaballa@udc.es	
Web	https://campusvirtual.udc.es/moodle/				
General description	Descriptores: Química Computacional. Química Física Supramolecular: catálisis supramolecular. Reconocimiento Molecular y Biocatálisis. Fotoquímica Aplicada: fotocatálisis. Electroquímica Aplicada: baterias, corrosión.				

Study programme competences	
Code	Study programme competences
A4	Coñecer en profundidade as características e fundamentos de diversos modelos químicos para o estudo de sistemas orgánicos, inorgánicos e biolóxicos, incluídos os materiais con proxección tecnológica.
A7	Coñecer o marco teórico e as aplicacións da electroquímica e da fotocatálise nos campos da enerxía e o medio ambiente.
A8	Coñecer os fundamentos das interaccións intermoleculares e as súas aplicacións no campo da catálise supramolecular,recoñecemento molecular e biocatálise.
A9	Coñecer algunhas aplicacións básicas da química computacional e dos programas de cálculo máis utilizados nos ámbitos da química e o medio ambiente.
A11	Coñecer as distintas técnicas experimentais e computacionales orientadas á caracterización de mecanismos de reacción.
A20	Coñecemento dos principais tipos de produtos naturais: enzimas, receptores moleculares, etc. Entender a súa participación en procesos de catálise e autoensamblaxe.
B1	Posuír e comprender coñecementos que acheguen unha base ou oportunidade de ser orixinais no desenvolvemento e/ou aplicación de ideas, a miúdo nun contexto de investigación.
B2	Que os estudantes saiban aplicar os coñecementos adquiridos e a súa capacidade de resolución de problemas en contornas novas ou pouco coñecidos dentro de contextos máis amplos (ou multidisciplinares) relacionados coa súa área de estudo.
B3	Que os estudantes sexan capaces de integrar coñecementos e enfrontarse á complexidade de formular xuízos a partir dunha información que, sendo incompleta ou limitada, inclúa reflexións sobre as responsabilidades sociais e éticas vinculadas á aplicación dos seus coñecementos e suizos.
B4	Que os estudantes saiban comunicar as súas conclusións e os coñecementos e razóns últimas que as sustentan a públicos especializados e non especializados dun modo claro e sen ambigüedades.
B5	Que os estudantes posúan as habilidades de aprendizaxe que lles permitan continuar estudando dun modo que haberá de ser en gran medida autodirixido ou autónomo.
B6	Ser capaz de analizar datos e situacións, xestionar a información dispoñible e sintetizala, todo iso a un nivel especializado.
B7	Ser capaz de planificar adecuadamente desenvolvementos experimentais, a un nivel especializado.
C1	Ser capaz de traballar en equipos, especialmente nos interdisciplinares e internacionais.
C4	Expresarse correctamente, tanto de forma oral coma escrita, nas linguas oficiais da comunidade autónoma.
C5	Dominar a expresión e a comprensión de forma oral e escrita dun idioma estranxeiro.
C6	Utilizar as ferramentas básicas das tecnoloxías da información e as comunicacións (TIC) necesarias para o exercicio da súa profesión e para a aprendizaxe ao longo da súa vida.
C9	Valorar criticamente o coñecemento, a tecnoloxía e a información dispoñible para resolver os problemas cos que deben enfrontarse.

C10	Asumir como profesional e cidadán a importancia da aprendizaxe ao longo da vida.
C11	Valorar a importancia que ten a investigación, a innovación e o desenvolvemento tecnolóxico no avance socioeconómico e cultural da sociedade.

Learning outcomes			
Subject competencies (Learning outcomes)	Study programme competences		
To acquire knowledge of new molecular structures, originating in solution, which are in borderline with biological systems. To know the applications of these media in the optimization of chemical separation processes, synthesis reaction, contaminant removal, etc..	AC4 AC7 AC8 AC9 AC11 AC20		
To analyze the properties of new microstructures, such as micelles, microemulsions, vesicles, liposomes, cyclodextrins, dendrimers, nanoparticles, etc. .. To explore new applications of these structures in basic processes, such as solubility, diverse equilibria, elimination processes, detection of compounds of interest .. ., and primarily on reactivity.		BC1 BC2 BC5 BC7	CC1 CC4 CC5 CC9 CC11
To acquire basic knowledge framed in Computational Chemistry, with special emphasis on the electronic structure calculations. To meet the most popular computer programs related to Computational Chemistry. To learn to make simple calculations of geometries, energies and other molecular properties.	AC9 AC11	BC2 BC3 BC4 BC5 BC6 BC7	CC1 CC4 CC5 CC6 CC9 CC10 CC11

Contents	
Topic	Sub-topic
TEMA 1.Computational Chemistry	Introduction Ab Initio Methods Functional Theory Density Semiempirical methods Base functions Molecular Mechanics Molecular dynamics. Computational Chemistry Programs Calculating properties
TEMA 2. Physical Chemistry Supramolecular	Surfactants in water. Surfactants in solvents. Chemical reactions in microheterogeneous media: the simple pseudophase model and the ion-exchange pseudophase model .
TEMA 3. Molecular Recognition and Biocatalysis	Host-guest systems. Typical hosts: cyclodextrins, polyethers, siderophiles, dendrimers, ..., DNA. Ligands of interest: ions, drugs, pesticides, cosmetics. Pharmacological and industrial applications.
TEMA 4 Applied Photochemistry	Photochemical reactions. photocatalysis Supramolecular Photochemistry. Fluorophores and microenvironment. Photochemical processes in supramolecular complexes. Fluorescence protein. DNA technology.

TEMA 5. Applied Electrochemistry	Potentiometric titrations. Ion-selective electrodes. Membrane potentials. Batteries and fuel cells. Corrosion.

Planning			
Methodologies / tests	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	20	20	40
Critical bibliographical	6	12	18
Seminar	8	16	24
Laboratory practice	24	36	60
Oral presentation	1	2	3
Long answer / essay questions	4	0	4
Personalized attention	1	0	1
(*)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	Oral presentation for the introduction of the different content of the course.
Critical bibliographical	Critical reading of scientific papers.
Seminar	Working Group for the study and discussion of scientific papers and other aspects with regard the understanding of the theoretical contents and laboratory experiments
Laboratory practice	Application of technologies and methodologies to the study and characterization of specific chemical systems related to the contents of the subject.
Oral presentation	Oral presentation of the results obtained from the experiments, techniques and methodologies used in joint and participatory seminar for all students.
Long answer / essay questions	Written test to measure comprehension ability, reasoning, synthesis, drafting, ..., of the student towards questions of certain extent.

Personalized attention	
Methodologies	Description
Critical bibliographical Laboratory practice	Help in interpreting scientific studies, in reviewing and providing related literature. Technical and methodological help for the development of Lab experiments.

Assessment		
Methodologies	Description	Qualification
Oral presentation	Oral presentation of results and analysis of the practical work. Assessed competencies: AM9, AM11, B2, B3, B4, B5, B6, C1, C4, C5, C6, C9, C10, C11.	25
Guest lecture / keynote speech	Participacion in lectures. Assessed competencies: AM9, AM11, B5, C4, C5, C10, C11.	5
Critical bibliographical	Critical analysis of scientific work. Discussion on study alternatives, improvement of results, future prespective showing the creative and innovative capacity of the student. Assessed competencies: AM9, AM11, B2, B3, B4, B5, B7, C4, C5, C6, C9, C10, C11.	20

Laboratory practice	Expertise, skills shown in the laboratory. Results obtained in the experimental work. Assessed competencies: AM9, AM11, B2, B3, B4, B5, B6, B7, C1, C4, C5, C9, C10, C11.	15
Long answer / essay questions	Degree of concepts' assimilation and comprehension. Ability to summarize and writing. Assessed competencies: AM9, AM11, A8, A20, B2, B3, B4, B5, B6, C4, C5, C6, C9.	30
Seminar	Participation in the discussion of the topics, development of theoretical activities, practical demonstrations and exercises solving. Assessed competencies: AM9, AM11, B1, B2, B3, B4, B5, B6, C4, C5, C9, C10, C11.	5

Assessment comments

Sources of information	
Basic	- Bockris, John O'M., Reddy, Amulya K.N. Gamboa-Aldeco, Maria. (2000). Modern electrochemistry 2B. Electrodics in chemistry, engineering, biology, and environmental science. New York : Kluwer Academic / Plenum Publishers] - Connors, K.A. (1987). Binding Constants. The Measurement of Molecular Complex Stability. . Wiley & Sons: New York, - Lewars, E. G. (2011). Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics. Springer - J. Szejtli (1988). Cyclodextrin Technology. Kluwer Academic Publishers (The Neherlands) - Hinchliffe, A. (2008). Molecular Modelling for Beginners. Wiley - J. R. Lakowicz (2006). Principles of Fluorescence Spectroscopy. Springer Science (New York) - V. Balzani, F. Scandola (1991). Supramolecular Photochemistry. Ellis Horwood (Chicherter, England) - M. J. Rosen (1989). Surfactants and Interfacial Phenomena. John Wiley & Sons - Raoutl Zana (1987). Surfactants in Solution. New Methods of investigation. Marcel Dekker (New York)
Complementary	- Cramer, C. A. (2004). Essentials of Computational Chemistry: Theories and Models. Wiley

Recommendations
Subjects that it is recommended to have taken before
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.