



Teaching Guide

Identifying Data				
Subject (*)			Code	2023/24
Applied Physical Chemistry			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	Optional	6
Language	SpanishEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador			E-mail	
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	Descriptors: Computational Chemistry; Supramolecular Chemistry: Supramolecular catalysis; Biocatalysis and Molecular Recognition. Applied Photochemistry: photocatalysis. Applied Electrochemistry: batteries, corrosion.			

Study programme competences

Code	Study programme competences
A1	Coñecemento das realidades interdisciplinares da Química e do Medio Ambiente, dos temas punteiros nestas disciplinas e das perspectivas de futuro.
A7	Coñecer o marco teórico e as aplicacións da electroquímica e da fotocatalise 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 biocatalise.
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 computacionais 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 coñecidas 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 suízos.
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.
C1	Ser capaz de traballar en equipos, especialmente nos interdisciplinares e internacionais.
C3	Ser capaz de adaptarse a situacións novas, mostrando creatividade, iniciativa, espírito emprendedor e capacidade de liderado.
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			
Learning outcomes	Study programme competences		
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 BC3 BC5	CC1 CC3 CC5 CC9 CC11
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..	AC1 AC7 AC8 AC9 AC11 AC20		
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.	AC1 AC7 AC8 AC9 AC11	BC1 BC2 BC3 BC5	CC1 CC3 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	Competencies	Ordinary class hours	Student's personal work hours	Total hours
Guest lecture / keynote speech	A7 A8 A9 A11 A20	15	15	30
Laboratory practice	B1 B5 C3 C1 C9 C11	20	40	60
Supervised projects	B1 B2 B3 C5 C6 C10	8	20	28
Long answer / essay questions	A1 A7 A8 A9 A20	4	8	12
Multiple-choice questions	A1 A7 A8 A9 A20	4	16	20
Personalized attention		0	0	0
(*)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	It will be described the general lines of the course and the introduction of its fundamental contents.
Laboratory practice	Application of technologies and methodologies to the study and characterization of specific chemical systems related to the contents of the subject.
Supervised projects	The student will read one or two recent articles related to supramolecular chemistry topics to prepare a report summarizing the relevant information and results.
Long answer / essay questions	Written test to evaluate the reasoning, synthesis, writing ability ... in practical questions of a certain extent.
Multiple-choice questions	Written test to measure comprehension ability, reasoning, synthesis, drafting, ..., of the student towards questions of certain extent.

Personalized attention	
Methodologies	Description
Supervised projects Laboratory practice	The use of tutorials is recommended (either in person, by email, through the Moodle forums or through Teams) to resolve any questions that arise in relation to any topic or type of methodology. Teachers will be available to solve any need or answer any questions during the established tutoring hours. Part-time students or those with academic attendance exemption will be attended in tutorials, both in person and by telematic means, whenever they need it.

Assessment			
Methodologies	Competencies	Description	Qualification
Supervised projects	B1 B2 B3 C5 C6 C10	The report is evaluated, which can be prepared following a questionnaire that specifies the system under study, the technique and methodology used, the results obtained, the most relevant conclusions and the future perspective proposed by the student.	40
Long answer / essay questions	A1 A7 A8 A9 A20	Reduced length test to measure the degree of assimilation and understanding of concepts and the ability to synthesize and write. It can be done through Moodle or in person.	10
Laboratory practice	B1 B5 C3 C1 C9 C11	Expertise, skills shown in the laboratory. Results obtained in the experimental work.	40
Multiple-choice questions	A1 A7 A8 A9 A20	Multiple-choice test to answer through Moodle in a limited time on basic and conceptual contents.	10

Assessment comments

Sources of information

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

Programa Green Campus Facultade de Ciencias Para axudar a conseguir unha contorna inmediata sustentable e cumprir co punto 6 da "Declaración Ambiental da Facultade de Ciencias (2020)", os traballos documentais que se realicen nesta materia: a. Solicitaranse maioritariamente en formato virtual e soporte informático. b. De realizarse en papel: - Non se empregarán plásticos. - Realizaranse impresións a dobre cara. - Empregarase papel reciclado. - Evitarase a realización de borradores. Perspectiva de xénero: Segundo se recolle nas distintas normativas de aplicación para a docencia universitaria incorpórase a perspectiva de xénero nesta materia, polo que deberás usarse linguaxe non sexista, utilizarase bibliografía de autores/as de diversos xéneros, propiciarse a intervención en clase de alumnos e alumnas.... Ademais, traballarase para identificar e modificar prexuízos e actitudes sexistas e influirase na contorna para modificalos e fomentar valores de respecto e igualdade. Prestárase atención á detectar situacións de discriminación por razón de xénero e proporanse accións e medidas para corrixilas.

(*)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.