| Teaching Guide | | | | |
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| Identifying Data | | | | 2020/21 |
| Subject (*) | Applied Physical Chemistry | | 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 | Optional | 6 |
| Language | SpanishEnglish | | | |
| Teaching method | Face-to-face | | | |
| Prerequisites | | | | |
| Department | Química | | | |
| Coordinador | Iglesias Martinez, Emilia | E-mail | emilia.iglesias@udc.es | |
| Lecturers | Iglesias Martinez, Emilia | E-mail | emilia.iglesias@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. | | | |
| Contingency plan | 1. Modifications to the contents<br>-No changes will be done<br>2. Methodologies<br>*Teaching methodologies that are maintained<br>(virtual format):<br>-Master session<br>-Tutored works<br>-Customized attention<br>-Multiple response test<br>-Assay test<br>*Teaching methodologies that are modified<br>-Laboratory experiments<br>3. Mechanisms for personalized attention to students<br>-e-mail , -Moodle forums -Teams<br><br>4. Modifications in the evaluation<br>-The Lab experiments mark will be added to the tutored work.<br>*Evaluation observations:<br><br>5. Modifications to the bibliography or webgraphy<br>-All material will be supplied by Moodle | | | |

| Study programme competences | |
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| 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 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. |

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| 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. |
| 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 | | | |
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| 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<br>BC2<br>BC3<br>BC5 | CC1<br>CC3<br>CC5<br>CC9<br>CC11 |
| To acquire knowledge of new molecular structures, originating in solution, which are in borderline with biological systems.<br>To know the applications of these media in the optimization of chemical separation processes, synthesis reaction, contaminant removal, etc.. | AC1<br>AC7<br>AC8<br>AC9<br>AC11<br>AC20 | | |
| To acquire basic knowledge framed in Computational Chemistry, with special emphasis on the electronic structure calculations.<br>To meet the most popular computer programs related to Computational Chemistry.<br>To learn to make simple calculations of geometries, energies and other molecular properties. | AC1<br>AC7<br>AC8<br>AC9<br>AC11 | BC1<br>BC2<br>BC3<br>BC5 | CC1<br>CC3<br>CC5<br>CC6<br>CC9<br>CC10<br>CC11 |

| Contents | |
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| Topic | Sub-topic |

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| TEMA 1.Computational Chemistry | Introduction<br>Ab Initio Methods<br>Functional Theory Density<br>Semiempirical methods<br>Base functions<br>Molecular Mechanics<br>Molecular dynamics. Computational Chemistry Programs<br>Calculating properties |
| TEMA 2. Physical Chemistry Supramolecular | Surfactants in water.<br>Surfactants in solvents.<br>Chemical reactions in microheterogeneous media: the simple pseudophase model and the ion-exchange pseudophase model . |
| TEMA 3. Molecular Recognition and Biocatalysis | Host-guest systems.<br>Typical hosts: cyclodextrins, polyethers, siderophiles, dendrimers, ..., DNA.<br>Ligands of interest: ions, drugs, pesticides, cosmetics.<br>Pharmacological and industrial applications. |
| TEMA 4 Applied Photochemistry | Photochemical reactions. photocatalysis<br>Supramolecular Photochemistry. Fluorophores and microenvironment.<br>Photochemical processes in supramolecular complexes.<br>Fluorescence protein. DNA technology. |
| TEMA 5. Applied Electrochemistry | Potentiometric titrations.<br>Ion-selective electrodes. Membrane potentials.<br>Batteries and fuel cells.<br>Corrosion. |

| Planning | | | | |
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| 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 | |
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| Methodologies | Description |
| Guest lecture / keynote speech | Il 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 |
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| Methodologies | Description |
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| Supervised projects<br>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.<br>Teachers will be available to solve any need or answer any questions during the established tutoring hours.<br>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. | 20 |
| 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. | 30 |
| Laboratory practice | B1 B5 C3 C1 C9 C11 | Expertise, skills shown in the laboratory. Results obtained in the experimental work. | 20 |
| Multiple-choice questions | A1 A7 A8 A9 A20 | Multiple-choice test to answer through Moodle in a limited time on basic and conceptual contents. | 30 |

| Assessment comments |
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| Sources of information | |
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| Basic | - J. R. Lakowicz (2006). Principles of Fluorescence Spectroscopy. Springer Science (New York)<br>- Connors, K.A. (1987). Binding Constants. The Measurement of Molecular Complex Stability. . Wiley & Sons: New York,<br>- V. Balzani, F. Scandola (1991). Supramolecular Photochemistry. Ellis Horwood (Chicherter, England)<br>- M. J. Rosen (1989). Surfactants and Interfacial Phenomena. John Wiley & Sons<br>- Raoutl Zana (1987). Surfactants in Solution. New Methods of investigation. Marcel Dekker (New York)<br>- J. Szejtli (1988). Cyclodextrin Technology. Kluwer Academic Publishers (The Neherlands)<br>- 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]<br>- Lewars, E. G. (2011). Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics. Springer<br>- Hinchliffe, A. (2008). Molecular Modelling for Beginners. Wiley |
| Complementary | - Cramer, C. A. (2004). Essentials of Computational Chemistry: Theories and Models. Wiley |

| Recommendations |
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| Subjects that it is recommended to have taken before |
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| Subjects that are recommended to be taken simultaneously |
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| Subjects that continue the syllabus |
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| Other comments |
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(*)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.