



| Teaching Guide           |   |        |                        |         |
|--------------------------|---|--------|------------------------|---------|
| Identifying Data         |   |        |                        | 2018/19 |
| 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                      | <a href="https://campusvirtual.udc.es/moodle/">https://campusvirtual.udc.es/moodle/</a>   |        |                        |         |
| General description      | Descriptors: Computational Chemistry; Supramolecular Chemistry: Supramolecular catalysis; Biocatalysis and Molecular Recognition. Applied Photochemistry: photocatalysis. Applied Electrochemistry: batteries, corrosion. |        |                        |         |

| Study programme competences / results |  |
|---------------------------------------|--|
| Code                                  | Study programme competences / results  |
| A1                                    | Coñecemento das realidades interdisciplinares da Química e do Medio Ambiente, dos temas punteiros nestas disciplinas e das perspectivas de futuro.   |
| 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 tecnolóxica.  |
| 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 xuízos. |
| 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.  |
| C3                                    | Ser capaz de adaptarse a situacións novas, mostrando creatividade, iniciativa, espírito emprendedor e capacidade de liderado.  |
| 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 afrontarse.              |
| 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 / results           |  |   |
| 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>AC4<br>AC7<br>AC8<br>AC9<br>AC11<br>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<br>BC2<br>BC5<br>BC7               | CC1<br>CC3<br>CC4<br>CC5<br>CC9<br>CC11         |
| 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.  | AC9<br>AC11                                     | BC2<br>BC3<br>BC4<br>BC5<br>BC6<br>BC7 | CC1<br>CC4<br>CC5<br>CC6<br>CC9<br>CC10<br>CC11 |

| Contents                                       |  |
|--|--|
| Topic  | Sub-topic  |
| 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                       |                          |                                      |                               |             |
|--------------------------------|--------------------------|--------------------------------------|-------------------------------|-------------|
| Methodologies / tests          | Competencies / Results   | Teaching hours (in-person & virtual) | Student's personal work hours | Total hours |
| Guest lecture / keynote speech | B3 B4                    | 13                                   | 13                            | 26          |
| Critical bibliographical       | B5 B6 B7 C5              | 1                                    | 10                            | 11          |
| Seminar                        | A9 A11 B2 C1             | 7                                    | 28                            | 35          |
| Laboratory practice            | B1 B5 B6 B7 C3 C9<br>C11 | 20                                   | 40                            | 60          |
| Oral presentation              | C4 C6 C10                | 1                                    | 5                             | 6           |
| Long answer / essay questions  | A1 A4 A7 A8 A20          | 3                                    | 9                             | 12          |
| 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 | 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   |
| Oral presentation              | Help in interpreting scientific studies, in reviewing and providing related literature. |
| Guest lecture / keynote speech | Technical and methodological help for the development of Lab experiments.               |
| Critical bibliographical       |   |
| Laboratory practice            |   |
| Long answer / essay questions  |   |
| Seminar                        |   |

| Assessment |
|------------|
|------------|



| Methodologies                 | Competencies / Results | Description   | Qualification |
|-------------------------------|------------------------|---|---------------|
| Oral presentation             | C4 C6 C10              | Oral presentation of results and analysis of the practical work.  | 15            |
| Critical bibliographical      | B5 B6 B7 C5            | Critical analysis of scientific work. Discussion on study alternatives, improvement of results, future perspective showing the creative and innovative capacity of the student. | 30            |
| Laboratory practice           | B1 B5 B6 B7 C3 C9 C11  | Expertise, skills shown in the laboratory. Results obtained in the experimental work.   | 15            |
| Long answer / essay questions | A1 A4 A7 A8 A20        | Degree of concepts' assimilation and comprehension. Ability to summarize and writing.   | 30            |
| Seminar                       | A9 A11 B2 C1           | Participation in the discussion of the topics, development of theoretical activities, practical demonstrations and exercises solving.   | 10            |

#### Assessment comments

#### Sources of information

|                      |   |
|----------------------|---|
| <b>Basic</b>         | <ul style="list-style-type: none"><li>- J. R. Lakowicz (2006). Principles of Fluorescence Spectroscopy. Springer Science (New York)</li><li>- Connors, K.A. (1987). Binding Constants. The Measurement of Molecular Complex Stability. . Wiley &amp; Sons: New York,</li><li>- V. Balzani, F. Scandola (1991). Supramolecular Photochemistry. Ellis Horwood (Chichester, England)</li><li>- M. J. Rosen (1989). Surfactants and Interfacial Phenomena. John Wiley &amp; Sons</li><li>- Raouf Zana (1987). Surfactants in Solution. New Methods of investigation. Marcel Dekker (New York)</li><li>- J. Szejtli (1988). Cyclodextrin Technology. Kluwer Academic Publishers (The Netherlands)</li><li>- Bockris, John O'M., Reddy, Amulya K.N. Gamboa-Aldeco, Maria. (2000). Modern electrochemistry 2B. Electrodes in chemistry, engineering, biology, and environmental science. New York : Kluwer Academic / Plenum Publishers]</li><li>- Lewars, E. G. (2011). Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics. Springer</li><li>- Hinchliffe, A. (2008). Molecular Modelling for Beginners. Wiley</li></ul> |
| <b>Complementary</b> | <ul style="list-style-type: none"><li>- Cramer, C. A. (2004). Essentials of Computational Chemistry: Theories and Models. Wiley</li></ul>   |

#### 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.