Study Plan

School: School of Sciences and Technology
Degree: Master
Course: Chemistry (cód. 725)

1st Year - 1st Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13540M	Analysis and Characterisation of Materials	Chemistry	6	Semester	156
QUI13541M	Porous Materials	Chemistry	6	Semester	156
QUI13538M	Applied Organic Chemistry	Chemistry	6	Semester	156
QUI13518M	Analysis and Characterization of Organic Compounds	Chemistry	6	Semester	156
QUI13520M	Environmental Chemistry	Chemistry	6	Semester	156

1st Year - 2nd Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13521M	Modeling and Simulation in Chemistry	Chemistry	6	Semester	156
QUI13544M	Catalysis and Catalytic Methods	Chemistry	6	Semester	156

Options

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13542M	Adsorption by Materials	Chemistry	6	Semester	156
QUI13527M	Functional Materials	Chemistry	6	Semester	156
QUI13549M	Polymers and Applications	Chemistry	6	Semester	156
QUI13522M	Medicinal Chemistry	Chemistry	6	Semester	156
QUI13537M	Synthesis of Bioactive Compounds	Chemistry	6	Semester	156
QUI13526M	Water Analysis and Treatment and Valorization of Liquid Effluents	Chemistry	6	Semester	156
QUI13523M	Solid Waste Valorization	Chemistry	6	Semester	156
QUI13524M	Electrochemistry and Corrosion	Chemistry	6	Semester	156
QUI13525M	Molecules and Technology	Chemistry	6	Semester	156

2nd Year - 3rd Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13543M	Seminar	Chemistry	3	Year	78
Dissertation					

2nd Year - 4th Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
Dissertation					

Conditions for obtaining the Degree:

*** TRANSLATE ME: Para conclusão do curso é necessário a aprovação (através de avaliação ou creditação) das seguintes unidades curriculares:

1.º Ano

1.º Semestre:

5 UC obrigatórias num total de 30 ECTS

2.º Semestre:

2 UC obrigatórias num total de 12 ECTS

3 UC optativas do Grupo Optativas num total de 18 ECTS

2.º Ano

3.º e 4.º Semestre:

1 UC obrigatória num total de 3 ECTS

Para obtenção do grau, é necessário também a aprovação na Dissertação com um total de 57 ECTS, no 3.º e 4.º Semestre. ***

Program Contents

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Analysis and Characterisation of Materials (QUI13540M)

Theoretical component

1.Vacuum systems, theory and equipments. 2.Surface chemistry. Insaturated centres, hydration and hydroxylation, Brønsted and Lewis acidity. Isoelectric point and point of zero charge. Boehm method. 3.Systematization of some techniques based on emission, absorption and dispersion of X rays. X ray diffraction. X ray photoelectron spectroscopy. 4.True, apparent and bulk density of solids. 5. Infrared, Raman and NMR spectroscopies. 6.Microscopy. 7.Thermal analysis and microcalorimetry. 8.Digestion of solid samples and analysis by ICP.

Practical component

Analysis and characterisation, by different techniques, of materials prepared in the curricular unit Porous Materials.

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Porous Materials (QUI13541M)

Theoretical component

Definitions and general principles. Main microporous and mesoporous materials and their relevance in scientific and technological contexts. Sol-gel method. Porous structure, fundamentals of methods of preparation, influence of conditions on the porosity and applications of porous materials, namely: carbon materials; zeolites and zeotypes; clays and pillared clays; ordered mesoporous materials; inorganic-organic hybrid materials; porous composite materials. Regeneration methods of porous materials. Modification methods to control the properties of materials.

Practical component

Preparation of microporous and mesoporous materials of various types under different conditions and by different methods. The materials will be characterised in the curricular unit Analysis and Characterisation of Materials.

Back

Applied Organic Chemistry (QUI13538M)

Anthropogenic organic compounds. Persistent organic pollutants (POPs), hydrocarbons, organic solvents and volatile organic compounds (VOCs), perfluorinated compounds (PFCs), flame retardants, cleaning agents and corrosion inhibitors, pharmaceuticals and personal care products, pesticides and others.
Reactions of organic compounds (such as drugs or pollutants etc) and mechanisms. Hydrolysis, reduction, oxidation and C-C bond forming reactions. The photochemical and electronic behaviour of conjugated and aromatic compounds. Photochemical reactions of selected compounds.
Biotransformations. Reactions mediated by microorganisms. Enzyme Catalyzed Reactions.

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Analysis and Characterization of Organic Compounds (QUI13518M)

Separation techniques and isolation of organic compounds:
Column chromatography, HPLC and GC.
Stationary phases, eluents and detection methods.
Hyphenated techniques (LC and GC-MS).
Advanced spectroscopic and spectrometric techniques for structural analysis of organic compounds:
One and two-dimensional of spectrometric techniques of NMR (1H, 13C, DEPT, COSY, HMBC, HMQC, INADEQUATE, NOESY, TOCSY,...).
NMR spectrometry of other important nuclei (15N, 19F, 31P and 29Si).
Infrared spectrometry (FT-IR).
Mass spectrometry.

Back

Environmental Chemistry (QUI13520M)

Air pollutants and its action. Stratospheric ozone. Photochemical smog. Acid rain. Air particles in suspension. Volatile organic compounds. Greenhouse effect gases. Metals and metallic compounds. Air pollutants monitoring. Environmental laws. Standard methods for monitoring the main air pollutants.
Chemical equilibriums in natural waters: acid-base equilibrium; solubility equilibriums; redox equilibriums. Natural cycle and regulation of trace metals in aquatic environments: Global cycling of metals; solid - water interface; complexation by humic substances; hydrophobic systems; regulation of heavy metals in rivers, lakes and oceans. Regulation of the chemical composition of natural waters: biogeochemical cycles of carbon, nitrogen and sulfur; Interdependence of biogeochemical cycles. Nature and types of aquatic pollutants: Eutrophication. Modelling applied to environmental systems.

Back

Modeling and Simulation in Chemistry (QUI13521M)

Molecular interactions. Intra-molecular and inter-molecular interaction models. Molecular mechanics and force-fields. Review of Statistical Mechanics fundamentals. Introduction to Molecular Simulations. Periodic boundary conditions. Trajectories and properties. Molecular dynamics. Simulations in the micro-canonical, canonical and isobaric ensembles. Metropolis Monte Carlo. Canonical, isothermal-isobaric, grand-canonical and Gibbs ensembles. Non-Boltzmannian sampling. Analysis of simulation results. Analysis of the simulation equilibration. Radial distribution functions. Mechanical properties. Correlation functions. Dynamical properties.
Examples of the use of Monte Carlo and Molecular Dynamics simulations for the calculation of properties (density, vapor pressure, diffusion coefficient, viscosity, solubility) and analysis of the structure of model systems involving aqueous solutions of pollutants, alternative solvents, gases dissolved in liquids, fuels and lubricants.

Back

Catalysis and Catalytic Methods (QUI13544M)

Importance of catalysis and mode of operation of catalysts. Overview of catalysis types.
Homogeneous catalysis. Fundamental concepts. Organometallic and coordination chemistry: concepts, fundamental reactions and processes. Role of the metallic center and ligands. Catalytic cycles, kinetic aspects and catalyst regeneration. New trends in homogeneous catalysts and new ligands.
Heterogeneous catalysis. Fundamental concepts. Materials for heterogeneous catalysis. Deactivation and preparation of catalysts. Kinetics and Mechanisms. Spectroscopic characterization of catalysts and surfaces. Introduction to catalytic reactors.
Bio-, electro and photocatalysis. Organocatalysis. Supramolecular catalysis. Immobilized organocatalysts. Ionic liquids as catalysts.
Case studies: applications in chemistry, energy sources from renewable resources and environmental remediation.

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Adsorption by Materials (QUI13542M)

Theoretical component
1. General concepts and terminology. The role of adsorption in different scientific and technological contexts. 2. Adsorption from the gas phase. Experimental methodologies. Adsorption mechanisms. Adsorption isotherms. Models and theories, and their application for textural characterisation. Comparative methods. Adsorption of probe molecules for the acidity evaluation. Thermodynamics of adsorption. Kinetics of adsorption. Examples of adsorption of different gases and vapours by different classes of materials. 3. Adsorption from the liquid phase. Experimental methodologies. Adsorption from dilute solutions. Classification and interpretation of isotherms. Kinetics of adsorption. Examples of adsorption of cations, organic solutes and biomolecules by different materials.

Practical component
Analysis of adsorption isotherms. Experimental determination of isotherms of adsorption from gas phase and aqueous solutions by materials prepared in the UC Porous Materials.

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Functional Materials (QUI13527M)

Concept of functional materials. Overview of functional materials and their applications.
Solar energy: photovoltaic, thermophotovoltaic and photoelectrochemical cells. Molecules for Dye-sensitized solar cells (DSSCs).
Hydrogen production and storage: electrolytic production and storage methods. Fuel cells: hydrocarbon processing and alternative fuels. Lithium-ion batteries and supercapacitors.
Materials for optoelectronics and photonics, electro- and photochromic materials, molecular switching, luminescent materials.
Chemical sensors and biosensors. Biomolecular labeling.
Intelligent controlled drug and other substances delivery materials. Biomaterials.
Materials for chemical and photocatalytic decomposition of organic compounds and removal of pollutants.

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Polymers and Applications (QUI13549M)

1: Introduction to Polymers. 2: Polymer Molecular Structure. 3: Polymerisation Mechanisms. 4: Polymer Properties. 5: Polymer Processing. 6: Elastomers and Gels. 7: Network Polymers. 8: Natural Polymers. 9: Syntheses of Polymers. 10: Polymers Characterisation. 11: Biomaterials. 12: Health, Energy, Transport, Construction and Environmental Applications. 13: Polymers on Circular Economy. 14: Future Perspectives.

Back

Medicinal Chemistry (QUI13522M)

- Introduction to Medicinal Chemistry, its importance and historical perspective. Nomenclature and classification of drugs.
- Mode of action of drugs and therapeutic targets: molecular mechanisms of drug action in lipids, carbohydrates, proteins and nucleic acids. Receptors. Molecular recognition and cellular communication.
- General cycle of drugs in the body. Pharmacokinetics: Absorption, Distribution, Metabolism and Excretion of drugs; prodrugs.
- Qualitative and quantitative structure-activity relationships (SARs).
- Main sources of obtaining drugs. Methods of searching, finding and isolating new drugs; development and production of new drugs.
- Development and production of new drugs.
- Study of some drugs: chemical structures, mechanisms of action, structure-activity relationship, pharmacodynamics, pharmacokinetics and applications.

Back

Synthesis of Bioactive Compounds (QUI13537M)

Importance of bioactive molecules and fields of action (drugs, biocides, etc). Chemical Synthesis in obtaining bioactive molecules. Chemical Synthesis in the "discovery" and "planning" of new bioactive molecules. Target-oriented synthesis, diversity-oriented synthesis and structure-based design. Retrossynthetic analysis. Interconversion of Functional Groups. Transition metal catalyzed cross coupling reactions: examples. Molecular rearrangements. Asymmetric synthesis. Stereoselectivity and Regioselectivity. Sustainable Chemical Synthesis; new synthesis processes with green technologies: biocatalysis, microwave assisted synthesis, etc. Synthesis of APIs on an industrial scale; approach to scale-up. Equipment, purity and control at different stages of synthesis at industrial level. Product separation, purification and drying. Dissemination of results and protection of intellectual property. Patents.

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Water Analysis and Treatment and Valorization of Liquid Effluents (QUI13526M)

1. Management of water supply systems
Qualitative and quantitative characterization of water
Main water treatment processes and operations
Design considerations of the main equipment
Treatment stages of water supply systems
2. Wastewater types
Wastewater constituents
Wastewater sources, flow rates and constituent loadings
Wastewater legislation
3. Wastewater treatment processes and operations
Types of physical, chemical and biological unit processes
Description, application and design considerations of the main equipment
4. Treatment stages of municipal and some industrial wastewaters
Main goals and processes in every treatment stage
5. Wastewater reclamation and reuse
Wastewater reuse applications
Public health and environmental issues
6. Sludge treatment, disposal and reuse
Sludge sources, characteristics and quantities
Treatment operations and processes. Main stages of sludge treatment
Regulations for reuse and disposal
7. Alternative or advanced treatment systems
8. Case studies

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Solid Waste Valorization (QUI13523M)

1-Introduction
2-Description and classification of residues
3-Characterization of the dangerousness of solid waste
4-National production of solid waste
5-Physical, chemical and biological characteristics of municipal solid waste (RSU);
6-Sources, types and characteristics of hazardous waste present in RSU;
7-Industrial and agricultural waste
8-Legislative, National and European framework;
9-Waste management: operators, infrastructures and facilities at national and regional.
9.1. Collection and transport of solid waste;
9.2. Solid waste separation and processing;
10. Valorisation of urban, industrial and agricultural solid waste
10.1. Energy recovery;
10.2. Composting;
10.3. Recycling and reuse;
10.4. Industrial valorisation.

Back

Electrochemistry and Corrosion (QUI13524M)

Relevance of Electrochemistry in the context of today's Society and of an effectively sustainable development.
Fundamental theoretical and practical aspects of electrochemistry in the bulk of conducting phases and at their interfaces.
Electrochemical characterization techniques of chemical species and new materials, processes and electrochemical devices.
Electrochemical conversion and storage of electrical energy: primary, secondary, fuel and photoelectrochemical cells and supercapacitors.
Electrosynthesis and electrochemical modification: electrolytic production and processing of inorganic and organic substances and new materials.
Electrochemical processes for treatment, recycling, degradation and purification of substances and materials, valuable or hazardous.
Electrometallurgy: metal production, metal finishing and metal processing.
Metallic corrosion: Fundamental concepts, negative impacts of the phenomenon, monitoring techniques, and protective and control measures.

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Molecules and Technology (QUI13525M)

Molecular technology. Fluorocarbons. Oxygen carrying. Density: measurement and estimation. Compressibility. Solubility of gases in liquids. Carbon capture. Gas permeation. Inhalation anaesthetics. Anaesthetic-cell membrane interaction. Vapour pressure: measurement and estimation. Ionic liquids: microstructure. Viscosity: measurement and estimation. Ionogels. Liquid crystals. Eutectic solvents and Green Chemistry. Liquid-liquid extraction of pollutants. Hydrogels. Rheology principles. Supercritical fluids. Supercritical extraction, reaction media and micronization. Critical constants: measurement and estimation. Drugs: processing. Co-crystalization and co-solvency. Drug delivery. Environmental fate and removal. Diffusion coefficient: measurement and estimation. Classical and alternative refrigerants. Latent heat of vaporization: measurement and estimation. Refrigerants as pollutants. Nanofluids: examples, principles and applications. Thermal conductivity: measurement and estimation.

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Seminar (QUI13543M)

The curricular unit contemplates two distinct but complementary components. On the one hand, the students should attend research lecturers and subsequently elaborate individually a written summary of selected lectures. The themes are not fixed, and some examples of invited lecturers are: "Molybdenum (VI) oxo complexes: versatile catalysts for olefin epoxidation"; "Highly active hydroformylation catalysts: development, performance and immobilisation"; "Silicatos e MOF microporosos e fotoluminescentes"; "Fluorescência molecular: dos vetores de fase aos OLEDs de 3ª geração".

On the other hand, in the other component of the curricular unit each student will do two individual oral presentations. The first will be on a theme established during the first classes and proposed by the lecturers and/or students, and which may be related with the theme of the student's dissertation. The second will be on the results obtained within the dissertation work.