Study Plan

School: School of Sciences and Technology
Degree: Master
Course: Chemistry (cód. 631)

Specialization Chemistry of Materials

1st Year - 1st Semester
Specialization Chemistry of Materials

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8461M	Analysis and Characterisation of Materials	Chemistry	5	Semester	130
QUI12185M	Porous Materials	Chemistry	6	Semester	156
QUI8465M	Modeling and Simulation in Chemistry	Chemistry	5	Semester	130
MAT10240M	Numerical Optimization	Mathematics	3	Semester	78
QUI8462M	Advanced Organic Chemistry	Chemistry	5	Semester	130
QUI8463M	Separation and Identification of Organic Compounds	Chemistry	6	Semester	156

1st Year - 2nd Semester
Specialization Chemistry of Materials

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8468M	Adsorption in Nanoporous Materials	Chemistry	5	Semester	130
QUI8467M	Homogeneous and Heterogeneous Catalysis	Chemistry	5	Semester	130
QUI8469M	Principles of Green Chemistry	Chemistry	2	Semester	52

Options Group I

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8470M	Chemistry of Polymers	Chemistry	6	Semester	156
QUI8473M	Electrochemistry and Corrosion	Chemistry	6	Semester	156
QUI8471M	Advanced Carbon Materials	Chemistry	6	Semester	156
QUI12187M	Technological Chemistry	Chemistry	6	Semester	156

Options Group II

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8476M	Functional Organic and Organometallic Materials	Chemistry	6	Semester	156
QUI8474M	Medicinal Chemistry	Chemistry	6	Semester	156
QUI8475M	Advanced Organic Synthesis	Chemistry	6	Semester	156
QUI12188M	Physical-Chemical Properties and Technology	Chemistry	6	Semester	156

1st Year - 2nd Semester
Specialization Chemistry of Materials

Component code	Name	Scientific Area Field	ECTS	Duration	Hours

Options Group III

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8478M	Materials for Eletronics and Optics	Chemistry	6	Semester	156
QUI8480M	Quantum Chemistry	Chemistry	6	Semester	156
QUI12189M	Forensic Chemistry B	Chemistry	6	Semester	156

2nd Year - 3rd Semester
Specialization Chemistry of Materials

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI12186M	Seminar	Chemistry	3	Year	78
Dissertation					

2nd Year - 4th Semester
Specialization Chemistry of Materials

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
Dissertation					

Specialization Organic Chemistry

1st Year - 1st Semester
Specialization Organic Chemistry

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8461M	Analysis and Characterisation of Materials	Chemistry	5	Semester	130
QUI12185M	Porous Materials	Chemistry	6	Semester	156
QUI8465M	Modeling and Simulation in Chemistry	Chemistry	5	Semester	130
MAT10240M	Numerical Optimization	Mathematics	3	Semester	78
QUI8462M	Advanced Organic Chemistry	Chemistry	5	Semester	130
QUI8463M	Separation and Identification of Organic Compounds	Chemistry	6	Semester	156

1st Year - 2nd Semester
Specialization Organic Chemistry

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8468M	Adsorption in Nanoporous Materials	Chemistry	5	Semester	130
QUI8467M	Homogeneous and Heterogeneous Catalysis	Chemistry	5	Semester	130
QUI8469M	Principles of Green Chemistry	Chemistry	2	Semester	52

1st Year - 2nd Semester
Specialization Organic Chemistry

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
Options Group I					

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8470M	Chemistry of Polymers	Chemistry	6	Semester	156
QUI8473M	Electrochemistry and Corrosion	Chemistry	6	Semester	156
QUI8471M	Advanced Carbon Materials	Chemistry	6	Semester	156
QUI12187M	Technological Chemistry	Chemistry	6	Semester	156

Options Group II

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8476M	Functional Organic and Organometallic Materials	Chemistry	6	Semester	156
QUI8474M	Medicinal Chemistry	Chemistry	6	Semester	156
QUI8475M	Advanced Organic Synthesis	Chemistry	6	Semester	156
QUI12188M	Physical-Chemical Properties and Technology	Chemistry	6	Semester	156

Options Group III

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI8478M	Materials for Eletronics and Optics	Chemistry	6	Semester	156
QUI8480M	Quantum Chemistry	Chemistry	6	Semester	156
QUI12189M	Forensic Chemistry B	Chemistry	6	Semester	156

2nd Year - 3rd Semester
Specialization Organic Chemistry

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI12186M	Seminar	Chemistry	3	Year	78
Dissertation					

2nd Year - 4th Semester
Specialization Organic Chemistry

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:

Área de Especialização em Química dos Materiais

1.ºAno

1.º Semestre:

6 UC obrigatórias num total de 30 Ects

2.º Semestre:

3 UC obrigatórias num total de 12 Ects

2 UC optativas do Grupo I de num total de 12 Ects

1 UC optativa do Grupo I, II ou III de num total de 6 Ects

2.º Ano

3.º e 4º Semestre:

1 UC obrigatória num total de 3 Ects

Área de Especialização em Química Orgânica

1.ºAno

1.º Semestre:

6 UC obrigatórias num total de 30 Ects

2.º Semestre:

3 UC obrigatórias num total de 12 Ects

2 UC optativas do Grupo II de num total de 12 Ects

1 UC optativa do Grupo I, II ou III de num total de 6 Ects

2.º Ano

3.º e 4º 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

Back

Analysis and Characterisation of Materials (QUI8461M)

Theoretical component:

1.Vacuum systems, theory and equipments. 2.Surface chemistry. Functional groups, 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.Helium and mercury pycnometry. Mercury porosimetry. 5. Infrared, Raman and NMR spectroscopies. 6. Microscopy. 7.Thermal analysis and microcalorimetry.

Practical component:

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

Back

Porous Materials (QUI12185M)

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 and influence of conditions on the porosity of porous materials, namely: aerogels, activated and super-activated carbons; molecular sieves; zeolites and zeotypes; clays and pillared clays; ordered mesoporous silicas, metalossilicates and carbons; inorganic-organic hybrid materials; porous composite materials. Modification and functionalization to control the properties of materials. Regeneration, importance and methods, of porous materials.

Practical component

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

Back

Modeling and Simulation in Chemistry (QUI8465M)

Molecular interactions. Models for the description of intramolecular and intermolecular interactions. Molecular mechanics and force fields. Parameterization of potentials. Reviews of Statistical Mechanics. Introduction to the molecular simulations. Periodic boundary conditions. Trajectories and properties. Ergodicity. The Molecular Dynamics method. Simulations in the microcanonical ensemble. Simulations in the canonical ensemble: the Nosé-Hoover and the Berendsen thermostats. Simulations in the isobaric ensemble: the Berendsen and the Parrinello-Rahman barostats. Geometry restrictions. The Monte Carlo method. Canonical ensemble, isothermal-isobaric ensemble, grand canonical ensemble and Gibbs ensemble. Non-boltzmann sampling. Analysis of simulations results. Radial distribution functions. Mechanical properties. Fluctuations. Correlation functions. Dynamical properties.

Back

Numerical Optimization (MAT10240M)

1. Scientific method and experimental design.
2. Analysis of variance models: fixed effects (single and multiple factor), random effects (single and multiple factor) and mixed effects.
3. Multiple comparisons.
4. Complete and incomplete block designs. Latin square designs.
5. Non-parametric approaches.
6. Simple linear regression model and multiple regression model (estimation, inference, prediction, model adequacy and validation). Diagnostics for influence points, outliers,
multicollinearity and autocorrelation. Model selection.
7. Nonlinear Regression.

Back

Advanced Organic Chemistry (QUI8462M)

Introduction to molecular orbital theory and pericyclic reactions. Stereoelectronic effects and their effect on chemical reactivity and selectivity, the anomeric effect and Baldwin's rules. Introduction to structure activity aspects in organic chemistry. Reactive intermediates: preparation and application. Rearrangements and fragmentations. All this material will be interconnected to the synthesis of high-added-value substances.

Back

Separation and Identification of Organic Compounds (QUI8463M)

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

Adsorption in Nanoporous Materials (QUI8468M)

Theoretical
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
Analysis of adsorption isotherms. Experimental determination of isotherms of adsorption from gas phase and aqueous solutions by materials prepared in Development of Advanced Porous Materials.

Back

Homogeneous and Heterogeneous Catalysis (QUI8467M)

Introduction to homogeneous and heterogeneous catalysis. Organometallic compounds in homogeneous catalysis: fundamental concepts, organometallic reactions and catalytic cycles.
Homogeneous catalysis in heavy chemistry and fine chemicals. Study of some important cases. Heterogeneous Catalysis: deactivation and preparation of catalysts. Catalytic activity of porous materials. Kinetics and mechanisms of heterogeneous catalysis. Introduction to catalytic reactors. Asymmetric catalysis: fundamental concepts and important reactions. Asymmetric organocatalysis. Application of enzymes. Asymmetric heterogeneous catalysis.

Back

Principles of Green Chemistry (QUI8469M)

- Introduction. Importance of Chemistry and Chemical Technology in Modern Society: Advantages vs. disadvantages.
- Chemistry and Sustainable Development.
- History and Evolution of Green Chemistry.
- The 12 Principles of Green Chemistry.
- Green Chemistry Metrics: Measuring and Monitoring Sustainable Processes
- Green Chemistry in different areas of chemistry. Success and false cases
- Green Chemistry in everyday life. Real cases.
- Life Cycle Assessment: a Tool for Identification of More Sustainable Products and Process
- The second 12 Principles of Green Chemistry.
- Nanoporous Materials as Catalysts in Green Chemistry.
- Seminars / Lectures on current topics within the Green Chemistry by invited specialists.

Back

Chemistry of Polymers (QUI8470M)

Theoretical: 1: Introduction to Polymers. 2: Polymer Molecular Structure. 3: Polymerisation Mechanisms. 4: Polymer Properties. 5: Liquid Crystals. 6: Polymer Processing. 7: Elastomers and Gels. 8: Network Polymers. 9: Natural Polymers. 10: Sol-Gel and Photochemical Syntheses. 11: Characterisation Techniques. 12: Biomaterials. 13: Health, Energy, Transport and Construction Applications. 14: Future Perspectives.
Practical: Synthesis and characterisation of some polymers.

Back

Electrochemistry and Corrosion (QUI8473M)

Importance of Electrochemistry in the context of actual Society: exhibition and conversation about common and vanguard cases.
Electrochemistry in the bulk of conducting phases (Review).
Electrochemistry at the interface of conducting phases.
Techniques of electrochemical characterization of chemical species and new materials, interfacial or non-interfacial processes, and electrochemical devices.
Electrochemical conversion and storage of electrical energy: electrochemical cells and supercapacitors.
Electrosynthesis and electrochemical modification: electrolytic production and processing of inorganic and organic substances and new materials.
Electrometallurgy: electrochemical techniques for metal production, metal finishing and metal processing.
Electrochemical processes for treatment, recycling and purification of substances and materials, valuable or hazardous.
Corrosion: Fundamental concepts and importance of its study.

Back

Advanced Carbon Materials (QUI8471M)

Short Program:
1: Presentation. 2: Structure. 3: Reactivity. 4: Precursors. 5: Textural Characterisation. 6: Chemical Characterisation. 7: Carbon Black. 8: Activated Carbon. 9: Carbon Membranes and Molecular Sieves. 10: Carbon Fibres and Composites. 11: Carbon in Metallurgy. 12: Fullerenes, Nanotubes and Graphene. 13: Carbon in Electrochemistry and Catalysis. 14: Diamond.
The theoretical program is complemented by a short laboratory project carried out in a block in the middle of the semester and by problems classes.

Back

Technological Chemistry (QUI12187M)

Production of goods in chemistry. The concept of commodity and chemical specialty. Examples of chemical processes of molecule production: basis to explain the most important concepts. The chemical process and its depiction. Material and energy balances. Applications. Process steps. Chemical reactors: material balances and sizing. Unit operations. Heat exchangers. Separation processes. The description of the most common separation processes. Distillation and liquid-liquid extraction: operation and design. Optimization and quality. Process and product quality control.

Back

Functional Organic and Organometallic Materials (QUI8476M)

Basic concepts of functional molecular materials: perspective of organic and organometallic compounds. Synthetic methods of organometallic and organic functional materials. Description of organometallic and organic materials for application in chemistry, physics and biology/medicine. Chemical sensors: fullerenes, macrocyclic compounds, polymeric and supramolecular architectures. Application in physics: drivers and molecular switches, LEDs, liquid crystals, luminescent materials, molecular nonlinear optoelectronic materials, photochromic materials, materials for solar panels, photovoltaic systems and optical recording, etc.). Application in biology and medicine: sensors, binding to DNA, anti-carcinogenic agents, degenerative diseases, etc.).

Back

Medicinal Chemistry (QUI8474M)

1.1. Introduction to Medicinal Chemistry.
1.2. Classification of drugs, molecular mechanisms of action and structure-activity relationships (SAR).
1.3. Pharmacokinetics. Prodrugs.
1.4. Methods of searching, discovery and isolation of new drugs; development and production of new drugs.
1.5. Study of some important drugs: sources, chemical structures, mechanisms of action, SARs, metabolism and applications of some drugs.
2.1. The chemistry of essential molecules in the cells.
2.2. Amino acids and proteins: structure and metabolic functions, reactivity and synthesis.
2.3. Carbohydrates: classification, structure, reactivity and metabolism.
2.4. Phosphates and the macromolecules derived from these units: structure and reactivity.
2.5. Lipids, their structural variety, importance and functions.
2.6. Nucleic acids: functions and genetic information.
2.7. Molecular recognition and cell communication.
2.8. Proteins as catalysts, mechanisms of enzymatic catalysis. Artificial enzymes.

Back

Advanced Organic Synthesis (QUI8475M)

Introduction to organic synthesis. Modern methods of organic synthesis. Synthesis of organometallic compounds. Asymmetric synthesis. Synthesis of some important natural products and pharmaceuticals. Introduction to retrosynthetic analysis. Green and alternative methods of organic synthesis. Combinatorial synthesis.

Back

Physical-Chemical Properties and Technology (QUI12188M)

Property prediction, estimation and correlation. Technological relevance of the physico-chemical properties. Fluid densities. Equations of state. Second virial coefficients and intermolecular forces. Estimation of densities. Vapour pressures of liquids and solids and enthalpies of vaporization and sublimation. Molecular interpretation. Vapour-liquid equilibrium of mixtures. Calculation and estimation of activity coefficients. Solubility of gases in liquids. Viscosity. Viscometers and rheometers. Viscosity calculation fundamentals and estimation. Thermal conductivity. Diffusion coefficients: principles and applications. Heat capacity and surface tension. Properties and technological application. Supercritical fluids: extraction and reactional medium. Micronization. Technological uses of fluorinated compounds and ionic liquids. Emulsions and bubbles of respiratory gases. Gaseous anaesthesia. Fluidity. Permeation.

Back

Materials for Eletronics and Optics (QUI8478M)

Materials with important electrical and magnetic properties for technological applications.
HTS: state of the art.
Ion conductors; fuel cells, electrodes and electrolytes.
Applications of dielectric materials.
Nanomaterials: effect "nano"in the properties and applications of traditional compounds under study.
Materials used in solar energy conversion, including materials with photoelectrochemical activity and photocatalytic activity.
Chemistry and technology of materials for optoelectronics and photonics. State of the art.
Devices and materials for optoelectronics. Liquid crystals. Photoconductors. Luminescent materials. Nonlinear optical properties. Data transmission. Magneto-optical recording.

Back

Quantum Chemistry (QUI8480M)

Reviews of quantum mechanics concepts. Postulates of quantum mechanics. Time independent perturbation theory. The hydrogen atom. The helium atom. Slater determinants. The Hartree-Fock method. The Koopman's theorem. Electronic correlation. The electron spin and the Pauli principle. Many-electron atoms. Homonuclear diatomic molecules. Ab-initio methods and the Density Functional Theory.

Back

Forensic Chemistry B (QUI12189M)

Introduction to forensic science and criminal investigation procedures.
How the forensic laboratory works.
Analytical methods in forensic chemistry.
Analysis of crime scenes.
Handling of physical evidence.
The chemistry of fingerprinting
The chemical treatment of fibres and forensic analysis of hair and fibres.
Analysis of drugs of abuse and their metabolites, presumptive and conclusive methods.
Poisons used in crimes, types of action and analysis.
Spectroscopic analysis of paints and plastics.
Inorganic systems as evidence, glass and soil.
Application of chemical methods in biological trace analysis.
Examination of questioned documents.
Characterization of the hydrocarbons mixture in arson investigations.
How to find out who shot and what weapon was used in the crime.

Back

Seminar (QUI12186M)

The curricular unit contemplates two distinct but complementary components. On the one hand, the students should attend research talks and subsequently elaborate, individually, a written summary. The themes are not fixed and some examples of invited talks are: "Molybdenum (VI) oxo complexes: versatile catalysts for olefin epoxidation", "Highly active hydroformylation catalysts: development, performance and immobilisation", "Mag(net)ic Molecules: Synthesis and Application", "Development and Applications of Biomaterials" and "Silicatos e MOF microporosos e fotoluminescentes".
On the other hand, the other component involves the elaboration of an individual monograph on a theme established during the first classes of the semester and proposed by the teaching team and/or the students, and which may be related with the theme of the student's dissertation. Each student must also make a Powerpoint presentation of the monograph, which will be followed by a discussion period.