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
QUI08461M	Analysis and Characterisation of Materials	Chemistry	5	Semester	130
QUI12185M	Porous Materials	Chemistry	6	Semester	156
QUI08465M	Modeling and Simulation in Chemistry	Chemistry	5	Semester	130
MAT10240M	Numerical Optimization	Mathematics	3	Semester	78
QUI08462M	Advanced Organic Chemistry	Chemistry	5	Semester	130
QUI08463M	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
QUI08468M	Adsorption in Nanoporous Materials	Chemistry	5	Semester	130
QUI08467M	Homogeneous and Heterogeneous Catalysis	Chemistry	5	Semester	130
QUI08469M	Principles of Green Chemistry	Chemistry	2	Semester	52

Options Group I

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI08470M	Chemistry of Polymers	Chemistry	6	Semester	156
QUI08473M	Electrochemistry and Corrosion	Chemistry	6	Semester	156
QUI08471M	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
QUI08476M	Functional Organic and Organometallic Materials	Chemistry	6	Semester	156
QUI08474M	Medicinal Chemistry	Chemistry	6	Semester	156
QUI08475M	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
QUI08478M	Materials for Eletronics and Optics	Chemistry	6	Semester	156
QUI08480M	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
QUI08461M	Analysis and Characterisation of Materials	Chemistry	5	Semester	130
QUI12185M	Porous Materials	Chemistry	6	Semester	156
QUI08465M	Modeling and Simulation in Chemistry	Chemistry	5	Semester	130
MAT10240M	Numerical Optimization	Mathematics	3	Semester	78
QUI08462M	Advanced Organic Chemistry	Chemistry	5	Semester	130
QUI08463M	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
QUI08468M	Adsorption in Nanoporous Materials	Chemistry	5	Semester	130
QUI08467M	Homogeneous and Heterogeneous Catalysis	Chemistry	5	Semester	130
QUI08469M	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
QUI08470M	Chemistry of Polymers	Chemistry	6	Semester	156
QUI08473M	Electrochemistry and Corrosion	Chemistry	6	Semester	156
QUI08471M	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
QUI08476M	Functional Organic and Organometallic Materials	Chemistry	6	Semester	156
QUI08474M	Medicinal Chemistry	Chemistry	6	Semester	156
QUI08475M	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
QUI08478M	Materials for Eletronics and Optics	Chemistry	6	Semester	156
QUI08480M	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

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Analysis and Characterisation of Materials (QUI08461M)

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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.

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Modeling and Simulation in Chemistry (QUI08465M)

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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.

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Advanced Organic Chemistry (QUI08462M)

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Separation and Identification of Organic Compounds (QUI08463M)

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Adsorption in Nanoporous Materials (QUI08468M)

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Homogeneous and Heterogeneous Catalysis (QUI08467M)

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.

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Principles of Green Chemistry (QUI08469M)

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Chemistry of Polymers (QUI08470M)

Back

Electrochemistry and Corrosion (QUI08473M)

Back

Advanced Carbon Materials (QUI08471M)

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.

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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 (QUI08476M)

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.).

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Medicinal Chemistry (QUI08474M)

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Advanced Organic Synthesis (QUI08475M)

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.

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Materials for Eletronics and Optics (QUI08478M)

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.

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Quantum Chemistry (QUI08480M)

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.

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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.

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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.