# Study Plan

**School:** Institute for Advanced Studies and Research
**Degree:** Doctorate
**Course:** Chemistry (cód. 629)

**1st Year - 1st Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| QUI12206D | Seminar in Chemistry I | Chemistry | 6 | Semester | 156 |

**Options**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| QUI8986D | Synthesis and Properties of Nanoporous Materials | Chemistry | 5 | Semester | 130 |
| QUI8987D | Methodologies for Characterization of Solids and Surfaces | Chemistry | 5 | Semester | 130 |
| QUI8988D | Advanced Methods in Organic Synthesis | Chemistry | 5 | Semester | 130 |
| QUI8989D | Mechanisms and Structure Determination in Organic Chemistry | Chemistry | 5 | Semester | 130 |
| QUI8990D | Advanced Methods in Computational Chemistry | Chemistry | 5 | Semester | 130 |
| QUI8991D | Supplements in Physical - Chemistry | Chemistry | 5 | Semester | 130 |
| QUI8992D | Advanced Analysis Techniques and Hyphens Techniques | Chemistry | 5 | Semester | 130 |
| QUI8993D | Microanalysis and in-situ Analysis Techniques | Chemistry | 5 | Semester | 130 |
| QUI12207D | Teaching practice | Chemistry | 5 | Semester | 130 |
| Free Option | | | | | |

Thesis

**1st Year - 2nd Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| QUI8983D | Seminar in Chemistry II | Chemistry | 6 | Semester | 156 |

**1st Year - 2nd Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| **Options** | | | | | |

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| QUI8986D | Synthesis and Properties of Nanoporous Materials | Chemistry | 5 | Semester | 130 |
| QUI8987D | Methodologies for Characterization of Solids and Surfaces | Chemistry | 5 | Semester | 130 |
| QUI8988D | Advanced Methods in Organic Synthesis | Chemistry | 5 | Semester | 130 |
| QUI8989D | Mechanisms and Structure Determination in Organic Chemistry | Chemistry | 5 | Semester | 130 |
| QUI8990D | Advanced Methods in Computational Chemistry | Chemistry | 5 | Semester | 130 |
| QUI8991D | Supplements in Physical - Chemistry | Chemistry | 5 | Semester | 130 |
| QUI8992D | Advanced Analysis Techniques and Hyphens Techniques | Chemistry | 5 | Semester | 130 |
| QUI8993D | Microanalysis and in-situ Analysis Techniques | Chemistry | 5 | Semester | 130 |
| QUI12207D | Teaching practice | Chemistry | 5 | Semester | 130 |
| Free Option | | | | | |

Thesis

**2nd Year - 3rd Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| QUI8984D | Seminar in Chemistry III | Chemistry | 4 | Year | 104 |
| Thesis | | | | | |

**2nd Year - 4th Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| Thesis | | | | | |

**3rd Year - 5th Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| QUI8985D | Seminar in Chemistry IV | Chemistry | 4 | Year | 104 |
| Thesis | | | | | |

**3rd Year - 6th Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| Thesis | | | | | |

**4th Year - 7th Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| Thesis | | | | | |

**4th Year - 8th Semester**

| Component code | Name | Scientific Area Field | ECTS | Duration | Hours |
|---|---|---|---|---|---|
| Thesis | | | | | |

### 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:

1 UC obrigatória num total de 6 Ects

2.º Semestre:

1 UC obrigatória num total de 6 Ects

No primeiro ano é necessário frequentar UC optativas conforme quadro de optativas num total de 10 Ects

2.º Ano

1 UC obrigatória num total de 4 Ects

3.º Ano

1 UC obrigatória num total de 4 Ects

Para obtenção do grau, é necessário também a aprovação na Tese com um total de 210 ECTS decorrente no 1.º, 2.º, 3.º e 4.º Ano ***

## Program Contents

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**Seminar in Chemistry I (QUI12206D)**

Seminar in Chemistry I involves gaining experience in a technique (or sequence of techniques), new for the student and of sufficient complexity, in the preparation of a monograph on the principles of the technique and results obtained, and their public oral presentation and discussion.
The themes are not fixed, but each theme is tailored to the particular needs of each student and needs prior approval of the jury of the curricular unit. It should be related to the topic of the student´s thesis and relevant in view of the objectives and skills that the Doctoral Program in Chemistry aims to develop. The monograph should include some results obtained by the student or on samples synthesized by the student and with analysis of the results carried out by the student. It may also include results collected from publications.
In addition, the students must attend scientific talks organized by the teaching team of the curricular unit and participate in the debate. The students can also take short courses.

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**Synthesis and Properties of Nanoporous Materials (QUI8986D)**

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 carbon; 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. These materials are characterised in the curricular unit of Methodologies of Characterisation of Solids and Surfaces.

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**Methodologies for Characterization of Solids and Surfaces (QUI8987D)**

Theoretical component

Vacuum theory, systems and equipment. Real, apparent and bulk density. Helium pycnometry and mercury porosimetry. Functional groups, coordinative unsaturation, hydroxylation, Brønsted and Lewis acidity. Isoelectric point and point of zero charge. Non instrumental methods for quantifying surface sites. Interaction of radiation with materials. Techniques for structural and surface characterization of materials. Microscopies (SEM, TEM, AFM, SFM). Techniques involving X rays (XRD, XRF, EDS, XANES, EXAFS, XPS, SAXS). Vibrational spectroscopies (FTIR, Raman) and NMR. Thermal analysis techniques and microcalorimetry (TGA, DTG, TPD, DTA, DSC, STA and Calvet calorimetry).

Practical component

Analysis and characterization by different techniques of materials prepared in the curricular unit Synthesis and Properties of Nanoporous Materials.

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**Advanced Methods in Organic Synthesis (QUI8988D)**

Advanced synthetic methodologies, including integrated analysis of some case studies. Application of organometallic compounds. Retrosynthetic analysis and synthetic strategy for key target compounds. Synthesis of some key pharmaceuticals and natural products. Methods for heterocyclic compound synthesis. Green and sustainable methods for the synthesis of important targets.

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**Mechanisms and Structure Determination in Organic Chemistry (QUI8989D)**

Advanced percyclic reactions - the inverse electron demand Diels-Alder and the hetero Diels-Alder reaction, the chelatropic and ene reactions. The effect of conformation on reactivity. The Hammett equation and the Hammond postulate. Investigation of mechanisms, kinetic studies, the deuterium isotope effect, detection of intermediates (IR, NMR, mass spectrometry, electron spin resonance (esr)). Alicyclic compounds - stability, reactivity and synthesis.

Advanced espectroscopic and espectrometric methods, 1D and 2D methods (1H, 13C, DEPT, COSY, HMBC, HMQC, INADEQUATE, NOESY, TOCSY,...). NMR of other common nuclei (15N, 19F, 31P e 29Si). Mass spectrometry.

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**Advanced Methods in Computational Chemistry (QUI8990D)**

Introduction to parallel computing and the different types of parallel architectures (Flynn's taxonomy). Identification of parallelism in an algorithm. Load balancing. Data parallelism (F95 and OpenMP). "Message Passing"(MPI). "Task farms".

Quantum Chemistry: Hückel, semi-empirical and ab initio methods. Density functional theory.

Quantum dynamics: Time evolution of a quantum system. Time dependent perturbation theory. Time dependent Density functional theory. Electronic transitions.

Molecular simulation: Molecular dynamics. Simulations in the microcanonical, canonical (Nosé-Hoover and Berendsen thermostats) and isobaric (Berendsen and Parrinello-Rahman barostats) ensembles. Geometry constraints. Metropolis Monte Carlo. Canonical, isothermic-isobaric, grand canonical and Gibbs ensembles. Non-Boltzmannean sampling. Thermodynamic perturbation theory. Thermodynamic integration method. Free energies calculations.

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**Supplements in Physical - Chemistry (QUI8991D)**

Common block

Statistical mechanics

Ensembles. Generalized ensembles. Non interacting particles sistems. Ising model, mean field theory and renormalization group theory.

Liquids

Forces and Intermolecular potentials. Radial distribution function. Correlation of molecular orientation. Self-organization. Liquids and solutions theories: net theories. Cell and mean field theories, pertubations and theories based on molecular fragments. High pressure phase diagrams.

Experimental thermodynamics

Densities. PVT relations. State equations. Liquid-vapor equilibrium. Vapor pressures. Excess functions. Activity coefficients. Viscosity. Viscosity in liquids. Diffusion. Heat capacities.

Biophysical techniques

Functional and structural characteristics of molecules and biological systems. Techniques used in biophysics: optical spectroscopies, magnetic resonance, dispersion techniques (of light) and diffraction, calorimetry, microscopy and computational techniques.

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**Advanced Analysis Techniques and Hyphens Techniques (QUI8992D)**

Sample preparation methods and chromatographic analysis

Sample preparation and analyte concentration methods. Review on the chromatographic techniques. New trends in chromatography: high temperature LC, microparticles and monolithic HPLC columns, ultrahigh pressure liquid chromatography, high speed-LC, multidimensional chromatography. Mass detectors, ionization modes and hyphenation with chromatography.

Electrochemical Methods

Bulk (Conductometry), static interfacial (Potentiometry) and dynamic interfacial methods (Voltammetry, Chronoamperometry, Chronocoulometry, Chronopotentiometry, Coulometric Titration, Electrochemical Impedance Spectroscopy , Electrochemical Quartz Crystal Microbalance, Electrochemical Mass Spectrometry, Electrochemical Scanning Tunneling Microscopy, Electrochemical Atomic Force and Scanning Electrochemical microscopy, Spectroelectrochemistry, Photoelectrochemistry and Electrochemiluminescence. New electrochemical sensors.

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**Microanalysis and in-situ Analysis Techniques (QUI8993D)**

1. Introduction: importance and use of analytical microprobe and in-situ techniques in Chemistry, applications and historical background.

2. Microanalysis techniques
2.1. Sampling techniques and microsample processing
2.2. Microscope based spectroscopic techniques (micro-FTIR and micro-Raman spectrometries)
2.3.Microprobe techniques (Electron microprobe, Proton microprobe, Photon microprobe, Ion microprobe, Laser ablation Inductively coupled plasma Mass spectrometry (LA-ICP-MS)).

3. In-situ techniques
3.1. Spectrometric techniques (in-situ FTIR, in-situ Raman, in-situ XRF and colorimetry)
3.2.Flow techniques (Flow Injection Analysis and Electrochemical probes)

4. Comparison between the analytical techniques: detection limits, analytical precision and accuracy, spatial resolution and applications.

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**Teaching practice (QUI12207D)**

Teaching activities associated to class monitor in a Chemistry 1st cycle curricular units related to their field of research, under the supervision of the professor who has teaching service allocated in the curricular unit.

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**Seminar in Chemistry II (QUI8983D)**

The syllabus is not fixed, but is tailored to the particular needs of each student. The theme to be treated needs prior approval of the jury of the curricular unit. It should be related to the topic of the student´s thesis project and should be relevant in view of the objectives and skills that the Doctoral Program aims to develop. In the monograph, the student may present a historical overview, but should emphasize the most outstanding recently published work and should also refer to the scientific and social implications. It may include results obtained by the student or obtained on samples synthesized by the student and with analysis of the results accomplished by the student. The conferences are not fixed having included, for example "Concentration and thermal applications of Solar Energy" (M. Collares Pereira, BES Renewable Energies Chair, UÉv); "Synthesis and evaluation of anti-tumoral/angiogenic potential of new heterocyclic compounds" (M.J. Queiroz, Chemistry Centre, U.Minho).

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**Seminar in Chemistry III (QUI8984D)**

The formal program consists of attendance at conferences organized under the Doctoral Program, usually in collaboration with the Évora Chemistry Centre, and the public presentation and discussion of the research work carried out during the year. Conferences organized by the teaching staff are indicated in the Class Summaries of the Chemistry Seminars. Some examples are: "Fluorescent membrane probes behaviour in lipid bilayers" (L.M. Loura, Chemistry Centre, U.Coimbra); "Design and synthesis of efficient organometallic molecules" (M.H. Garcia, Centre for Molecular Sciences and Materials, U.Lisbon); "Sustainable Use of Solid Residues" (L. Oliveira, U.Federal de Minas Gerais, Brazil).
In addition to attendance at conferences organized by the teaching staff, students are encouraged to undertake courses in their specific area of research, and to participate in other conferences/congresses related to the general area of their research taking place either at U.Év or at another institution.

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**Seminar in Chemistry IV (QUI8985D)**

The formal program consists of attendance at conferences organized under the Doctoral Program, usually in collaboration with the CQE, and the public presentation and discussion of the research work carried out. Conferences organized by the teaching staff are indicated in the Class Summaries of the Chemistry Seminars. Examples are: "Structure Analysis of Porous Materials by EM" (X.D. Zou, Director of Berzelii Center EXSELENT on Porous Materials, U.Stockholm, Sweden); "Synthesis, Properties and Applications of IoNanofluids" (C.N. Castro, Director of Centre for Molecular Sciences & Materials, U.Lisbon); "Natural Products as Inspiration and Challenge" (H.G. Schmalz, U.Cologne, Germany).
In addition to attendance at conferences organized by the teaching staff, students are encouraged to undertake courses in their specific area of research, and to participate in other conferences/congresses related to the general area of their research taking place either at U.Év or at another institution.