Study Plan

School: Institute for Research and Advanced Training
Degree: Doctorate
Course: Chemistry (cód. 727)

1st Year - 1st Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13575D	Chemistry Seminar I	Chemistry	6	Semester	156

***** TRANSLATE ME:Grupo de Optativas de Competências Transversais *****

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
FIL13966D	Epistemology of Science	Philosophy	3	Semester	78
VIS13967D	Communication techniques	Education Sciences Design Linguistics	3	Semester	78
HIS13970D	Open Science and strategies of science communication and dissemination	Design History Informatics	3	Semester	78
LLT13973D	Academic writing skills in English I	Linguistics	3	Semester	78
LLT13974D	Academic writing skills in English II	Linguistics	3	Semester	78
PSI13968D	Personal Career Management	Psychology	3	Semester	78
INF13969D	LaTex Introdution	Informatics	3	Semester	78
GES13975D	Project Planning and Management	Management	3	Semester	78
MAT14055D	Fundamentals of Data Analysis in Environment R	Mathematics	6	Semester	156
FIL13971D	Ethics and Research	Philosophy	3	Semester	78
GES14077D	Start-up PhD	Management	3	Semester	78
MAT15034D	Numerical Tools with Python	Informatics Mathematics	6	Semester	156
FIS15035D	History of Sciences	Physics History	3	Semester	78
HIS15036D	Introduction to automatic bibliographic reference systems	History	3	Semester	78
PSI15037D	Emotions in learning contexts	Psychology	3	Semester	78

1st Year - 1st Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
Options					

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13579D	Synthesis and Properties of Nanoporous Materials	Chemistry	6	Semester	156
QUI13580D	Methodologies of Characterisation of Solids and Surfaces	Chemistry	6	Semester	156
QUI13581D	Advanced Methods in Organic Synthesis	Chemistry	6	Semester	156
QUI13582D	Mechanisms and Determination of Structure in Organic Chemistry	Chemistry	6	Semester	156
QUI13583D	Advanced Methods in Computational Chemistry	Chemistry	6	Semester	156
QUI13584D	Advanced Analytical Techniques and Hyphenated Techniques	Chemistry	6	Semester	156
QUI13585D	Microanalysis and In-Situ Analysis Techniques	Chemistry	6	Semester	156
Free option					

Thesis

1st Year - 2nd Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13576D	Chemistry Seminar II	Chemistry	6	Semester	156

1st Year - 2nd Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours

***** TRANSLATE ME:Grupo de Optativas de Competências Transversais *****

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
FIL13966D	Epistemology of Science	Philosophy	3	Semester	78
VIS13967D	Communication techniques	Education Sciences Design Linguistics	3	Semester	78
HIS13970D	Open Science and strategies of science communication and dissemination	Design History Informatics	3	Semester	78
LLT13973D	Academic writing skills in English I	Linguistics	3	Semester	78
LLT13974D	Academic writing skills in English II	Linguistics	3	Semester	78
PSI13968D	Personal Career Management	Psychology	3	Semester	78
INF13969D	LaTex Introdution	Informatics	3	Semester	78
GES13975D	Project Planning and Management	Management	3	Semester	78
MAT14055D	Fundamentals of Data Analysis in Environment R	Mathematics	6	Semester	156
FIL13971D	Ethics and Research	Philosophy	3	Semester	78
GES14077D	Start-up PhD	Management	3	Semester	78
MAT15034D	Numerical Tools with Python	Informatics Mathematics	6	Semester	156
FIS15035D	History of Sciences	Physics History	3	Semester	78
HIS15036D	Introduction to automatic bibliographic reference systems	History	3	Semester	78
PSI15037D	Emotions in learning contexts	Psychology	3	Semester	78

Options

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13579D	Synthesis and Properties of Nanoporous Materials	Chemistry	6	Semester	156
QUI13580D	Methodologies of Characterisation of Solids and Surfaces	Chemistry	6	Semester	156
QUI13581D	Advanced Methods in Organic Synthesis	Chemistry	6	Semester	156
QUI13582D	Mechanisms and Determination of Structure in Organic Chemistry	Chemistry	6	Semester	156
QUI13583D	Advanced Methods in Computational Chemistry	Chemistry	6	Semester	156
QUI13584D	Advanced Analytical Techniques and Hyphenated Techniques	Chemistry	6	Semester	156
QUI13585D	Microanalysis and In-Situ Analysis Techniques	Chemistry	6	Semester	156
Free option					

Thesis

2nd Year - 3rd Semester

Component code	Name	Scientific Area Field	ECTS	Duration	Hours
QUI13577D	Chemistry Seminar III	Chemistry	3	Year	78
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
QUI13578D	Chemistry Seminar IV	Chemistry	3	Year	78
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 (componente curricular) é necessário a aprovação (através de avaliação ou creditação) das seguintes unidades curriculares:

1.º Ano

1 UC obrigatória num total de 6 ECTS no 1º semestre

1 UC obrigatória num total de 6 ECTS no 2º semestre

UC optativas livres - Competências transversais num total de 12 ECTS

UC optativas do grupo de optativas num total de 12 ECTS

2.º Ano

1 UC obrigatória num total de 3 ECTS

3.º Ano

1 UC obrigatória num total de 3 ECTS

Para obtenção do grau, é necessário também a aprovação na Tese com um total de 198 ECTS decorrente no 1.º, 2.º, 3.º e 4.º Ano ***

Program Contents

Back

Chemistry Seminar I (QUI13575D)

The theme to be treated by each student is not fixed and 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 in Chemistry aims to develop. The monograph should include some results obtained by the student and with analysis and discussion of the results carried out by the student. It may also include results collected from publications that illustrate applications of the technique. Students are also encouraged to attend conferences.

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Epistemology of Science (FIL13966D)

1. Contemporary Epistemology and the contributions of the History and Philosophy of Science, Studies of Science and Technology.
2. The Scientific Revolution and its repercussions. The unit of knowledge and the organization of the disciplines. The problem of demarcation: science and common sense, religion, art and power.
3.Beliefs, methodologies, scientific truths and justification. The epistemological virtues. Normal science, controversies and innovation.
4.The scientific veracity: the logical-formal, empirical and hermeneutic dimensions. Practices and 'trading zones". The logic of discovery and of justification. Personae, objectification and ontologies.
5.Special epistemologies: the epistemologies of the social sciences, of life sciences, of engineering and technologies, of arts. Interdisciplinarity, multidisciplinarity and transdisciplinarity.
6.The dynamics of scientific communities an the challenges of the globalization of science: problems of culture, functioning and scientific et

Back

Communication techniques (VIS13967D)

1. Communication:
- general concepts
- channels, codes, meanings and contexts
- noise and communication facilitators
- style
- verbal and nonverbal communication
- oral and written communication

2. Written communication:
- different types of writing: formal, informal, academic, literary, journalistic, technical, advertising; social media
- subjectivity vs objectivity
- techniques of plain language writing
- typography, layout and graphics
- non-formal science communication writing
- writing press releases
- writing emails
- writing on social media

3. Oral communication:
- different types of oral communication: informative and persuasive
- preparation of an oral presentation
- techniques for facing, captivating and persuading the audience
- the importance of storytelling
- the tone of voice
- nonverbal communication
- visual aids to oral communication - information design
- interviews and press conferences
- debates: the art of disagreeing and arguing
- job interviews

Back

Open Science and strategies of science communication and dissemination (HIS13970D)

1. Fundamental concepts and topics on Open and Citizen Science and their emergent contexts.
2. How to publish?
2.1. The various types of scientific texts and disciplinary areas.
2.2. The peer review.
2.3. Indexed publications and impact factors.
2.4. The h-index.
3. The problems of opening and sharing data: from ethical issues to data intelligibility.
3.1. Copyright and creative commons licenses. Permanent links. The patents.
3.2. The metadata
3.3.The institutional repositories.
4. Open and shareable data requirements: from data management plan to preservation issues
5. Interoperability.
6. Information Representation and Retrieval
7. Data Security
8. Science communication strategies
8.1. The history of science communication and the challenges of modern societies
8.2. How to stimulate the intellectual pleasure of critical and scientific thinking?
8.3. Strategies to attract and build audiences: emotional design

Back

Academic writing skills in English I (LLT13973D)

Unit 1. The writing process: (a) the purpose, types and features of academic writing; (b) types of academic texts; (c) the development of critical reading approaches; (d) planning and brainstorming; key points & note-making; (e) paraphrasing & summarizing; (f) references & quotation; (g) rewriting & proofreading.
Unit 2. Elements of writing: (a) argument and discussion; (b) cause and effect; (c) cohesion; (d) comparison; (e) examples; (f) generalization.

Back

Academic writing skills in English II (LLT13974D)

Unidade 1. Accuracy in writing: (a) academic vocabulary; (b) conjunctions, nouns & adjectives, prepositions; (c) punctuation; (d) verbs: passive, referencing, tenses.
Unidade 2. Writing models: (a) reports, case studies and literature reviews; (b) designing and reporting surveys; (c) essays; (d) the PhD thesis.

Back

Personal Career Management (PSI13968D)

1. Work and career
1.1. The changing nature of work in a globalized society
1.2. The importance of personal career management in globalized societies
1.3. Models and practices of personal career management

2. The development of personal career management skills
2.1. My career
2.2. Identity
2.3. Career adaptability resources
2.4. Barriers and supports to personal career management
2.5. The implementation of personal career management strategies

3. Research on personal career management

Back

LaTex Introdution (INF13969D)

1. Document Organization: Document divisions, Lists.
2. Common Documents: Presentations, Tables and Figures.
3. Academic Publications: Acronyms, Bibliographies & References.
4. Monographs and Books: Multi-File Documents.
5. Advanced Topics: Mathematical Expressions, Hyperlinks, Indexes, Graphics.

Back

Project Planning and Management (GES13975D)

1. Project planning, programming and control
2. Project programming with deterministic durations
3. Project programming with stochastic durations
4. Project planning and financial management
5. Presentation, resolution and discussion of research project exemples

Back

Fundamentals of Data Analysis in Environment R (MAT14055D)

1. Introduction to the R language
i. Installation of R, R Studio and libraries
ii. Use of R as a calculator: mathematical and logical operations
iii. Data storage: variables, vectors, matrices and lists
iv. Object classes and object conversion into different classes
v. Data import, export and storage
vi. Data manipulation: filters, selections, renames, groupings, sorts, etc.
vii. Pipe Operator
2. Graphical data visualization: categorical, discrete and continuous data
i. Static graphs
ii. Dynamic graphs
iii. Recording graphs in several formats
3. Summary measures
i. Location
ii. Dispersion
iii. Form
iv. Association
4. Hypothesis tests
i. Parametric
ii. Non-parametric

Back

Ethics and Research (FIL13971D)

I. INTRODUCTION - THE PLACE OF ETHICAL QUESTIONING IN SCIENTIFIC AND TECHNOLOGICAL RESEARCH
I. 1. Research and Science
I. 2. Science, Technique and Technology
I. 3. Technological development and Ethics
II. CONCEPTS, VALUES AND ETHICAL PRINCIPLES IN RESEARCH
II. 1. Safeguarding human rights by the ethical regulation of research
II. 2. The common heritage of obligations of information professionals and researchers
II. 3. The criteria of freedom and responsibility in research
III. LICITUDE AND LEGALITY IN RESEARCH PROJECTS
III. 1. Issues of authorship - the rights and duties of the researcher
III. 2. Ethics Committees, codes or letters of conduct and personal decision
III. 3. Digital Age and research integrity

Back

Start-up PhD (GES14077D)

I. Navigating the Entrepreneurs' Sea: why are there start-ups that fail and others that are successful?
• What is an entrepreneur and what is entrepreneurship made of?
• Entrepreneurial personality, entrepreneurial skills and entrepreneurship teams.
• The power of innovation and ingredients to innovate.
• Entrepreneurship and critical sense - identify your own weaknesses and threats through SWOT analysis.
II. Designing a Value Proposition
• The validation of needs.
• How to eliminate the problems of a target audience?
• The conceptualization of a solution / prototype.
• Test and get feedback.
III. Minimum Viable Product (MVP): from the commitment of features to rapid prototyping
IV. Lean start-up: an integrated model
• From business strategy to business model: a roadmap for the future.
• The power of business communication.
V. Intellectual Property and Protection of Innovation
VI. Funding Sources: from investment rounds to crowdfunding

Back

Numerical Tools with Python (MAT15034D)

1. Introduction to SageMath software. Installation.
2. SageMath as a calculator: first calculations, elementary functions, Python variables, symbolic variables, first graphs.
3. Representation of floating point numbers: properties, rounding.
4. Programming and data structure: algorithms (loops, conditions and functions), lists and other data structures.
5. Analysis: symbolic expressions and simplifications, elementary mathematical functions, explicit resolution of equations. Sums, limits, sequences, series, derivatives and integrals. Solving differential equations.
6. Linear algebra: vector and matrix computation, solving linear systems, eigenvalues and eigenvectors computation, matrix decomposition.
7. Graphics: graphical representation of functions, parametric curves, curves in polar coordinates, implicitly defined curves, representation of discrete data, representation of the solution of differential equations.

Back

History of Sciences (FIS15035D)

Plurality of approaches in the history and philosophy of science and their interest in pedagogy and integral and humanistic training.
Aristotelian worldview.
Navigations and the preconditions of the Scientific Revolution.
Scientific Revolution: from Copernicus to Newton.
Kant and the theory of knowledge.
Lavoisier: Chemistry and the respiration of animals.
Laplacian Cosmovision and the development of Thermodynamics.
The consilience of inductions.
The Biological transformism and the anthropological model.
Overcoming mechanism, history and epistemology.
Quanta, relativity: overcoming the classical paradigm.
The history of science place.
Homo faber and the educational value of the history of science.
Institutionalization of HFC: creation of magazines and organization of conferences.
The modular structure of scientific theory.
Contemporary technoscience.
Material culture (laboratories, instruments, collections, etc).
The circulation of knowledge.
Science and values. Science and gender

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Introduction to automatic bibliographic reference systems (HIS15036D)

Introduction
1. Software installation
2. The importance of state of art and the difficulties in doing it
3. The main text formats used in the academic world
4. Zotero in the context of automatic management systems of bibliographic references
5. University libraries, available databases and the Web of Knowledge
Part I - Using Zotero to create my library
1. Collecting bibliography with Zotero
2. The organization of the library
3. Exploration of reading
4. Searching within the library
Part II - Reading with Zotero
Part III - Using Zotero for writing academic texts
1 Making the notes.
2. Styles
3.Automatically producing the final bibliography and changinge it
Part IV - Sharing with Zotero
1. E-mailing bibliographic references
2.Creating groups and sharing a library

Back

Emotions in learning contexts (PSI15037D)

1- Models and explanatory theories on the relationship between emotion and cognition.
2- Emotions and feelings in learning experiences
3- Emotional regulation in learning contexts

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Synthesis and Properties of Nanoporous Materials (QUI13579D)

Theoretical component

Definitions and general principles. Main nanoporous 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 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 nanoporous 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 of Characterisation of Solids and Surfaces (QUI13580D)

Theoretical component

Vacuum theory, systems and equipment. Adsorption methodologies. Helium pycnometry. 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 (TGA, DTG, TPD, DTA, DSC and STA).

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 (QUI13581D)

Target-oriented synthesis, diversity-oriented synthesis and sustainable synthesis.
Modern catalytic methods, chemocatalytic and biocatalytic methods, organocatalysis and metal-based coupling procedures.
Advanced retrosynthetic analysis.
Heterocycle synthesis.
Modern enabling technologies; alternative solvents, continuous flow processes, microwave assisted synthesis.
Radical based synthesis (photocatalysis).
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 and purification.

Back

Mechanisms and Determination of Structure in Organic Chemistry (QUI13582D)

Provide knowledge on important issues regarding the reactivity of organic compounds, such as advanced pericyclic reactions, mechanisms and their determination, quantitative activity-structure relationships (QSAR) and the stability and reactivity of cyclic compounds.
Provide knowledge on the various spectroscopic and spectrometric techniques for structural analysis of organic compounds.

2D NMR (COSY, HMBC, HMQC, INADEQUATE, NOESY, TOCSY,...).
NMR of other important nuclei (15N, 19F, 31P e 29Si).

Mass spectrometry; analysis of the decomposition profiles of various organic compounds.

Back

Advanced Methods in Computational Chemistry (QUI13583D)

Quantum Chemistry: Hückel, semi-empirical and ab initio methods. Density functional theory.
Quantum dynamics: Time evolution of a quantum system. Time dependent Density functional theory. Electronic transitions.
Molecular simulation: Molecular dynamics. Simulations in the micro-canonical, 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.
Intelligent Systems: Knowledge and Knowledge Representation; Reasoning; Degree of Confidence and Quality of Information. Methods and Techniques. Applications to the area of chemistry. In silico experimentation.

Back

Advanced Analytical Techniques and Hyphenated Techniques (QUI13584D)

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): Miniaturization of electrochemical cells, new sensors, applications.

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Microanalysis and In-Situ Analysis Techniques (QUI13585D)

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. Imaging techniques (IR reflectography, radiography, hyperspectral imaging, photogrammetry)

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

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Chemistry Seminar II (QUI13576D)

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 in Chemistry 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 societal implications. It may include results obtained by the student and with analysis of the results accomplished by the student. Students must also attend conferences. Examples of conferences organized by the teachers of the curricular unit: "Concentration and thermal applications of solar energy" (M. Collares Pereira, UÉ); "Porous carbon: An efficient and sustainable material for catalysis"(I. Matos, REQUIMTE).

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Chemistry Seminar III (QUI13577D)

The formal program consists of attendance at conferences organized under the Doctoral Program 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 curricular unit. Some examples are: "Fluorescent membrane probes behaviour in lipid bilayers" (L.M. Loura, U.Coimbra); "Design and synthesis of efficient organometallic molecules" (M.H. Garcia, U.Lisbon); "Carbon xerogels: from the lab to the industry" (INCAR, Spain); "Carbon dioxide utilization: opportunities of a global threat" (M.N. Ponte, REQUIMTE).
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 UÉ or at another institution.

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Chemistry Seminar IV (QUI13578D)

The formal program consists of attendance at conferences organized under the Doctoral Program in Chemistry 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 curricular unit. Some examples are: "Structure analysis of porous materials by EM" (X.D. Zou,, U.Estocolmo, Suécia); "Synthesis, properties and applications of ionanofluids" (C.N. Castro, U.Lisboa); "Nanostructuring conjugated polymers and polyelectrolytes" (H. Burrows, U. Coimbra); "Sustainability in view of drug delivery"(A. A. Ricardo, REQUIMTE).
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 UÉ or at another institution.