Objectives of the specialty:

All courses will be taught in English. The first half will be organized in clusters around a major route accounting for 15 ECTS. It will cover the following thematic areas: Molecular Chemistry (MoChem), Physical Chemistry for nanoscience (PCNano) and Theoretical Chemistry and Spectroscopy (TCN). Within each course an optional module (UE) (one of the other themes to choose) helps strengthen interdisciplinarity in an individual way. A strong core ensures that spirit through unifying modules such as molecular modeling, supramolecular chemistry and energy, and nanoscience. The module General Instruction enables students support in English and science communication. Regular participation in research seminars and conferences invited researchers provides important insight on issues and current topics. The last semester of the master will be entirely devoted to a long internship in the lab and will be completed by a bibliographic project giving rise to a defense and the summer school of the master. In addition to the defenses, lectures by faculty members and researchers will be given there.

<table>
<thead>
<tr>
<th>Speciality</th>
<th>Frontiers in Chemistry</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Common core</strong></td>
<td></td>
</tr>
<tr>
<td><strong>In charge</strong></td>
<td>Bernd Schöllhorn Olivia Reinaud</td>
</tr>
</tbody>
</table>

- UE 1: General instruction
- UE 2: Molecular modelling
- UE 3: Supramolecular chemistry
- UE 4: Energy and nanosciences

**Credits:** 15 ECTS

**Evaluation:** full compensation
Detailed description of the courses (UE):

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers: O. Reinaud, B. Schöllhorn, Matteo Merzagora, Sabine Michelon</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE: UE 1</td>
<td></td>
</tr>
<tr>
<td>ECTS: 6</td>
<td></td>
</tr>
<tr>
<td><strong>Teaching language:</strong> English</td>
<td></td>
</tr>
<tr>
<td><strong>In charge:</strong> O. Reinaud, B. Schöllhorn</td>
<td></td>
</tr>
</tbody>
</table>

**OBJECTIVES**

La participation régulière aux séminaires de recherche et aux conférences de chercheurs invités donne un aperçu important sur les divers aspects de la recherche et le développement scientifique. La pratique de l’anglais ainsi qu’un module sur la communication scientifique constituent un soutien important et une préparation à la vie professionnelle. Des conférences de professionnels du privé permettront d’acquérir quelques notions du R&D tels que les règlements européens ou la propriété intellectuelle ainsi que des discussions avec les invités.

**Pre-required notions:** Master 1 level

**PROGRAM**

A) **Research and development – research seminars**, TP: 10h P5 et 10 P7 (2 ECTS)
   - **Scientific seminars**
     6 seminars, 3 at Paris Descartes and 3 at Paris Diderot (report)
   - **European Economics, Human Resources and Legal Environment (invited lecturers)**
     a) Patents, trademarks, industrial and intellectual property: Invention, patents.
     b) Research and Development (R&D): Pharmaceuticals, materials.
     c) Environment, health and safety: European legislation – standards and norms (REACH…)

B) **Communication and human resources**, 20h HC (2 ECTS)
   Communication, job interview, cv …

C) **Foreign language**, 20h HC (2 ECTS), English (2 groups)

**Deliverables:** Analyse de conférences scientifiques. Notions du R&D. Communication scientifique (présentation orale et écrite). L’anglais (ou français pour les étrangers anglophones)

**Grading:** written reports, presentation, article analysis and control (complete compensation)
# UE 2 Computational project: 
How molecular modeling can assist the chemist?

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers:</th>
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</thead>
<tbody>
<tr>
<td>CODE : UE 2</td>
<td>F. Barbault</td>
</tr>
<tr>
<td>ECTS : 3</td>
<td>A. Perrier</td>
</tr>
<tr>
<td></td>
<td>M. Seydou</td>
</tr>
<tr>
<td>Teaching language:</td>
<td>F. Maurel</td>
</tr>
<tr>
<td>In charge:</td>
<td>I. Kleiner</td>
</tr>
</tbody>
</table>

## Objectives

The purpose of this UE is to illustrate how molecular modeling may decipher experimental data and/or predict chemical properties. Accordingly, this UE will be organized around several projects, each chosen by one or two students, and supervised by a teacher. The courses, 25% of time, will be adapted in accordance with the student’s scientific background and their project objectives. Some proposed projects might mix computational and experimental aspects.

**Pre-required notions:** Master 1 level

## Program

6h lecture + 24h TP

The student should choose one project among the following (non-exhaustive) list:
- How to predict ligand/protein interactions?
- How are molecules organized on a surface?
- How to model a chemical reaction?
- How to simulate and interpret a vibrational or a UV-Visible spectrum?

For the project picked by the student, technical and theoretical courses (25% of time) will be adapted. Students will have to provide two reports. The first one will be a bibliographic report, aiming at providing the state of the art of the project, and the second one will summarize the methods and results and will be written as a scientific article. Finally, a project defense will be made by the student.

## Deliverables:

At the end of this UE the students will be able to: manage a computational project; undertake meaningful calculations according to experimental data; master molecular modeling results interpretations/discussions/critics; write and defend the computational results.

**Grading:** The evaluation will take into account the two reports (50% of the mark) and the oral defence (50%).
### UE 3: Supramolecular Chemistry

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers:</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE: UE 3</td>
<td>Olivia Reinaud, Benoit Colasson, Bernd Schöllhorn, +...</td>
</tr>
<tr>
<td>ECTS: 3</td>
<td></td>
</tr>
</tbody>
</table>

**Teaching language**: English

**In charge**: O. Reinaud

---

**OBJECTIVES**

This class will give the students more insights into modern supramolecular chemistry. The notions in molecular recognition will be developed such as for the control of the reactivity within a supramolecular system. Also, new properties stemming from the supramolecular aspect of the objects will be discussed (for instance, the stereochemistry in supramolecular systems).

**Pre-required notions**: Master 1 level

---

**PROGRAM**

**A/ Supramolecular chemistry, 10h (1 ECTS)**

Reactivity in supramolecular chemistry.

- a) reactions in a confined space (artificial or biological)
  - (stereo)selectivity - stabilization of intermediates vs. rate acceleration
- b) supramolecular combinatorial chemistry (search for new catalysts, drug discovery)

**B/ Lectures and conferences on selected aspects of supramolecular chemistry by invited professors (2 ECTS)**

**Deliverables**:

**ÉVALUATION**: Final exam
<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers:</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE : UE 4S</td>
<td>Marc Robert</td>
</tr>
<tr>
<td>ECTS : 3</td>
<td>Cyril Costentin</td>
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<tr>
<td></td>
<td>François Mavré</td>
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<tr>
<td></td>
<td>Benoit Limoges</td>
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<td></td>
<td>Pascal Martin</td>
</tr>
<tr>
<td></td>
<td>Hyacinthe Randriamahazaka</td>
</tr>
</tbody>
</table>

| Teaching language | In charge: M. Robert |

<table>
<thead>
<tr>
<th>OBJECTIVES</th>
</tr>
</thead>
<tbody>
<tr>
<td>This course is intended to give a detailed introduction to the contemporary challenges associated to the development of renewable energy, mainly solar energy, at a global scale, and the role of emerging nanosciences in designing and inventing molecular systems as well as new materials able to store and/or produce energy using renewable energies as a primary source.</td>
</tr>
</tbody>
</table>

| Pre-required notions: Master 1 level |

<table>
<thead>
<tr>
<th>PROGRAM</th>
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</table>

1. **Molecular electrochemistry**
   - Activation of small molecules (10h)
   - Nanomaterials for storing and producing energy (6-8h)

2. **Lectures and conferences on selected topics** (6-12h) (invited researchers…)

| Deliverables: |

| EVALUATION: Final exam |
Objectives of the major:

This major will be delivered at the University Paris-Descartes with various aspects on molecular chemistry from chemical synthesis to the interface with biology. The lectures provide the tools for investigating the selective activation of molecules allowing the functionalization and synthesis of complex compounds. The reactivity in biological systems will be developed on one side through redox reactivities catalyzed by metallo-enzymes and the conception of biometric systems, and on the other side through nucleic acids.

- UE 5.1: Organic reactivity
- UE 5.2: Smart molecules
- UE 5.3: Redox bio-inorganic chemistry
- UE 5.4: Bio-organic chemistry
- UE 5.5: Option (1UE to be chosen from the other majors)

Credits: 15 ECTS

Evaluation: total compensation within each course (UE).

Detailed description of the courses (UE):
# UE 5.1: Organic Reactivity

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
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<tr>
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<table>
<thead>
<tr>
<th>Lecturers</th>
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<tbody>
<tr>
<td>Laurent Micouin</td>
</tr>
<tr>
<td>Stellios Arseniyadis,</td>
</tr>
<tr>
<td>Guillaume Prestat</td>
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<tr>
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<tbody>
<tr>
<td>English</td>
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<table>
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<tr>
<th>In charge</th>
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<tr>
<td>L. Micouin</td>
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</table>

## OBJECTIVES

To master the selective activation of a complex molecule. To master the selective functionalization of a non-functional compound.

### Pre-required notions:

- Master 1 level

## PROGRAM

- Transition metal catalysts as carbophilic Lewis Acid
- Pd(II) activation of unsaturated C-C bonds, TM-Cat Conia-ene reaction, Gold Chemistry
- Metathesis in organic synthesis
- Transition metal catalyzed Csp2-H activation
- Radical chemistry
  - G. Prestat (10h CM + tutoring 5h)

- Stoichiometric aromatic and heteroaromatic C-H or C-X bound activation
- Directed metalation, halogen-metal exchange, oxidative additions
  - L. Micouin (5h CM + 2h of tutoring)

- Aliphatic C-H bounds activation using transition metals, carbenes, nitrenes, C-C and C-X bound formation
- Application of C-H bounds activation in total synthesis
  - S. Arseniyadis (5h CM + 3h of tutoring)

### Deliverables:

- Rules and methods of selective activation of complex molecules, for the synthesis of complex organic molecules or molecular objects.

### Grading:

- Final exam 100%
# UE 5.2: Smart molecules

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers: Mélanie Ethève-Quelquejeu, Marc Lecouvrey, Isabelle Leray</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE: UE 5.2</td>
<td>Teaching language: English</td>
</tr>
<tr>
<td>ECTS: 3</td>
<td>In charge: Mélanie Ethève-Quelquejeu</td>
</tr>
</tbody>
</table>

## OBJECTIVES

**Pre-required notions:** Master 1 level

## PROGRAM

### I. Chemistry of Peptides and Proteins: (14h: CM)
- Solid phase synthesis
- Native chemical ligation
- Biorthogonal labelling of Proteins by chemical modification or by the ribosomal machinery

### II. Fluorescence spectroscopy (CM: 8h, ED: 2h)
- Photophysical properties of molecules
- Fluorescent probes for the detection of ions and neutral molecules

### III. Probes associated to other detection methods (6h: CM)
- Luminescence
- Molecular probes and nanochemistry

### IV. Article Analysis

## Deliverables:
Knowledge and understanding of the strategies for the conception of molecular probes for biology.

## Grading:
Final exam 100%
# UE 5.3 : Redox bioinorganic chemistry

## IDENTIFICATION
- **CODE**: UE 5.3
- **ECTS**: 3

## Lecturers:
- Olivia Reinaud
- Jean-Pierre Mahy
- Frédéric Banse
- Peter Faller

## Teaching language:
- English

## In charge:
- O. Reinaud

## OBJECTIVES
- Structure, mechanism and reactivity of major classes of metallo-enzymes (Fe, Zn, Cu) involved in redox processes
- Activation of small molecules (H₂O₂, O₂)
- Biomimetic systems

## Pre-required notions:
- Master 1 level

## PROGRAM

### Hemoproteins (6h lecture + 4h tutoring)
- Control and tuning of the heme reactivity by the protein backbone: electron transfer, O₂ (P-450, cyclooxygenase) and H₂O₂ (peroxidases, catalase) activation
- Rational design of biomimetic system for oxidation catalysis

### Non-heme Fe-enzymes (5h lecture + 3h tutoring)
- Non-heme active site for oxidation catalysis: catechol dioxygenase, aromatic-hydroxylase, alpha-ketoglutarate enzymes

### Copper proteins (8h lecture + 4h tutoring)
- Types 1 et A: electron transfer
- Type 2: oxidase (with a co-factor) or monoxygenase (with a reductant) activity
- Type 3: from O₂ transport O₂ activation (hemocyanine, catecholase, tyrosinase)
- 4 electron reduction of O₂: laccases, cytochrome c oxidase
- Biomimetic systems

## Deliverables:
- Knowledge and understanding at the molecular level of redox reaction catalyzed by metallo-enzymes and design of biomimetic systems

## Grading:
- Final exam 100%, 2h
### UE 5.4 : Bio-organic Chemistry

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers:</th>
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</thead>
<tbody>
<tr>
<td>CODE : UE 5.4 ( \text{(commune M Frontiers)} )</td>
<td>Mélanie Etheve-Quelquejeu</td>
</tr>
<tr>
<td>ECTS : 3</td>
<td>Dominique Padovani</td>
</tr>
<tr>
<td>Teaching language : English</td>
<td>Erwan Galardon</td>
</tr>
</tbody>
</table>

**In charge:** Mélanie Etheve-Quelquejeu

### OBJECTIVES

Nucleic Acids and Chemistry. Function and structure; Synthesis of chemically modified oligonucleotides. Nucleic acid analogues

Oxidative modifications on cysteines and redox signaling.

Biochemistry of sulfur metabolic compounds (cofactors and radical chemistry).

**Pre-required notions:** Master 1 level in Organic Chemistry

### PROGRAM

**Chemistry of nucleic acids:**

Synthesis of chemically modified oligonucleotides The post-synthetic approach by solid phase synthesis (with modified –nucleobase, sugar or phosphoramidite), by enzymatic process, by semi-synthesis.

Nucleic acid analogues (PNA, LNA, triazole-linked DNA).

**Oxidative modifications on cysteines and redox signaling:**

Oxygen and nitrogen reactive species (ROS/RNS): formation and reactivity. Biological chemistry of sulfinic acids and nitrosothiols.

**Sulfur metabolic compounds and hydrogen sulfide:**

Overview of sulfur compounds metabolism in mammals. Focus on S-adenosylmethionine as a source of chemical groups and hydrogen sulfide (biogenesis, degradation and reactivity).

**Deliverables:** Knowledge and understanding of the nucleosides and nucleotides chemistry.

**Grading:** final exam 2h (80%) and tutoring (20%)
Master de Chimie
M2 - Parcours Frontiers in Chemistry

<table>
<thead>
<tr>
<th>Specialty</th>
<th>Frontiers in Chemistry (M2S3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Major</td>
<td>Physical chemistry for Nanosciences (PCnano)</td>
</tr>
<tr>
<td>In charge</td>
<td>Nordin Félidj</td>
</tr>
</tbody>
</table>

Objectives of the major:

The proposed lectures of the major PCnano (physical chemistry for nanoscience) are an introduction in the principal concepts of physical chemistry at nanometric scale and resulting applications. Physical and chemical surface properties and the different characterization methods of interfaces are presented and microscopic as well as spectroscopic aspects will be discussed. Nanoelectrochemistry and molecular electronics, physical chemistry of polymers for electronic components, properties of nanostructured surfaces, metal nano-structures and nanotubes are included in the program. The students will be also taught the comprehension of tools and strategies for elaboration, functionalization and characterization of surfaces as well as the fabrication of nanostructured objects and materials. This major will finally focus on the numerous connections between nanosciences and biology and the interest to combine these two disciplines for the development of innovative devices and systems. At the end of those lectures, students will have a detailed knowledge of the technological and fundamental challenges of nanochemistry and nanobiotechnologies.

- UE 6.1: Physical chemistry of surfaces
- UE 6.2: Materials and nanomaterials for electronics and optics
- UE 6.3: Surface functionalization
- UE 6.4: Nano-biotechnologies
- UE 6.5: Option (1UE to be chosen from the other themes)

Credits: 15 ECTS

Evaluation: total compensation within each course (UE).

Detailed description of the courses (UE):
# UE 6.1: Physical chemistry at nanometric scale

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers: Nicolas Battaglini, Claire Mangeney, Jean Christophe Lacroix, Jalal Ghilane</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE: UE 6.1</td>
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<tr>
<td>ECTS: 3</td>
<td></td>
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<tr>
<td>Teaching language: English</td>
<td>In charge: J. C. Lacroix</td>
</tr>
</tbody>
</table>

## OBJECTIVES

This course is an introduction in the principal concepts of physical chemistry at nanometric scale and resulting applications. Physical and chemical surface properties and the different characterization methods of interfaces are presented and microscopic as well as macroscopic aspect will be discussed. The third part is focused on force field and tunneling microscopy, nowadays frequently used in physics, chemistry and biology laboratories. The students will learn how to extract topographic information using these techniques and how to determine the physical and chemical properties of a given sample with high spatial resolution.

### Pre-required notions:

Master 1 level in physical chemistry

## PROGRAM

1) **Physical and chemical surface properties** (C. Mangeney, 8h)
   - Introduction: ideal and real surfaces; interfaces and characterization methods
   - Microscopic aspects: surface/molecule interactions
   - Macroscopic aspects
   - Molecular adhesion

2) **Molecular electronics and Nanoelectrochemistry** (J-C. Lacroix, 8h)
   - General concepts on the process of molecular recognition.
   - Description of intramolecular electron transfer mechanisms and examples in research

3) **Force field microscopy** (N. Battaglini, 8h)
   - Introduction: Historical aspect of the technique, microscopy with a local probe
   - Tunneling microscopy (STM): instrumentation, applications
   - Force Field Microscopy (AFM): different working procedures

4) **Scanning electrochemical microscopy** (J. Ghilane, 2h + 4h TP, 1-2 groupes)

### Deliverables:

Connaissances approfondies des méthodes actuelles de type top-down et bottom-up, Compréhension des phénomènes plasmoniques localisés et de l'impact de la nanostructuration ...

### Grading:

Final exam 100%
**UE 6.2 : Materials and nanomaterials for electronics and optics**

**IDENTIFICATION**

<table>
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<th>CODE</th>
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<tr>
<td>UE 6.2</td>
<td>3</td>
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</table>

**Lecturers:**
- Jean-Christophe. Lacroix,
- Nordin Féridj
- Marc Lamy de la Chapelle,
- Samir Farhat

**Teaching language:** English

**In charge:** N. Féridj

**OBJECTIVES**

Nanoelectrochemistry and molecular electronics; physical chemistry of polymers for electronic components; nanostructured surfaces, metal nano-structures; nanotubes.

**Pre-required notions:** Master 1 level in physical chemistry

**PROGRAM**

1) *Physico-chimie des composants électroniques plastiques (diode, transistor, photovoltaïque)* (J. C. Lacroix, 8h)

Organic (or plastic) electronics is an emerging domain that aims at realizing electronics devices made of organic materials (polymers and small molecules). This lecture is an introduction to this new domain. First, we show how some organic materials behave as semiconductors, and in what they differ from their inorganic counter-parts, like silicon. Next, we present various organic electronic devices (diodes, transistors, opto-electronic devices) and detail their operating mode. Finally, we describe the specific fabrication techniques of organic electronics.

2) *Nanostructured surfaces, metal nano-structures: optical properties* (N. Féridj, 8h)

Metallic nanoparticles (mainly gold, copper, silver) which size is much smaller than the incident light wavelength, lead to collective oscillation of conductive electrons at the particle surface, the so-called “localized surface plasmon”. Such an optical phenomenon leads to a very high electric field enhancement at the particle surface. The goal of this lecture is to show all the possible applications using plasmonics structures in the context of high sensitive spectroscopies such as fluorescence or Raman scattering.

3) *Nanotubes* (M. Lamy de la Chapelle, S. Farhat, 10h)

Chemistry of nanotubes: nanotube synthesis (catalytic synthesis, growth processes...) polymorphism and nanotube structures, thermodynamic, synthesis of hetero-atomic nanotubes. Physics of nanotubes: structural properties, interaction light-matter, electronic properties, mechanical properties, vibrational properties, properties determination (characterization methods, measurements...) Applications: composite, biological applications, field emission, energy storage, nanoelectronics...

**Deliverables:** Nanoelectrochemistry and molecular electronics; physical chemistry of polymers for electronic components; nanostructured surfaces, metal nano-structures; nanotubes.

**Grading:** Final exam 100%
# UE 6.3: Surface Functionalization

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers:</th>
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<tbody>
<tr>
<td>CODE: UE 6.3</td>
<td>Benoit Piro, Bernd Schöllhorn, Roberta Brayner, Philippe Lang</td>
</tr>
<tr>
<td>ECTS: 3</td>
<td>In charge: B. Schöllhorn</td>
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<tr>
<td>Teaching language: English</td>
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</table>

## OBJECTIVES

During the three courses the students will be taught the comprehension of the tools and the strategies for elaboration, functionalization and characterization of surfaces as well as the fabrication of nanostructured objects and materials.

**Pre-required notions:** Master 1 level in physical chemistry and L3/M1 level in organic chemistry

## PROGRAM

1) **Chemical Functionalization of Surfaces - Electronic Conducting Polymers** (B. Piro, 8h)
   - Elaboration and properties of modified electrodes.
   - Structure and properties correlation
   - New trends and applications: an Overview

2) **Organic and organometallic monolayers** (B. Schöllhorn 8h, P. Lang 6h)
   - Methods for elaboration and characterization of molecular monolayers
   - Applications in research and industrial technology.

3) **Synthesis of materials at the nanoscale: magnetic properties** (R. Brayner, 4h)
   - Methods for preparing nanostructured materials (physical, chemical and mechanical).
   - Synthesis of nanoparticles by chemical liquid phase nucleation and growth
   - Energetic contributions: Effects of size, Size characteristics; Magnetic materials and sample applications

**Deliverables:** strategies for the elaboration and the functionalization of surfaces and selected characterization techniques; applications of functionalized surfaces; methods for the fabrication of nanostructured objects with magnetic properties.

**Grading:** Final exam 100%
### UE 6.4: Nanobiotechnologies

<table>
<thead>
<tr>
<th>Identification Code: UE 6.4</th>
<th>ECTS: 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lecturers:</td>
<td>Benoit Piro, Marion Giraud, Claire Mangeney, Damien Marchal, Vincent Noel</td>
</tr>
<tr>
<td>Teaching language:</td>
<td>English</td>
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<tr>
<td>In charge:</td>
<td>B. Piro</td>
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</table>

#### OBJECTIVES

This course focuses on the numerous connections between nanosciences and biology and the interest to combine these two disciplines for the development of innovative devices and systems. By the end of the course, students will have a detailed knowledge of the technological and fundamental challenges of nanobiotechnologies.

**Pre-required notions:** Master 1 level in physical chemistry

#### PROGRAM

1. **Nanomaterials: Imagery and Therapy** (C Mangeney/M. Giraud, 8h?)
   - Vector-mediated drug delivery
   - Chemical Physics of Colloids applied to Biology, Organic Nanomaterials.
   - Colloidal systems for Imagery and Therapy, Cells Labelling and Contrast Agents, Cellular Hyperthermia.

2. **DNA/Proteins/glycosides chips**: (B. Piro, D. Marchal, 8h?)
   - Functionalization and Sensing strategies,
   - Fields of Application - research, diagnostic, health, agribusiness ,..,

3. **Contribution of Biology to Nanostructures Building**: (R. Brayner, V. Noel, 8h?)
   - Biomimetic materials,
   - Programmed Supramolecular Architectures based on Biomolecules and Nano-object

#### Deliverables:

#### Grading:
Final exam 100%
Objectives of the major:

**Analytical Chemistry for natural and anthropogenic complex systems.**

The objective of this major is to teach scientific knowledge and practice on advanced analytical chemistry applied on natural system or the anthroposphere. The students will be prepared for academic research but also for R&D in companies: control needs are increasing at the same time as worldwide trade, complexity of industrial fabrication processes as well as impact on human health. Today, identified targets for employment are laboratories working on environment issues, in pharmaceutical / para-pharmaceutical industry or food industry as well as in the field of energy. This course is included in a wider context thus improving skills and competences of the future graduated students.

*Pre-required notions:* A theoretical background on chemistry and analytical chemistry (M1 level) is required.

**ECUE composant l'UE**

- UE 7.1 Performing analyses in the environment and complex systems
- UE 7.2 Heterogeneity and complexity
- UE 7.3 Processes in aquatic systems and at geo-interfaces
- UE 7.4 New tools and technologies in analytical chemistry
- UE 7.5 Option (1UE to be chosen from the other themes)

**Faculty**

Souad AMMAR (PR), Marc BENEDETTI (PR), Christine CORDIER (MCF HDR), Alexis GROLEAU (MCF), Didier JEZEQUEL (MCF), Rémi LOSNO (PR), Jean Yves PIQUEMAL (MCF HDR), François PREVOT (MCF), Yann SIVRY (MCF).

**Credits:** 15 ECTS

**Evaluation:** total compensation within each course (UE).

**Detailed description of the courses (UE):**
## UE 7.1: Analyses in environment and complex systems

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers: Didier Jézéquel, Rémi Losno, Yann Sivry, Souad Ammar, Jean-Yves Piquemal</th>
</tr>
</thead>
<tbody>
<tr>
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<tr>
<td>Teaching language: English</td>
<td>In charge: Yann Sivry</td>
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</tbody>
</table>

### OBJECTIVES

The purpose of this course is to provide an overview of i) the main issues relatives to analytical measurement on complex matrix; ii) the specificity of techniques used for such measurements; iii) the most recent developments on this subject.

**Pre-required notions:** A theoretical background on chemistry and analytical chemistry (M1 level) is required to attempt to this UE.

### PROGRAM

*(26h cours + tutoring)*

The overall goal of this UE is to present the main issues relative to analytical measurement on environmental and complex systems, from the sampling strategy to the use of analytical techniques dedicated to such systems in the current scientific state of the art.

This objective will be reached thanks to the development, during the lectures and tutorials, of specific themes:

1. Sampling strategy, sample preparation and preservation for multiphase and/or complex systems (RL, 6 h);
2. Analytical techniques using spectrometry (AAS, ICP-AES, ICP-MS and XRF), chromatography, electrochemistry and coupled devices (YS/DJ, 8 h);
3. Isotopic determinations as a tool to decipher complex systems (YS, 6 h);
4. X-Rays diffraction (XRD) (SA/JYP, 6 h);
5. Trace Metal speciation determination (YS, 4 h)

Both analytical development challenges and applied case studies will be presented in this course.

**Deliverables:** Advanced method and technics for elemental, isotopic and molecular inorganic analyses in heterogeneous and variable systems.

**Grading:** Oral presentation and examination *(100%)*. Each student will have to give a 15 min talk dealing with either a case study of complex system analysis, an analytical method specifically dedicated to environment and complex system analyses or a comparison of data obtained with various analytical techniques. The student ability to criticize the choice of the techniques and the analytical precisions will be taken into account. This presentation will be followed by an oral examination of 15 min.
Master Chimie Sorbonne Paris Cité - Frontiers in Chemistry

<table>
<thead>
<tr>
<th>UE 7.2 : Heterogeneity and complexity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>IDENTIFICATION</strong></td>
</tr>
<tr>
<td>CODE : UE 7.1</td>
</tr>
<tr>
<td>ECTS : 3</td>
</tr>
<tr>
<td><strong>Lecturers :</strong></td>
</tr>
<tr>
<td>Mehrdad Nikravech (Paris 13)</td>
</tr>
<tr>
<td>Rémi Losno</td>
</tr>
<tr>
<td>François Prévot</td>
</tr>
<tr>
<td>Alexis Groleau</td>
</tr>
<tr>
<td><strong>Teaching language :</strong></td>
</tr>
<tr>
<td>English</td>
</tr>
<tr>
<td><strong>In charge:</strong></td>
</tr>
<tr>
<td>F. Prévot</td>
</tr>
</tbody>
</table>

**OBJECTIVES**

Analytical chemistry of complex systems produces lots of data in short periods to take into account the time evolution and the spatial heterogeneity of the systems. Understand the meaning of the data stream is a challenge but necessary to understand the fate and behaviour of the investigated system. Most of the useful information can be hidden in the data flow and the objective of this course is to learn how to extract the maximum information with the minimum of work. Most of the complexity of analytical systems is caused by its heterogeneity and temporal variability. Consequences of spatial and temporal heterogeneity in fluid systems are presented here.

**Pre-required notions:** A theoretical background on chemistry and analytical chemistry (M1 level) is required to attempt to this UE.

**PROGRAM**

(26h cours + tutoring)

1) Mass and heat transfer: Principles, basic equations, numerical solutions and examples (MN 10h cours + 2h tutoring). (1 ECTS)

Fluid dynamic applied to advection, convection and transportation. Conservation equations for heat and mass transfer.
Diffusion (Fick's law).
Small systems dynamic: active and passive accumulation devices and membranes.
Large systems: convection and stability in gas and liquids.
Time and space scale relationships.
Application: From plants to global environment.

2) Data analyses (14h cours + 4h tutoring) (2 ECTS)
Review of statistical methods used for measurements and time series processing (RL, 4h).
Accuracy. Errors and uncertainties. Error propagations. (RL, 2h)
Analyses certification. Instrument stability check. (FP, 4h)
Monitoring tools for natural and industrial environment (FP, 4h).
Training on computer: Spread-sheet organisation, R software with statistical plugins. (AG, 4h)

**Deliverable :** Knowledge of physical and mathematical tools to work in a complex environment.

**Grading:** Written examination (60%), oral examination (40%)
UE 7.3: Processes in aquatic systems and at geo-interfaces

**IDENTIFICATION**
- **CODE**: UE 7.1
- **ECTS**: 3

**Lecturers**: Didier Jézéquel, Yann Sivry, Marc Benedetti

**Teaching language**: English

**In charge**: Marc Benedetti

**OBJECTIVES**

The purpose of this course is to provide an understanding of the fundamental geochemical processes that govern the chemical composition of natural waters and the environmental fate of chemical species in natural waters.

**Pre-required notions**: A theoretical background on chemistry and analytical chemistry (M1 level) is required to attempt to this UE.

**PROGRAM**

*(26h cours + tutoring)*

Thermodynamics and kinetics processes regulating the chemistry of surface and groundwater in natural and polluted environments, with particular emphasis on explaining the aqueous concentrations of chemical species and controlling geochemical factors in the hydrosphere.

**Lectures list**:
- Introduction (MB, 2h)
- Complexation Reactions (MB, 4h)
- Chemical Weathering (MB, 2h)
- Sorption and Desorption (YS, 4h)
- Modeling interface processes (MB, 8h)
- Redox Chemistry (DJ, 6h)
- Kinetics (DJ, 4h)

**Presentations**: Each student is required to give two 15 min talks to the class on a specific research topic related to the material covered in class. The talks will be based on a literature search involving journal papers.

Tutorials will require the use of the geochemistry program Visual MINTEQ. A download copy (free) is available at http://www.lwr.kth.se/English/OurSoftware/vminteq/ (this program is designed to operate in Windows).

**Most Relevant Journals**: Applied Geochemistry, Aquatic Geochemistry, Chemical Geology and Geochim et Cosmochim Acta, Environmental Sciences and Technology.

**Reference Books**:
- The Geochemistry of Natural Waters (JI Drever), Prentice Hall
- Aquatic Chemistry (W Stumm and JJ Morgan), Wiley-Interscience

**Deliverables**: Knowledge of fundamental processes at solid-liquid and liquid-gas interfaces.

**Grading**: Final exam (60%), Research Presentations (40%)
# UE 7.4: New tools and technologies in analytical chemistry

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<thead>
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<th>IDENTIFICATION</th>
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<tbody>
<tr>
<td>CODE: UE 7.1</td>
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<tr>
<td>ECTS: 3</td>
</tr>
</tbody>
</table>

**Lecturers:**
- Marc Benedetti
- Alexis Groleau
- Didier Jézéquel
- Rémi Losno
- François Prévot
- Christine Cordier
- Yann Sivry

**Teaching language:** English

**In charge:** Didier Jézéquel

## OBJECTIVES

Knowledge of the capability and limitations of analytical instruments. Choosing the right method for the appropriate problem. The student will work on a proposed personal research project.

**Pre-required notions:** A theoretical background on chemistry and analytical chemistry (M1 level) is required to attempt to this UE.

## PROGRAM

*(26h cours + tutoring)*

This course will present techniques, methods and principles at the more advanced state of the art level for operating chemical analyses. The teaching team is wide for this title because the covered domain is large and needs specific knowledge.

**Part 1:** Instrumental techniques (8h cours + 2h tutoring) *(1 ECTS)*

- Detectors and associated technologies. Signal computation, application to particles (photons, ions, electrons, neutrons) counting, data processing advancements for new instrumentation (FP).
- Separation of analytes (DJ)
- Inorganic and organic carbon measurements, isotopic determinations (MB)

**Part 2:** Analytical issues (13h cours + 2h tutoring) *(1.5 ECTS)*

- Applied spectroscopy to chemical analyses: IR, UV, Raman, NMR (CC)
- Ultra-trace analyses (RL)
- Measuring isotopes. (YS)
- Coupling separation and analyses (MB/DJ)

**Part 3:** New trends in instrumentation (5h cours) *(0.5 ECTS)*

- Progresses in technology (MB)
- Future needs for science and society (AG)

**Deliverables:** Knowledge of the most recent techniques for analytical material and methods with an emphasis to inorganics. Knowledge of the most adapted methodologies to solve an analytical challenge in a complex system.

**Grading:** written exam (60%), project presentation (40%)
Objectives of the major:

The goal of the lectures is to study the behavior of molecules in different environments (gaz, surface, liquid) using quantum chemistry, molecular mechanics, experimental and theoretical spectroscopies. Many applications will be proposed: studies of earth atmosphere, astrophysical systems, photochemistry, intramolecular dynamics, bio-informatics. A special focus will be made on climate change and air pollution which are two key issues in current atmospheric research. Examples of observation of atmospheric key species by satellites and ground-based observatories will be given. The process of deducing mixing ratios from atmospheric spectra (retrieval) will be described and detailed.

ECUE composant l’UE

- UE 8.1 Laser chemistry
- UE 8.2 Modern Spectroscopy for Atmospheric and astrophysical applications
- UE 8.3 Computational chemistry
- UE 8.4 Molecular modelling of large systems
- UE 8.5 Option (1UE to be chosen from the other themes)

Credits: 15 ECTS

Evaluation: total compensation within each course (UE).

Detailed description of the courses (UE):
This course is intended to give an introduction to modern experimental spectroscopic techniques for the study of molecular and supramolecular systems. For this, we will make use of examples of state-of-the-art research in experimental spectroscopy (all wavelength domains). Emphasis will be laid on low divergence light sources used in modern spectroscopy, such as lasers and synchrotron radiation. Special attention will also be paid to scientific methodologies that couple spectroscopy to theoretical chemistry.

We address gas phase techniques as well as surface and condensed phase spectroscopic and micro-spectroscopic techniques. We will also show that also gas phase spectroscopic studies are highly relevant not only for the study of diluted matter but also for biomolecular systems that normally evolve in the condensed phase.

**Pre-required notions:** Master 1 level. Basic knowledge in spectroscopy L3/M1 level.

**Program**

<table>
<thead>
<tr>
<th>1. Lasers as tools in experimental physical chemistry and spectroscopy (0.5 ECTS)</th>
</tr>
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<table>
<thead>
<tr>
<th>2. Synchrotron radiation (SR) as a light source (0.5 ECTS)</th>
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</thead>
<tbody>
<tr>
<td>General mode of operation: electron storage rings, dipole and undulator beamlines, use of synchrotron radiation for different scientific applications (UV/VUV and other spectral domains, condensed and gas phase):</td>
</tr>
<tr>
<td>Examples: photoionization mass spectrometry, photoelectron spectroscopy and e/*i coincidence spectroscopy, FT VUV spectroscopy, inner shell spectroscopy (soft X).</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>3. Advanced MW, THz and IR gas phase spectroscopy (1 ECTS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MW spectroscopy, FTIR spectrometers, use of synchrotron radiation in the IR/THz domain, tunable diode laser spectroscopy in the IR/THz domain, cavity ring down spectroscopy (CRDS), cavity enhanced spectroscopy, femtosecond comb spectroscopy</td>
</tr>
</tbody>
</table>

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<tr>
<th>4. Surface and condensed phase techniques (0.5 ECTS)</th>
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<tbody>
<tr>
<td>Optical microscopy, scanning near field optical microscopy (SNOM), atomic force microscopy (AFM), scanning tunneling microscopy (STM), surface-enhanced Raman scattering (SERS), XPS.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>5. Practical work in the form of mini projects. Visit Synchrotron Soleil (0.5 ECTS)</th>
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<table>
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<tr>
<th>6. Modelling the phochemical reactivity</th>
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</thead>
<tbody>
<tr>
<td>ab-initio methods for excited states</td>
</tr>
<tr>
<td>potential energy surfaces, ground and first excited states, photochemical reaction path</td>
</tr>
<tr>
<td>Dynamical aspects</td>
</tr>
<tr>
<td>Application: azobenzene photoreactivity</td>
</tr>
</tbody>
</table>

**Deliverables:** Knowledge of the most recent techniques of spectroscopy in research laboratory

**Grading:** Final exam (80%), Practical work (20%)
The purpose of this course is to introduce the underlying spectroscopy linked to atmospheric and astrophysical studies. A special focus will be made on climate change and air pollution which are two key issues in current atmospheric research. Examples of observation of atmospheric key species by satellites and ground-based observatories will be given. The process of deducing mixing ratios from atmospheric spectra (retrieval) will be described and detailed.

Pre-required notions: Connaissances de base en spectrométrie de niveau L3/M1 chimie ou physique. Notions de physico-chimie de l'atmosphère et astrophysique.

PROGRAM

(26h cours + tutoring)

Synchrotron radiation (SR) as a light source:
- General mode of operation: electron storage rings, dipole and undulator beamlines
- Different spectral domains: IR, VUV, soft X, hard X, examples of different scientific applications (condensed and gas phase examples)

Advanced laboratory spectroscopy in the MW, THz, IR and UV spectral domain for astrophysical and atmospheric applications
- Measurement of high quality spectroscopic data in the laboratory for the interpretation of observational data. Spectroscopic measurements at different temperatures and pressures.
- MW spectroscopy, FTIR spectrometers, use of synchrotron radiation in the IR/THz domain, tunable diode laser spectroscopy in the IR/THz domain, cavity ring down spectroscopy (CRDS), cavity enhanced spectroscopy, femtosecond comb spectroscopy
- UV and VUV laboratory spectroscopy
- Examples of the study of stable and unstable species of atmospheric and astrophysical interest

LiDAR: Light Detection And Ranging

Atmospheric and Astrophysical applications
- Structure of the Earth's atmosphere
- Climate change and air pollution: key chemical and physical processes
- Atmospheric sounding: satellites and ground based observatories
- Chemistry in the interstellar medium and planetary atmospheres (including exoplanets).
- Spectroscopic observation: microwave and submillimeter telescopes, IR observatories, observation in the UV and VUV spectral regime from satellites.
- Laboratory Astrophysics: measurement of high quality spectroscopic data for the interpretation of observational data. Spectroscopic measurements at different temperatures and pressures, examples of the study of species of atmospheric and astrophysical interest.

Practical work in the form of mini-projects
- Visit to Créteil Atmospheric Infrared observatory OASIS
- Analysis of an atmospheric spectra

Deliverables: Connaitre et appréhender les techniques d'observations utilisant des méthodes spectroscopiques en sciences de l'univers, initiation à l'analyse des spectres atmosphériques et méthodes d'inversion.

Grading: Final exam (80%), Practical work (20%)
OBJECTIVES
The purpose of the first part of this course is to give an overview of advanced computational methods and to apply these theoretical approaches to molecular systems ranging from simple organic molecules to complex assemblies (supramolecular or biological systems for instance). The theoretical basis of \textit{ab initio} methods and density functional theory will be covered in depth.

This second part of this course is intended to present advanced methods of theoretical molecular spectroscopy, applied for the study of different isolated molecular systems, from small (in)organic molecules to more complex molecules which can mimic parts of biomolecules (small peptides, sugars, amino acids ...). Experimental aspects of high resolution spectroscopy will be treated too where necessary. Emphasis will be put on the quantum mechanical approaches necessary to model high resolution spectra in terms of line positions, line intensities and line shape. We will show how the spectroscopic data can be used for structure determination.

Pre-required notions: M1 level in theoretical chemistry and spectroscopy.

PROGRAM

\textbf{Quantum chemistry methods (2 ECTS)}
Potential Energy Surface (PES)
Electronic correlation
Post Hartree-Fock methods
Density Functional Theory
Determination of molecular properties (Charge distribution, dipole moment, Raman/IR, RMN, RPE, UV-visible spectra...)
Chemical reactivity

\textbf{Advanced Theoretical spectroscopy (Lecture 10h)}
Modeling of IR and MW spectra
Fermi-type and Coriolis type, vibration-rotation interactions
Models and theory for analyzing microwave and infrared spectra
Modeling of line positions, intensity and line shape

Structure determination
Molecular spectra and structure determination from rotational constants
Applications to molecules of atmospheric and astrophysical interest
Applications to small peptide biomimetics in the gas phase

Deliverables: The goal of this teaching unit is to provide the principles, advantages and limits of the various techniques of \textit{ab-initio} quantum chemistry and advanced theoretical spectroscopy.

Grading: Final exam (80%) and continuous assessment (20%)
<table>
<thead>
<tr>
<th><strong>IDENTIFICATION</strong></th>
<th><strong>Lecturers</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE : UE 7.4</td>
<td>François Maurel</td>
</tr>
<tr>
<td>ECTS : 3</td>
<td>Florent Barbault</td>
</tr>
<tr>
<td><strong>Teaching language</strong> : English</td>
<td>Mahamadou Seydou</td>
</tr>
<tr>
<td><strong>In charge</strong>: Mahamadou Seydou</td>
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</table>

**OBJECTIVES**

This course aims at enhancing the knowledge of computational chemistry toward the applications of modern research topics:

I. **Surfaces and nanomaterials,**
II. **Biological compounds**

At the end of the courses the students will be able to lead meaningful molecular modeling calculations within an experimental framework.

**Pre-required notions**: M1 level in theoretical chemistry.

**PROGRAM**

(26h cours + tutoring)

**Surfaces and nanomaterials modelling**
- Models for metallic systems, surfaces and nanomaterials
- Tight binding bond model to study surfaces and nanomaterials
- Electronics, optical and thermals properties calculations
- Applications to supra molecular networks on surface and carbon nanotubes

**Simulations of biological compounds**
- Molecular docking and virtual screening of ligands
- Explore the biological flexibility through molecular dynamics
- Ligand/protein recognition process
- Applications to rational drug discovery
- Biomacromolecular structures

**Deliverables**: Understand and use computer simulations techniques applied to experimental chemistry

**Grading**: Final exam (100%)
### Specialty

<table>
<thead>
<tr>
<th>Specialty</th>
<th>Frontiers in Chemistry (M2S4)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Common core</td>
</tr>
<tr>
<td>In charge</td>
<td>Bernd Schöllhorn</td>
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<tr>
<td></td>
<td>Olivia Reinaud</td>
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</table>

- UE 9: Bibliographic project
- UE 10: Research internship

**Credits:** 30 ECTS

**Evaluation:** total compensation within each course (UE).

**Detailed description of the courses (UE):**

#### UE 9: Bibliographic project

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE : UE 8</td>
<td>O. Reinaud, B. Schöllhorn</td>
</tr>
<tr>
<td>ECTS : 5</td>
<td>M. Branca, F. Mavré, F. Maurel, F. Barbault, M. Giraud, N. Félidj</td>
</tr>
</tbody>
</table>

**Teaching language:** English

**In charge:** O Reinaud, B. Schöllhorn

**OBJECTIVES**

Bibliographic project: Literature research and analysis

**Pre-required notions:** Master 1 level

**PROGRAM**

Le stagiaire est supervisé et aidé dans la réalisation d'un projet bibliographique sur un sujet scientifique proposé.

**Deliverables:** Literature research and analysis

**Grading:** oral presentation (100%)
# UE 10 Research Internship

<table>
<thead>
<tr>
<th>IDENTIFICATION</th>
<th>Lecturers:</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE: UE 9</td>
<td>Claire Fave</td>
</tr>
<tr>
<td>ECTS: 25</td>
<td>Claire Mangeney</td>
</tr>
<tr>
<td></td>
<td>Olivia Reinaud</td>
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<tr>
<td></td>
<td>Bernd Schöllhorn</td>
</tr>
<tr>
<td></td>
<td>Benoit Colasson</td>
</tr>
<tr>
<td>Teaching language: English/French</td>
<td></td>
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<tr>
<td>In charge: C. Mangeney, O. Reinaud</td>
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</tbody>
</table>

## OBJECTIVES

Ce stage long permet de confronter et compléter les enseignements théoriques et méthodologiques reçus lors de la formation par une mise en situation d'activité. Véritable expérience professionnelle, il donne la possibilité à l'étudiant d'acquérir un savoir-faire mais également un savoir-être au contact de professionnels expérimentés et ceci dans le domaine de la recherche. Il s'agit d'une formation approfondie par la recherche.

**Pre-required notions**: Master 1 level

## PROGRAM

Research internship in an academic or private laboratory (5 to 6 months) including a written report and an oral presentation in English followed by a short discussion with the jury.

**NB**: The internship should be performed in one of the laboratories of University Sorbonne Paris Cité. Exceptions only possible after approval by the head of the master.

**Grading**: Written report 50 %, oral presentation 50% in English.