M2 COURSE DESCRIPTION

Academic Year 2026 – 2027

General guidelines

Semester 1: Fundamental and transversal courses (30 ECTS)

- A total of 30 ECTS is required to validate the semester.
- Transversal courses may not exceed 8 ECTS.
- External courses (outside the catalogue) may be selected – subject to an agreement with the host program and approval from your year supervisors – up to a max. of 12 ECTS for fundamental courses and 8 ECTS for transversal courses.
- Extra courses (not validating) may be taken beyond the required 30 ECTS. However, it is recommended not to exceed 36 ECTS in total.

Semester 2: Research internship (5-6 months, 30 ECTS)

A full-time 5-6 month research internship is mandatory to validate the semester (30 ECTS).

Specialties

One or several specialties can be obtained; however, having a specialty is not mandatory for completing the degree. A specialty may be earned through one of the following options:

(1) validate three 6 ECTS courses for which it is the primary specialty (P), and select an internship aligned with the specialty.

(2) validate two 6 ECTS courses for which it is the primary specialty (P) and two 6 ECTS courses for which it is the secondary specialty (S), and select an internship aligned with the specialty.

Apprentice track

An apprenticeship track is possible. A total of 30 ECTS is required for both semesters. In Semester 1, courses must be selected so as to leave two days per week available for work within the host company. In Semester 2, the internship is carried out in the same company. Students are responsible for securing their own host company.

List of courses – Semester 1

Fundamental courses					
MHMCHIM#	Course title	Slot	Specialties		ECTS
			Scientific	Transversal	
301	Emergent activation methods, synthetic strategies and technologies in synthesis	Fr-PM			6
302	Organometallic Chemistry and Catalysis	We-AM		-	6
303	Design, Synthesis and Characterization of Advanced Polymers	Th-PM			6
304	Valorization of bioresources / Valorisation des bioressources	Tu-AM			6
305	Medicinal products from biotechnology	Th-AM			6
330	Total synthesis of natural products and bioactive compounds	Tu-AM		-	6
306	Materials for environment	Tu-PM			6
307	Materials for energy devices	Fr-PM			6
308	Materials for optics	Tu-AM			6
309	Polymers and Soft Matter: Design and Applications	Th-AM			6
310	Biomaterials: from materials engineering to biomedical devices	Mo-PM			6
311	Probing, controlling, elaborating surfaces at the nanometric scale	We-AM			6
312	Statistical mechanics and simulations for biomolecular systems	Th-AM			6
313	Data Science and AI for Chemistry	We-PM			6
314	Theory of Chemical Reactivity	Tu-PM			6
315	Modelling Materials	Th-PM			6
316	Omics	Th-PM			6
317	New molecular and particle-based systems for diagnostics and therapeutics	Mo-PM			6
318	Key issues in modern separation sciences and technologies	We-PM			6
319	Electrochemistry for Sustainability, Diagnosis and Global change	Th-AM		-	6
320	Magnetic resonance	Mo-PM		-	6
321	Multimodal imagings with contrast agents for theranostics	We-AM			6
322	Inorganic Chemical Biology	We-PM			6
323	Dynamics of Biological processes	Fr-PM		-	6
324	Chemical Biology	Tu-PM			6
325	Fluorescent probes for advanced cell imaging	Tu-AM			6

Scientific Specialties:

- Molecular design and synthetic tools
- Analytical and physical chemistry
- Smart materials
- Chemistry and life sciences
- Theoretical chemistry and modelling

Transversal Specialties:

- Digital Chemistry
- Nanotechnologies
- Environment
- Renewable energies
- Health

Transversal courses			
MHMCHIM#	Course title	Slot	ECTS
326	Scientific communication, with project	Tu-PM	6
327	Scientific communication, without project	Tu-PM	4
328	Research design	Fr-AM	6
329	Seminar cycle	Mo-AM	2

MHMCHIM301

<table>
<tr><td colspan="2" rowspan="2">M2 S1</td><td colspan="2">Emergent activation methods, synthetic strategies and technologies in synthesis</td></tr>
<tr><td colspan="2">Keywords: Photocatalysis, Organocatalysis, Biocatalysis, Flow chemistry, Mechanochemistry, Electrosynthesis, Electrophotocatalysis</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Maxime R. Vitale (maxime.vitale@ens.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Kevin Cariou; Laurence Grimaud; Benjamin Laroche; Jean-Francois Soulé; Maxime R. Vitale</td></tr>
<tr><td colspan="2">Language of instruction</td><td colspan="2">English</td></tr>
<tr><td colspan="2">Specialties
(P = primary ;
S = secondary)</td><td colspan="2">Molecular design and synthetic tools (P)
Renewable energies (S)</td></tr>
<tr><td colspan="2"></td><td>Total teaching hours: 48 h
- Lectures : 28 h
- Tutorials: 16 h
- Invited speakers (2 x 2h) : 4 h</td><td>Grading:
- written exam: 75 %
- oral exam / presentation: 25 %</td></tr>
<tr><td colspan="4">Course description and content

This course explores cutting-edge methodologies and technologies in chemical synthesis, emphasizing innovative activation techniques. Topics include:

• Photocatalysis: Harnessing light to drive chemical reactions.
• Organocatalysis: Utilizing small organic molecules as catalysts.
• Biocatalysis: Leveraging enzymes for sustainable synthesis.
• Flow Chemistry: Continuous processing for scalable and efficient reactions.
• Mechanochemistry: Solid-state reactions activated by mechanical force.
• Electrosynthesis: Electrochemical methods for sustainable synthesis.
• Electrophotocatalysis: Combining light and electrochemical activation.

Students will gain insights into integrating these methods to solve complex synthetic challenges.</td></tr>
<tr><td colspan="4">Learning goals

The student should be able to:
- Understand emergent activation methods
- Learn the pros and con of the different activation method/technology
- Learn to understand different kind of catalytic cycles
- Develop the ability to select the most appropriate activation method or synthetic strategy to achieve the desired outcome efficiently and sustainably</td></tr>
<tr><td colspan="4">Prerequisites

Advanced knowledge of organic chemistry and organometallic catalysis (M1 level)</td></tr>
</table>

MHMCHIM302

M2	S1	Organometallic Chemistry and Catalysis	
		Keywords: cross-coupling reactions, earth-abundant metal catalysis, gas utilization and valorization, C-H bond activation, metathesis, mechanism understanding	
Coordinator		Amandine Guérinot (amandine.guerinot@espci.fr)	
Instructor(s)		Laurence Grimaud; Amandine Guérinot; Phannarath Phansavath; Jean-François Soulé; Maxime Vitale	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Molecular design and synthetic tools (P)	
		Total teaching hours: 48 h - Lectures: 34 h - Seminar: 2 h - Tutorials: 12 h	**Grading:** - written exam: 75 % - oral exam / presentation: 25%

Course description and content

Over the past 50 years, metal catalysis has emerged as a key strategy to produce complex molecular architectures for pharmaceuticals, agrochemicals or materials. A panel of synthetic methods relying on organometallic chemistry and catalysis will be presented, with a special focus on recent developments and future challenges in the context of sustainable chemistry. The first section will be devoted to mechanistic studies in palladium-catalyzed cross-coupling reactions. An introduction to earth-abundant metal catalysis will be then provided. In a subsequent section, synthetic strategies based on C-H activation will be discussed. Another module will be dedicated to gas (CO, H_2, CO_2) incorporation and valorization. Finally, olefin metathesis will be examined. In all the sections, both reactivity and mechanistic aspects will be addressed. Interactivity will be favored through several tutorial sessions.

Learning goals

The course will provide the students with a strong knowledge in organometallic chemistry, catalysis and mechanism investigations. The students will be able to:

- devise synthetic pathways including metal-catalyzed reactions
- understand and analyze a research article dealing with organometallic catalysis
- propose a mechanism for classical metal-catalyzed reactions

Prerequisites

M1 level in organic chemistry, basics in catalysis (Pd-catalyzed cross-coupling reactions), basics in kinetics

MHMCHIM303

M2	S1	Design, Synthesis and Characterization of Advanced Polymers	
		Keywords: controlled radical polymerization, metal-catalyzed polymerization, photopolymerization, emulsion polymerization, supramolecular assembly and polymerization, covalent adaptable networks, material properties, microscopy and scattering techniques	
Coordinator		Renaud Nicolaÿ (renaud.nicolay@espci.psl.eu)	
Instructor(s)		Stefano Aime; Costantino Creton; Emmanuel Lacôte; Renaud Nicolaÿ; Christophe Thomas; Nathan Van Zee	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Molecular design and synthetic tools (P); Smart Materials (P); Environment (S); Nanotechnologies (S)	
		Total teaching hours: 48 h - Lectures : 43 h - Tutorials : 5 h	**Grading:** - written exam: 66 % - report: 17 % - oral exam / presentation: 17 %

Course description and content

The goal of the course is to provide students with a solid and versatile toolbox to design and prepare functional polymers, including self-healing. Special emphasis will be placed on sustainability, recyclability and upcycling issues. To this end, various polymerization techniques (controlled radical polymerization, photopolymerization, metal-catalyzed polymerization, supramolecular polymerization), processes (emulsion polymerization, reactive processing) and characterization techniques (rheology, light, X-ray and neutron scattering, thermomechanical characterization, microscopy) will be presented and discussed in detail. The acquired knowledge will allow to correlate the macroscopic properties of polymeric materials with their structure.

Learning goals

The course will provide all students with a strong background in polymer synthesis, characterization, and properties. Students will be able to:
- choose the monomer(s) and polymerization methods to design (co)polymers with tunable molar masses, topology, composition and functionality;
- Correlate structure, properties and processability of polymeric materials;
- Select appropriate characterization techniques to investigate specific properties of polymeric materials;
- Design and characterize self-healing and recyclable polymers.

Prerequisites

M1 level in polymer chemistry, basics in organic and organometallic chemistry, and physicochemical and mechanical properties of polymers.

MHMCHIM304

<table>
<tr><td rowspan="2">M2</td><td rowspan="2">S1</td><td colspan="2">Valorization of bioresources</td></tr>
<tr><td colspan="2">Keywords: biomass, biofuels, lignocellulose pre-treatment, biosourced platform molecules, other molecules of biosourced interest, biomater</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Frédéric de Montigny (frederic.de-montigny@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Frederic de Montigny; Christophe Thomas; Regis Gauvin; Michel Minier; Hubert Chapuis; Isabelle Ziegler-Devin; Vincent Semetey</td></tr>
<tr><td colspan="2">Language of instruction</td><td colspan="2">French</td></tr>
<tr><td colspan="2">Specialties
(P = primary ;
S = secondary)</td><td colspan="2">Molecular design and synthetic tools (P); Environment (P); Renewable energies (S)</td></tr>
<tr><td colspan="2"></td><td>Total teaching hours: 48 h
- Lectures : 27 h
- Tutorials: 18 h</td><td>Grading:
- written exam: 50 %
- oral exam / presentation: 50 %</td></tr>
<tr><td colspan="4">Course description and content

- Presentation of the issues related to plant chemistry and concepts ranging from biomass to biomaterials and platform molecules...
- Presentation of the concepts of plant chemistry allowing to replace fossil carbon by plant carbon, either by a substitution strategy or by the development of new biosourced materials.
- The concepts covered will include : biomass, biofuels, lignocellulose pre-treatment, biosourced platform molecules, other molecules of biosourced interest, biomaterials.</td></tr>
<tr><td colspan="4">Learning goals

The student should be able to:
Presentation of tools for the design and the implementation of industrial processes that meet the challenges of sustainable development: use of renewable materials from biomass, improvement of eco-compatibility of processes, development of industrial synthesis strategies considering all sustainability criteria.</td></tr>
<tr><td colspan="4">Prerequisites</td></tr>
</table>

MHMCHIM305

M2	S1	Medicinal products from biotechnology	
		Keywords: biotechnology, biotherapy, gene therapy, oligonucleotides, recombinant proteins	
Coordinator		Pascal Bigey (pascal.bigey@parisdescartes.fr)	
Instructor(s)		Pascal Bigey; Céline Hoffman	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Molecular design and synthetic tools (P); Health (P)	
		Total teaching hours: 48 h - Lectures: 38 h - Personal work : 10 h	**Grading:** - written exam: 80 % - report / assignments: 20 %

Course description and content

- Recombinant DNA technology : molecular biology, sequencing techniques and applications, PCR techniques, genome editing
- Basic introduction to epigenetics
- Recombinant proteins drugs, particularly monoclonal antibodies
- Oligonucleotide as drugs: design and synthesis of oligonucleotide, base modifications, formulation of oligonucleotides

Definition and mechanism of antisense oligonucleotides, splicing modulators, aptamers, DNA baits, RNA interference and description of the existing drugs

- In vivo gene therapy using viral (AAV, HSV) and non viral vectors. Description of the challenges and the encountered problems.
- Ex vivo gene therapy using viral vectors : y retroviruses, lentiviruses Description of the existing gene therapy products and perspectives
- Cell therapy : cancer immunotherapy and CAR-T cells
- Vaccination : all types of vaccines with a particular emphasis on genetic vaccines (DNA and mRNA)

Learning goals

The student should be able to:
- understand how works any biotherapy drug.
- know the different classes of biotherapy drugs, how they are made, and their main field of use
- understand the main challenges in designing such drugs
- read and understand any scientific publication related to biotherapy

Prerequisites

Knowledge of cell biology, particularly transcription- - translation, and basic immunology

MHMCHIM330

<table>
<tr><td colspan="2">M2 S1</td><td colspan="2">Total synthesis of natural products and bioactive compounds</td></tr>
<tr><td colspan="2"></td><td colspan="2">Keywords: Strategies in multistep organic synthesis, Total synthesis of natural products, Synthetic approaches to bioactive molecules, Retrosynthetic analysis and route design, Role of heteroatoms in reactivity and functional group transformations, Stereoselective and asymmetric synthesis, Radical reactions and radical cyclization methodologies</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Benjamin Laroche (benjamin.laroche@espci.fr)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Kevin Cariou; Amandine Guérinot; Benjamin Laroche; Christophe Meyer; Phannarath Phansavath; Maxime Vitale</td></tr>
<tr><td colspan="2">Language of instruction</td><td colspan="2">English</td></tr>
<tr><td colspan="2">Specialties
(P = primary ;
S = secondary)</td><td colspan="2">Molecular design and synthetic tools (P)</td></tr>
<tr><td colspan="2"></td><td>Total teaching hours: 48 h
- Lectures : 27 h
- Tutorials: 18 h</td><td>Grading:
- written exam: 50 %
- oral exam / presentation: 50 %</td></tr>
<tr><td colspan="4">Course description and content

This course explores synthetic strategies used in the design and execution of complex organic syntheses, with a particular focus on natural products and bioactive molecules. Students will learn how multistep synthetic pathways are planned, emphasizing retrosynthetic analysis, functional group interconversions, and the strategic use of heteroatoms to control reactivity. Key stereochemical concepts will be illustrated through representative examples of stereoselective and asymmetric total synthesis of complex molecules. The course also introduces radical-based methodologies, including radical cyclization reactions that enable efficient construction of polycyclic molecular frameworks. By examining representative case studies, learners will gain insight into how synthetic design connects with drug discovery and the development of structurally intricate organic compounds.</td></tr>
<tr><td colspan="4">Learning goals
The course will provide the students with broad and advanced knowledge in organic synthesis. The students will be able to:
• Apply traditional and modern synthetic strategies to the construction of complex organic molecules.
• Use retrosynthetic analysis to design and assess synthetic routes.
• Evaluate stereochemical challenges and select appropriate strategies to address them.
• Integrate structural, mechanistic, and strategic reasoning when planning synthetic pathways.</td></tr>
<tr><td colspan="4">Prerequisites
M1 level in organic chemistry</td></tr>
</table>

MHMCHIM306

M2	S1	Materials for environment	
		Keywords: GHGs – Carbon capture and valorisation – Depollution – Heat transfer – Porous materials – Inorganic materials – molten salts.	
Coordinator		Georges Mouchaham (georges.mouchaham@ens.psl.eu)	
Instructor(s)		Georges Mouchaham; Christian Serre; Virginie Lair; Caroline Mellot-Draznieks	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Smart materials (P); Environment (P); Renewable energies (S)	
		Total teaching hours: 48 h - Lectures: 34 h - Tutorials: 8 h - Seminars: 6 h	**Grading:** - written exam: 60 % - report / assignments: 20 % - project (20%)

Course description and content

This module will focus on the features of materials (organic, inorganic, hybrid; porous or not) for their use and application (capture and/or conversion) in:

- CO_2 capture and valorisation: CO_2 cycle; effect of CO_2 and GES on climate change; the state-of-the-art and current challenges in the field, from capture (capture technologies: pros/cons), to catalytic transformation/valorisation (thermal-, photo-, electro- C plasma-assisted catalysis) into valuable molecules and energy vectors.
- Air and water depollution/remediation: overview on the main pollution sources from domestic and industrial uses; small gas and vapors and some other problematic molecules (e.g., NOx, VOCs, PFAS) separation and degradation with porous materials and related composites; water harvesting from air; new detection systems.
- Heat transfer: introduction to heat management and the impact of the porous solids in related applications such as heat reallocation for low energy cooling/heating systems.

Moreover, this course will also provide an overview on molten salts and their use for CO_2 capture and conversion. This part will encompass the fundamentals about molten salts, the approaches to CO_2 capture and recovery, and up to Industrial applications and prospects.

Learning goals

The student should be able to:

- establish a general overview on the state of the art and current challenges in the field of materials for the environment from depollution to heat-management; a must to have in view of understanding and developing more sustainable alternatives.
- acquire a comprehensive and fair vision of this domain of major importance related to the energy transition.
- make a tight link between the materials and their applications, throughout an integrative approach (i.e., from detection and capture to conversion and remediation).

Prerequisites

Basics in solid state chemistry (electronic structure, transition metal complexes, crystalline solids); knowledge on porous materials (gas/vapor sorption and interaction with porous media).

MHMCHIM307

M2	S1	Materials for energy devices	
		Keywords: Batteries – Hydrogen - Fuel Cells – composite materials – electro catalysis	
Coordinator		Vanessa Pimenta (vanessa.pereira-pimenta@espci.fr)	
Instructor(s)		Vanessa Pimenta; Sathiya Mariyappan; Jolanta Swiatowska; Domitille Giaume; Christian Serre; Loïc Assaud; Virginie Lair	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Smart materials (P); Renewable energies (P)	
		Total teaching hours: 48 h - Lectures: 33 h - Tutorials: 9 h - Seminars: 6 h	**Grading:** - written exam: 60 % - report / assignments: 20 % - oral exam / presentation: 20 %

Course description and content

This module will be focused on the characteristics of emerging materials (organic, inorganic, and hybrid), their application in energy systems, and the challenges related to interfacial phenomena and stability:

• Batteries: this section will cover the principles of lithium-ion batteries and the main drawbacks driving the development of beyond lithium-ion technologies: emerging materials for Na-ion, metal-air, Li-S, and all solid-state batteries (including design strategies for electrode and electrolyte materials, interfacial reactivity, and interphases).

• Hydrogen: this section will include de basic principles for hydrogen production, distribution, storage and valorization. The fundamentals of catalytic processes for hydrogen production (photo and electro catalysis) will be studied, including water splitting processes. The fuel cells and electrolysers of the future for energy production and storage will be presented, with a focus on improving performance, enhancing durability, and reducing costs.

The working principles and the design of new composite membranes for PEMFC and composites for ammonia fuel cells, focusing on the development of innovative materials and new technologies, will be introduced.

Learning goals

The student should be able to:

- establish a general overview of the state of the art and the current challenges in the field of emerging materials for energy storage and conversion systems
- acquire a comprehensive understanding of interfacial phenomena and the challenges in designing sustainable materials
- analyze electrochemical conversion mechanisms
- develop a broader vision of alternative energy systems
- propose a selection of materials for the design of new devices

Prerequisites

Basics of solid state chemistry (electronic and crystallographic structures); basics of materials chemistry; basics of electrochemistry.

MHMCHIM308

M2	S1	Materials for optics	
		Keywords: Inorganics and hybrids materials for optical applications such as photovoltaics, lighting, quantum information, imaging, sensors	
Coordinator		Thierry Pauporté (thierry.pauporte@chimieparistech.psl.eu)	
Instructor(s)		Philippe Goldner; Sandrine Ithurria; Thierry Pauporté; Thomas Pons; Antoine Tissot; Alexandre Tallaire	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Smart materials (P); Nanotechnologies (P); Environment (S); Renewable energies (S)	
		Total teaching hours: 48 h - Lectures: 43 h - Tutorials: 1 h - Practicals: 4 h	**Grading:** - written exam: 87.5 % - oral exam / presentation: 12.5 %

Course description and content

- Basics and mechanisms of luminescence- Applications and devices (9h) (Th. Pauporté, CNRS, Chimie Paristech)

- Photovoltaic materials and technologies (12h): Introduction to semiconductors and to semiconductor junctions; fabrication of photovoltaic devices and modules; silicon technologies, emerging technologies (Th. Pauporté, CNRS, Chimie Paristech)

- Engineering of colloidal optical inorganic nanomaterials (12h). Semiconductor and metal nanocrystals; synthesis; characterization; surface and interface, functionalization; applications in optoelectronics, biology and photocatalysis (T. Pons, INSERM, ESPCI; S. Ithurria, ESPCI)

- Materials for optical quantum technologies (9h): introduction to quantum technologies, material design and fabrication, rare earth doped crystals, color centres in diamond, applications to quantum memories and sensors. (Ph. Goldner, CNRS, Chimie Paristech; A. Tallaire, CNRS, Chimie Paris Tech)

- Switchable hybrid materials (6h): spin crossover, photomagnetism, porosity, chemosensing. (A. Tissot, CNRS)

Learning goals

The student should be able to:

- Acquire advanced notions of optical spectroscopy and light matter interactions
- Identify the relationship between materials composition, structure and optical properties for different applications
- Identify the preparation methods and characterization tools adapted to a specific optical materials
- Understand the functioning of photovoltaic solar cells and acquire the knowledge of the various technologies

Prerequisites

Basics of inorganic materials; structures and properties, basics of optical spectroscopies; notions about materials characterization (structural and electronic properties)

MHMCHIM309

M2	S1	Polymers and Soft Matter: Design and Applications	
		Keywords: soft matter, polymer, hydrogel, self-assembly, colloid, membrane, bio-based polymer, biomaterial, actuator, stimuli-responsive, adsorption, adhesion	
Coordinator		Yvette Tran (yvette.tran@espci.psl.eu)	
Instructor(s)		Yvette Tran; Anniina Salonen; Christophe Tribet; Min-Hui Li; Laurent Corté	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Chemistry and life science (P); Smart materials (P); Nanotechnologies (P); Environment (S); Health (S)	
		Total teaching hours: 48 h - Lectures: 36 h - Tutorials: 12 h	**Grading:** • **Terminal grading** - written exam: 60 % - oral exam / presentation: 40 %

Course description and content

The objective of this course is to give an overview of the engineering of polymers and soft matter and the applications for materials and for biology. The approaches are as close as possible to those currently developed in PSL research laboratories (ESPCI, ENS, Chimie ParisTech).

Polymer thermodynamics and physico-chemistry properties. Tune weak and reversible molecular interactions to change macroscopic properties. Sol-gel transition. Focus on stimuli-responsive hydrogels and surfaces.

Light-responsive assemblies. Control of complex and dynamic systems by light. Latest methods and design strategies for light-switchable surfactant and polymer-based systems. Illustrations of out-of-equilibrium dynamics: microflow, microswimmers.

Self-assembling on liquid crystal polymers. Thermotropic LC polymers and elastomers as soft actuators and sensors. Lyotropic LC polymers with amphiphilic block copolymers self-assembled in water, polymer micelles and vesicles.

Design of self-assemblies and interfaces using bio-sourced and bio-based building blocks and polymers. Recent innovations in the field of biomaterials and biotechnologies. Adsorption and adhesion properties. Biomedical applications.

Learning goals

The student should be able to:
- link molecular and macromolecular engineering and more general soft matter design
- relate macroscopic behavior to microscopic phenomena
- mobilize knowledge to solve a complex problem involving polymers and soft matter
- critically analyze scientific publications

Prerequisites

Basic knowledge of macromolecular chemistry and physical chemistry
Basic knowledge of thermodynamics: entropy, enthalpy, free energy, phase separation, molecular forces
Knowledge of biology is not required

MHMCHIM310

M2	S1	Biomaterials : from materials engineering to biomedical devices	
		Keywords: Biomaterials, Biopolymers, Biominerals, Biocompatibility, Hydrogels, Interfaces	
Coordinator		Sophie Griveau (sophie.griveau@chimieparistech.psl.eu)	
Instructor(s)		Christophe Tribet; Fan Sun; Anouk Galtayries; Thibaud Coradin; Christophe Thomas; Sophie Griveau	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Chemistry and life science (P); Smart materials (P); Health (S)	
		Total teaching hours: 48 h - Lectures: 38 h - Tutorials : 6 h	**Grading:** - written exam: 30 % - report: 20 % - oral exam / presentation: 20 % - intermediate written exam: 30 %

Course description and content

This teaching unit offers courses covering the different types of materials used in biomedical applications of biomaterials (metals, biominerals, biopolymers, hydrogels), on the material/living interface (biomolecule/surface interaction, functionalization strategies) and on more forward-looking aspects of biomaterials science (controlled-release systems, for example). The courses will present necessary theoretical backgrounds while illustrating the concepts with the cutting-edge advances in biomaterials research.

The teaching approach will be interdisciplinary, combining chemistry, mechanics and biology. Fundamental aspects and more applied aspects directly related to the major types of applications (cardiovascular, orthopedic, dental, etc.) will be covered simultaneously.
The course will be organized in two main parts:

- Most courses focus on the different types of biomaterials: polymeric (nano)materials, biominerals, hydrogels, and metallic materials and their applications for biomaterials;
- Another section focuses on the material/living interface, biomolecule/surface interactions, and functionalization strategies and their characterizations.

The courses will be completed by seminars, based on research work in companies, start-ups and/or academic laboratories.

Students will work on a bibliographical project on a research theme of their choice. The aim will be to deepen their knowledge and critical thinking in one or more of the areas of biomaterials, while using their scientific skills developed in this module from others for in-depth understanding of the implemented strategies and in the analysis of the results.

Learning goals

The student should be able to:

- Define (multi-parametric) specifications for the design of a medical device
- Have a deep knowledge of the scientific vocabulary in biomaterials-
- Choose a family of materials on the basis of chosen criteria, based on these specifications
- Select appropriate approaches to material surface functionalization based on specifications
- Propose physico-chemical characterization methods for biomaterials
- Analyze scientific literature on the chemical aspects of biomaterials

Prerequisites

Undergraduate study in chemistry of materials, molecular chemistry and physical chemistry

MHMCHIM311

M2	S1	Probing, controlling, elaborating surfaces at the nanometric scale	
		Keywords: Physicochemical properties of surfaces; surface energies; surface stress; Nanostructuring and self-organization; surface analysis techniques	
Coordinator		Anouk Galtayries (anouk.galtayries@chimieparistech.psl.eu)	
Instructor(s)		Anouk Galtayries; Frédéric Wiame	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Analytical and physical chemistry at all scales (P); Smart materials (P); Nanotechnologies (P); Renewable energies (S)	
		Total teaching hours : 48 h - Lectures : 32 h - Tutorials : 8 h - Practicals : 8 h	**Grading:** - written exam: 60 % - intermediate written exam: 40 %

Course description and content

The aims of this module are to provide a general understanding of the physicochemical properties of surfaces and the atomic mechanisms involved in surface reactivity.
Knowledge of the structural and electronic properties of a surface at the nanometric and atomic scales is essential for understanding the behaviour of materials and for anticipating and controlling their properties and changes. The development of materials with innovative properties requires the characterization and control of surfaces on a nanometric scale.
This module should enable students to acquire a complete interdisciplinary body of knowledge to understand the physical chemistry of the surfaces of different materials.
Application exercises will reinforce the understanding of the principles. Demonstrations on equipment in research laboratories will give concrete expression to research work on surfaces.
State-of-the-art experimental tools for characterizing surfaces by microscopy, spectroscopy and spectrometry (STM, AFM, LEED, XPS, ToF-SIMS, etc.) will be described, compared and presented.
Illustrations of their performance will be presented for various materials application fields (energy, catalysis, biomaterials, corrosion, microelectronics, aeronautics, etc.).

Course outline
1) Introduction to the physical chemistry of surfaces
2) Surface reactivity
3) Surface characterization techniques
4) Nanostructured surfaces

Learning goals

The student should be able to:
- Identify and explain the constraints and main technological challenges associated with surface characterization
- Determine the structure, characteristics and basic properties of a given surface
- Identify the appropriate surface analysis technique for obtaining specific information, based on its operating principle and main characteristics
- Discuss the influence of surface structure and composition on the mechanisms and kinetics of reactivity.

Prerequisites

M1 level in chemical physics

MHMCHIM312

<table>
<tr><td rowspan="2">M2</td><td rowspan="2">S1</td><td colspan="2">Statistical mechanics and simulations for biomolecular systems</td></tr>
<tr><td colspan="2">Keywords: molecular modeling; (bio)molecular function and reactivity; multiscale approaches; statistical mechanics; thermodynamics</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Guillaume Stirnemann (guillaume.stirnemann@ens.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Élise Duboué-Dijon; Fabio Sterpone; Davide Avagliano</td></tr>
<tr><td colspan="2">Language of instruction</td><td colspan="2">English</td></tr>
<tr><td colspan="2">Specialties (P = primary ; S = secondary)</td><td colspan="2">Chemistry and life science (P); Theoretical chemistry and modelling (P); Analytical and physical chemistry at all scales (S); Digital Chemistry (S)</td></tr>
<tr><td colspan="2"></td><td>Total teaching hours: 48 h
- Lecture: 28 h
- Tutorials: 6 h
- Practicals:14 h</td><td>Grading:
- written exam: 50%
- intermediate written exam: 20 %
- report / assignments: 30 %</td></tr>
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Course description and content

Building upon core concepts of classical mechanics, statistical thermodynamics, and quantum chemistry, this class provides a large overview of the modern molecular simulation techniques that can be used to study chemical, biochemical and biophysical processes

- Classical mechanics, equations of motion, propagators
- Simulation ensembles and thermodynamic conditions (thermostat, barostat)
- Enhanced sampling techniques (Umbrella Sampling, Metadynamics, Replica Exchange, Steered MD, etc.)
- Mixed quantum/classical approaches: concept, applications
- Beyond the molecular scale: coarse grained techniques, mesoscale techniques (eg Brownian dynamics, Dissipative Particle Dynamics, Lattice Boltzmann MD), principle of multi-scaling.

The core concepts of the class will be demonstrated through various examples and applications, including enzymatic reactivity, conformational sampling, and protein diffusion in crowded environments. Students will gain practical experience through hands-on sessions, where they will learn to use popular molecular dynamics (MD) engines and analyze simulation trajectories effectively.

Learning goals

The student should be able to:

- Master core notions of statistical mechanics applied to molecular dynamics simulations
- Understand the available simulation toolbox to study biomolecular phenomena
- Perform and to analyze molecular dynamics simulations

Prerequisites

Notions of thermodynamics (energy, entropy, free-energy, first and second principles)
Newtonian mechanics
Notions of statistical mechanics (thermodynamic ensemble, ensemble average, Boltzmann statistics, phase space)
Some literature can be suggested ahead of the class to catch up on some of these concepts, if necessary.

MHMCHIM313

M2	S1	Data Science and AI for Chemistry	
		Keywords: artificial intelligence, machine learning, data science, databases, chemical data, deep learning	
Coordinator		François-Xavier Coudert (fx.coudert@chimieparistech.psl.eu)	
Instructor(s)		François-Xavier Coudert; Thijs Stuyver; Guillaume Stirnemann; Damien Laage; Carlo Adamo	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Theoretical chemistry and modelling (P); Digital Chemistry (P)	
		Total teaching hours: 48 h - Lectures : 36 h - Practicals : 12 h	**Grading:** - written exam: 50 % - report: 50 %

Course description and content

Fundamentals of machine learning:

- Fundamentals of statistical learning: machine learning, supervised and unsupervised learning, classification and regression algorithms, optimization
- Evaluating machine learning models: training/testing/validation, complexity, bias and variance
- Representation of chemical structures (2D and 3D): cheminformatics, molecular descriptors
- Deep learning and neural networks
- Generative models and their application in chemistry
- Databases in chemistry: chemical formats, metadata, storage and curation, API, databases, open science

Applications:

- Structure/property, structure/activity relationships, QSAR/QSPR methods
- Machine learning for theoretical chemistry: functionals, reactive force fields, exploration and collective variables, etc.
- Large-scale screening for pharma applications, docking and advanced methods
- The modern cheminformatics toolbox

Group projects (12 h):

Students will develop their ability to perform statistical analysis of chemical datasets through a modern Python-based toolchain, train their own models, test their accuracy, and validate the choice of hyperparameters. Among topics that can be chosen, we provide a diversity of examples, including: prediction of molecular properties, classification of chemical compounds based on physical properties, clustering of molecules for similarity, prediction of spectroscopic data, prediction of solid-state properties, etc.

Learning goals

The student should be able to:

- Understand the nature of data being produced in chemical research, its representation, and know common databases in chemical sciences
- Identify key types of machine learning tasks and the methods suited for each task
- Train ML models, choose hyperparameters and understand the bias–variance tradeoff
- Understand the fundamental workings of neural networks and generative models, their use in chemical applications and their current limitations

Prerequisites

BSc-level mathematics and statistics (probability distribution, optimization, Bayes theorem), MSc-level physical chemistry and theoretical chemistry (molecular dynamics, force fields, Density Functional Theory)

MHMCHIM314

M2	S1	Theory of Chemical Reactivity	
		Keywords: DFT, ab initio electronic structure methods, reaction rate theory, chemical dynamics, machine learning, data science, reaction optimization	
Coordinator		Thijs Stuyver (thijs.stuyver@chimieparistech.psl.eu)	
Instructor(s)		Thijs Stuyver; Fréderic Labat; Ilaria Ciofini; Damien Laage	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Theoretical chemistry and modelling (P); Digital Chemistry (S), Nanotechnologies (S)	
		Total teaching hours: 48 h - Lectures : 32 h - Practicals/projects : 16 h	**Grading:** - written exam: 50 % - report: 50 %

Course description and content

Part 1: Ab-initio electronic structure methods and multilayer approaches (24 h)

Electronic structure methods enable the explicit simulation of chemical processes and reactions at the molecular level, facilitating the characterization of their mechanisms and the theoretical rationalization of their efficiencies. In this part, state-of-the-art *ab initio* simulation techniques will be illustrated, focusing on Density Functional Theory (DFT) and introducing post-Hartree-Fock methods. Next, the application of these methods to investigate (photo)catalytic processes will be discussed. Subsequently, techniques to model environmental effects, including explicit and implicit solvation approaches will be introduced. Advanced multilayer techniques, combining quantum mechanical and classical frameworks, offering tools to simulate complex systems like solvated molecules, interfaces, and catalytic environments, will be presented.

Part 2: Machine learning for mechanistic rationalization and optimization of reaction conditions (12h)

In recent years, purely *data-driven* methods have emerged as complementary tool to study chemical reactivity. On the one hand, machine learning techniques can provide (indirect) insights into reaction mechanisms, and on the other hand, they provide powerful frameworks to rationally optimize reaction conditions. In this part, the main concepts of machine learning and cheminformatics will be presented concisely, after which a range of applications to chemical reactivity will be discussed critically. At the end of this part, experiment planning (for reaction optimization) through Bayesian Optimization will be introduced.

Part 3: Reaction Rate Theory and Chemical Dynamics (12h)

Understanding chemical reactions at a fundamental level requires bridging electronic structure and statistical mechanics to describe reaction dynamics. This part of the course starts with transition-state theory and progresses to modern approaches like reactive flux methods and time-dependent friction. Nuclear quantum effects on reaction rates will be addressed using ring-polymer molecular dynamics, while non-adiabatic dynamics will be discussed with techniques such as Ehrenfest and surface hopping dynamics to go beyond the Born-Oppenheimer approximation. Altogether, these advanced methods offer a comprehensive view of reaction dynamics.

Learning goals

The student should be able to:

- Identify, explain and apply appropriate theoretical approaches based on electronic structure methods that can be used and combined to untangle complex reaction mechanisms
- Identify, explain and apply theoretical approaches to model large systems and complex environments
- Identify and critically discuss opportunities for machine learning in chemical reactivity studies
- Apply standard machine learning algorithms to chemical reactivity datasets and interpret the results
- Understand and apply experiment planning techniques based on Bayesian Optimization
- Derive chemical rate constants from molecular simulations and determine molecular factors controlling the kinetics of a reaction
- Apply molecular simulation techniques to chemical systems with nuclear quantum effects or with non-adiabatic transitions

MHMCHIM314

Prerequisites

BSc-level mathematics and statistics (probability distribution, optimization, Bayes theorem), MSc-level physical chemistry and theoretical chemistry (statistical mechanics, molecular dynamics, quantum mechanics)

MHMCHIM315

M2	S1	Materials Modelling	
		Keywords: DFT, TDDFT, MD, AIMD, CSP, Response Properties	
Coordinator		F. Labat (frederic.labat@chimieparistech.psl.eu)	
Instructor(s)		C. Adamo; D. Avagliano; F.-X. Coudert; F. Labat; R. Vuilleumier	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Theoretical chemistry and modelling (P); Smart Materials (P)	
		Total teaching hours: 48 h - Lectures : 32 h - Tutorials : 16 h	**Grading:** - final written exam: 50 % - intermediate written exam: 50 %

Course description and content

This module introduces the main techniques and approaches for the modelling of the structural, mechanical, electronic, optical, and response properties of materials. It is organized into four main parts, each presented with illustrating examples, mainly chosen in the fields of photonic, biomimetic and energy materials.
The main topics covered are:

- molecular dynamics and ab initio molecular dynamics
- electronic structure of solids, surfaces, interfaces, lattice dynamics and crystal structure prediction
- structural and mechanical properties, framework materials and porous materials
- optical and response properties

Learning goals

The student should be able to:

- Know the theoretical approaches that can be used and combined to model different classes of materials
- Know the theoretical approaches that can be used to compute the structural, mechanical, electronic, optical, and response properties of materials, with different time and/or length scales
- Understand the structure/property relationship of selected classes of materials

Prerequisites

- Prior knowledge of classical and quantum mechanical approaches for the modelling of molecules and solids (M1)
- M1 level of statistical physics and molecular simulation fundamentals
- Prior knowledge in crystallography (L3)
- Students are expected to be familiar with linear algebra, matrices and matrix operations, operators, Dirac notation, and the concept of generalized inner products (L3)

MHMCHIM316

M2	S1	Omics: collective characterization and quantification of biological molecules	
		Keywords: Metabolomics, Interactomics, Genomics, Proteomics, Volatomics	
Coordinator		Yann Verdier (Yann.Verdier@espci.fr)	
Instructor(s)		Audrey Combes; Mathilde Lepoitevin; Anne Varenne; Jérôme Vial; Yann Verdier	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Analytical and physical chemistry at all scales (P); Chemistry and life science (P); Health (S)	
		Total teaching hours: 48 h - Lectures: 30 h - Tutorials: 12 h - Practicals : 8 h - Seminars : 8 h	**Grading:** - written exam: 80 % - report: 20 %

Course description and content

1- Introduction: the challenges of the different omics approaches

2- Common aspects of omics approaches :
- Instrumentation: chromatographic and electrokinetic separative methods, coupling with mass spectrometry (focus on the different analysers depending on the analytical problem)
- Data acquisition and processing; identification of markers (T1-2-3)

3-Specific aspects :
- Genomics/Transcriptomics (P1-2)
- Proteomics (T1-2)
- Metabolomics (T3)
- Interactomics
- Volatolomics: gas sample; GCxGC-MS

Tutorials
T1 :Genomic data analysis
T2 :Proteomic data analysis
T3 :Metabolomic data analysis

Practicals
P1: Construction of nanopore system for DNA analysis
P2: DNA Sequencing

Cross-disciplinary seminars
Glycomics and other omics; Multi-omics approach for the characterization of biological samples

Learning goals

The student should be able:
- to know how to operate within an experimental park and choose the right analytical strategy for the omics problem under consideration;
- to know how to link the different approaches and complementarities of omics;
- to understand and use data processing tools.

MHMCHIM316

Prerequisites

- Molecular structure and functions of the main biological molecules (DNA, RNA, proteins, lipids, carbohydrates, metabolites) UE Biology for chemistry
- Principle of liquid and gas chromatography

MHMCHIM317

M2	S1	**New molecular and particle-based systems for diagnostics and therapeutics: from conception to applications**	
		Keywords: Specific molecular recognition elements; Nanomaterials; Physicochemical characterizations; bioassays formats; nanotoxicity	
Coordinator		Laura Trapiella (laura.trapiella@chimieparistech.psl.eu)	
Instructor(s)		Fanny d'Orlyé; Audrey Combes; Anne Varenne; Bich-Thuy Doan	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Analytical and physical chemistry at all scales (P); Smart Materials (S); Nanotechnologies (P); Health (S)	
		Total teaching hours: 48 h - Lectures : 28 h - Tutorials: 12 h - Practicals : 8 h	**Grading:** • **Terminal grading** *(obligatoire)* - written exam: 50 % • **Additional intermediate gradings** - Continuous assessment (written/oral): 15 % - report / assignments: 10 % - oral exam / presentation: 25 %

Course description and content

This UE is devoted to give a general overview of the strategies for diagnostics and therapeutics based on the use of new affinity ligands and nanostructured systems. The students will discover the main nanostructures used in the field as well as the ways for their synthesis and characterization. In the view to design more specific systems a panel of new molecular recognition elements and the principal strategies to couple to the nanostructured systems as well as the trending strategies for the evaluation of their specific and non-specific interaction for targeting will be afforded. Finally in vitro bioassays formats for diagnostics and in vivo theragnostic approaches will be presented. For in vivo applications the assessment of the toxicity is a must so the guideline to perform such evaluation will be revised.

The content of the UE will be presented to the students in different pedagogic formats:

- Interactive lectures to afford the main theoretical concepts
- Case of study or applicable problems will be treated to facilitate the comprehension and illustrate the theoretical concepts
- Practical sessions in the laboratory to make hands in the conception and application of those novel systems
- Seminars on innovative materials dedicated to a specific application based on the current research developed at PSL on the topic

The final goal of this UE is to provide to the students with the competences to design and understand the development of novel tools based on new molecular and particle-based systems for diagnostics and therapy aligning material-property-application chain

Learning goals

The student should be able to:

- Identify the main current strategies for diagnostic C Therapy based on the use of affinity ligand and nanomaterials
- Know the principal ways of synthesis and biofunctionalization of nanomaterials
- Apply the best physicochemical characterizations to elucidate the structure, properties, interactions of this new tools
- Select the appropriate toxicity test to evaluate the adequation of the proposed system for in vivo applications
-Design of new diagnostic C therapeutic tools based on molecular and particle-based systems

MHMCHIM317

Prerequisites

- Knowledge in the following fields are required: Analytical Chemistry, Biochemistry, Material Sciences (see related courses from M1)

MHMCHIM318

M2	S2	Key issues in modern separation sciences and technologies	
		Keywords: Analytical separations, coupling, sample processing, lab-on-a chip devices	
Coordinator		Fanny d'Orlyé (fanny.dorlye@chimieparistech.psl.eu) Jerome Vial (jerome.vial@espci.psl.eu)	
Instructor(s)		Anne Varenne; Fanny d'Orlyé; Jerome Vial; Michel Sablier; José Dugay; Audrey Combes	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Analytical and physical chemistry at all scales (P); Environment (S); Health (S); Renewable energies (S)	
		Total teaching hours: 48 h - Lectures: 24 h - Tutorials: 12 h - Practicals: 12 h	**Grading:** - final exam: 30 % - intermediate exam: 30 % - report / assignments: 20 % - oral exam / presentation: 20 %

Course description and content

Handling complex samples requires the implementation of hyphenated techniques. Among them the most used are the coupling of separation techniques with mass spectrometry. The different interfaces and their characteristics will be presented along with the specific capabilities of the various mass analyzers available for these coupling. An opening will be proposed towards other online or hyphenated detection techniques (based on spectrophotometry, electrochemistry or spectroscopy), and discussed in terms of analytical performance and complementarity towards dual detection modes.

However, the one-dimension separation before detection is not always sufficient. To address this issue, 2D chromatographic and electrophoretic separations could be considered. After general consideration on fundamental aspects of 2D separations covering both orthogonality considerations and the mode (heart cutting and comprehensive), a focus will be put on the interface between both dimensions: the modulator. The different technologies that could be implemented will be discussed.

The miniaturization of analytical systems and their integration on microfluidic chips will also be considered to help overcoming technological bottlenecks at the bench scale towards fully integrated and automatized analytical strategies. Practical examples of applications in the fields of energy, environmental monitoring, medical diagnosis and circular economy will illustrate the relevance of such approaches.

To widen the scope of analysis to sample matrices (like gases or solids) not directly compatibles with analytical separation conditions, different sample processing methodologies could also be considered. Coupling techniques like condensation, thermos-desorption or pyrolysis together with preconcentration strategies are among solutions that will be discussed.

The methodological and technological developments presented in this course will be put into context, offering analytical solutions to tackle societal issues in health, environment, energy and circular economy.

This teaching module comprises 12 hours of practical work in chromatography and mass spectrometry applied to the fields of the environment, health, and food safety.

Learning goals

The student should be able to conceive, develop or select the most adapted strategy to current analytical challenges they could face, in terms of analytical design, technological set up and methodological performance.

MHMCHIM318

Prerequisites

Students should have basic knowledge in the mechanisms involved in chromatographic and electrophoretic separations and must be familiar with concepts like retention factors, selectivity, efficiency, resolution. The thermodynamic and kinetic aspects of interfacial systems must also be acquired.

MHMCHIM319

M2	S1	**Electrochemistry : Fundamentals and applications in Sustainability, Diagnosis and Global change**	
		Keywords: electrochemical methods, energy, environment, characterization, analysis	
Coordinator		Sophie Griveau (sophie.griveau@chimieparistech.psl.eu) Laurent Thouin (laurent.thouin@ens.psl.eu)	
Instructor(s)		Alexander Oleinick; Dimitri Mercier; Kevin Ogle; Armelle Ringuedé; Laurent Thouin; Sophie Griveau	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Analytical and physical chemistry at all scales (P); Chemistry and life science (S); Smart materials (S);	
		Total teaching hours: 48 h - Lectures:48 h - Tutorials: 4 h - Practicals: 4 h	**Grading:** - written exam: 75 % - report / presentation: 12.5 % - intermediate written exam: 12.5 %

Course description and content

The course aims to cover the fundamental aspects of electrochemistry while addressing new innovative strategies for coupling with other modern physicochemical methods of interest. By extending the value of electrochemistry beyond a general introduction to electrochemical methods, this course highlights its role in solving societal challenges and its contribution to sustainable and efficient practices, in fields as diverse as health, materials and energy.
The course content is organized into two main parts.

- The first part is dedicated to the fundamentals in electrochemistry and the modeling of electrochemical reactions. The aim is to provide students with a complete understanding of electrochemical processes at the interface: Electrochemical thermodynamics, charge transfer, mass transport, coupled chemical reactions… Theory via numerical simulations is emphasized to stress the foundations but also to highlight key phenomena.
- The second part addresses the development of electroanalytical methods in relation with advances in complementary in-situ microscopies, spectroscopies, spectrometric techniques etc…. Some combinations are discussed to provide information about structure changes, reaction pathways, and local events taking place during chemical or biological reactions. Miniaturization and implementation of electrochemical measurements in confined space or microfluidic environments are also addressed.

Complementary to the courses, applications in areas of major societal challenges such as environmental monitoring, diagnostics for materials, health and medicine, energy storage…, will be covered by conferences from researchers and/or from companies in the fields.

Students will be asked for bibliographic projects to illustrate how electrochemistry can contribute to elucidating complex issues in physicochemical processes and how modern electrochemistry can promote the development of technologies and processes in relation to sustainable practices.

Learning goals

The student should be able to:
- Understand key electrochemical processes and electrochemical methods
- Analyze and interpret experimental results with numerical modeling
- Apply advanced electrochemical methods to elucidate physicochemical reactions at complex interfaces

MHMCHIM319

Prerequisitess

Redox reactions, Electrochemical equilibria, Basics in electrode processes and mass transport, steady-state voltammetry

MHMCHIM320

M2	S1	Magnetic Resonance	
		Keywords: Nuclear Magnetic Resonance; Electron Paramagnetic Resonance; Two-Dimensional Spectroscopy; Biological Magnetic Resonance; Magnetic Resonance of Materials; Hyperpolarization	
Coordinator		Fabien Ferrage (Fabien.Ferrage@ens.psl.eu)	
Instructor(s)		Kong Ooi Tan; Fabien Ferrage; Laurent Binet; Jean-Baptiste d'Espinose	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Analytical and physical chemistry at all scales (P); Chemistry and life science (S) OR Smart materials (S) based on project choice	
		Total teaching hours: 48 h - Lectures: 35 h - Tutorials: 9 h - Presentations: 4 h	**Grading:** - written exam: 50% - intermediate written exam: 20% - oral exam / presentation: 30%

Course description and content

This course provides an in-depth exploration of magnetic resonance spectroscopies. These methodologies are fundamental tools for elucidating molecular structure, dynamics, and interactions across a wide range of chemical, biological, and material systems. By bridging theoretical concepts with experimental applications, this course equips participants with the expertise to apply magnetic resonance techniques to contemporary challenges in science and engineering.

In this class, you will gain a broad culture of the fields of magnetic resonance. You will be able to comprehend MR and uncover the wealth of information it can provide about biomolecular systems and materials. The class will explore the following topics:

1. Introduction to magnetic resonance, Hamiltonian operators, energy levels, vector model of NMR and application to diffusion measurements.
2. Nuclear spin relaxation: a simple model of transverse relaxation, longitudinal relaxation, models of molecular motions, nuclear Overhauser effect, Overhauser dynamic nuclear polarization.
3. Continuous-wave EPR: examples of applications, practical aspects of EPR, spin hamiltonian, g-factor, hyperfine interaction, liquid state EPR (radicals) and solid-state EPR of S=½ systems.
4. Quantum description of solution state NMR: product operator formalism, polarization transfer, 2D NMR: theory and use of: HSQC, COSY, NOESY, HMBC, TOCSY, introduction to triple-resonance experiments
5. Solid-state NMR: anisotropic interactions, magic-angle spinning, cross polarization, recoupling and decoupling experiments, quadrupolar nuclei.
6. Pulsed EPR: Instrumentation, ENDOR and DEER
7. Hyperpolarization methods: Dynamic nuclear polarization mechanism and instrumentation

Each section will feature examples in the fields of materials chemistry, chemistry and life sciences, heritage science.

The class includes a project to explore in detail a particular field: detecting protein-ligand binding with NMR, NMR of large biomolecules with transverse relaxation-optimized spectroscopy, exploring numerical simulation of mechanisms that drive dynamic nuclear polarization, solid-state NMR spectroscopy, EPR of transition metal complexes.

Learning goals

After following this class, students should be able to:

- understand how solution and solid-state NMR and EPR experiments work from quantum mechanics principles
- choose NMR and EPR experiments to answer scientific questions in a breadth of fields from synthetic chemistry to material sciences and structural biology
- use numerical tools to understand and analyze experiments

MHMCHIM320

Prerequisites

Basic mathematics (linear algebra, calculus: differential equations/integrals, Fourier transform)
Quantum mechanics: Dirac notation and algebra in Hilbert spaces, Pauli matrices, angular momentum operators and their properties
Electronic structure of molecules and coordination complexes, ligand, and crystal field theories
Basic classical physics: angular momentum, magnetic/electric dipole, and dipole-dipole interactions

MHMCHIM321

M2	S1	Multimodal imagings with contrast agents for theranostics	
		Keywords: Bioimagings, chemical probes, diagnostics, theranostics	
Coordinator		Bich-Thuy Doan (bich-thuy.doan@chimieparistech.psl.eu)	
Instructor(s)		Guillaume Bort; Jérome Gateau; Nicolas Tsapis; Yves Frapart; Thomas Viel; Olivier Clément; Philippe Goldner; Min-Hui Li; Christian Serre; Pierre Mesdom	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Chemistry and life science (P); Smart materials (S); Health (P); Nanotechnologies (S)	
		Total teaching hours: 48 h - Lectures: 34 h - Tutorials: 2 h - Practicals: 12 h	**Grading:** - written exam: 75 % - report: 25 %

Course description and content

The Module is an advanced course dedicated to engineers, chemists and biologists.
To answer the need for personalized and precision medicine and to investigate novel therapy against diseases, the course will provide extensive expertise in multimodal imagings with contrast agents, associated with molecular and nanoparticular science. Several multimodal imagings methods will be explored with various facets of molecules and nanoparticles from their design to their evaluation, dedicated to their applications in biology and medicine. This comprehensive perspective will equip students with the ability to handle methodology of bioimagings, and to conceptualize the design of molecules and nanoparticles tailored to specific biological applications for bioimaging and guided diagnosis and therapy in vivo.
The field of medical imaging has evolved into a distinct specialization, with advanced research in chemistry playing a pivotal role in this biomedical domain. The development of this discipline is intricately tied to the ongoing development of new imaging probes for both diagnosis or therapy, often associated with nanoparticles to create a form of therapy known as nanomedicine, that will be designated as theranostics when diagnostic information can be provided concurrently.
Several modern imaging modalities and methodology using these molecules and nanoparticles will be featured including optical, magnetic resonance, US, and positron emission tomography, US, thermal imaging, either in single or multimodal formats. Fluorescent, plasmonic, magnetic, organic and inorganic nanoparticles, included up to date activable theranostics will be presented together with their biomedical applications, spanning from cellular studies to in vivo preclinical and clinical settings.
The lessons will be structured into general courses, including practical exercises and case study sessions.
These sessions will focus on mastering the design and the evaluation of theranostics agents, and methodology of imagings. Furthermore, they will work on developing a complete project centered on diagnostic methodologies and therapy evaluation, with the imaging agents, aimed at addressing healthcare challenges through image-guided therapy. These projects may mirror real-world scenarios encountered in academic or industrial laboratory settings.
Lessons content:
- Understanding fluorescent, magnetic, radioactive to organic and inorganic nanoparticles, with the incorporation of multimodal imaging components, their design and imaging properties.
- Evaluating of the agents in using and developping imagings methods in vivo in preclinics to clinics for diagnosis and therapy.
- solving a chemical or biological, biomedical problematics using the bioimaging probes for image-guided therapy during case study sessions.

Learning goals

The student should be able to:
- know the biomedical and clinical imagings, associated with commercial imaging probes.
- know how to use them to provide a diagnosis in their in vitro and in vivo applications in the biomedical or medical field. It includes their operating principles, the biophysical or biochemical principles of their operation.
- propose innovative solutions designing chemical imaging probes, using physicochemical and bioimaging techniques to develop them and explain how functionalized probes can be developed.

Prerequisites

Spectroscopy UV vis, fluorescence, NMR spectroscopy, nanoparticles, polymer, inorganic and molecular chemistry, biomaterial sciences knowledges

MHMCHIM322

M2	S1	Inorganic chemical biology	
		Keywords: Inorganic Medicinal Chemistry, Inorganic Chemical Biology, Photodynamic Therapy, Bioorganometallic Chemistry, Metalloproteins, Metallomics, Dioxygen Activation.	
Coordinator		Gilles Gasser (gilles.gasser@chimieparistech.psl.eu)	
Instructor(s)		Gilles Gasser; Clotilde Policar	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Chemistry and life science (P); Molecular design and synthetic tools (P); Health (P); Environment (S)	
		Total teaching hours: 48 h - Lectures: 48 h	**Grading:** - written exam: 100 %

Course description and content

Firstly, we intend to illustrate that metal-containing species play a great role in biology. Indeed, nature uses metal ions to accomplish most of the essential biological functions. Due to their different kinetic, geometric and electronic properties, metal complexes can undergo reactions which are not possible with organic agents, providing nature with a wider chemical repertoire. We therefore intend to describe the variety of the role of endogenous metal ions, including metallo-biomolecules and metalloproteins and detail their mechanism at the molecular level, with a special focus on hydrolytic processes, electron exchange and dioxygen transport and activation. We will also show how chemists can get bioinspired by metallo-biomolecules to design molecular systems on interest (bio-inspired catalysts) on selected examples.
In addition, metal-containing species have great potential as therapeutic agents. With the exception of cisplatin and its derivatives, metal-containing drugs, particularly organometallics, have been, until very recently, largely neglected by both the pharmaceutical industry and academia. Over the last few years, however, things have changed, and significantly! Indeed, “inorganic drug candidates” are beginning to enter clinical trials, with more promising lead structures in the pipeline. We will point out the latest advances in the field of medicinal inorganic chemistry with an emphasis on the discovery of new inorganic compounds with proven anti-cancer activity, enzyme inhibition, or anti-malarial properties. Moreover, the specific mechanisms of action of the metal-based drugs will be presented in detail.

Learning goals

By the end of this UE, each student should be able to:
-outline and explain the specific use and reactivity of metal ions in a complex biological environment
-outline the mechanisms of metalloproteins and define the design of molecular systems mimicking their functions
-describe the mechanism of action of important metal-based drugs
-predict potential targets of a random metal-based drug candidate
-read and provide critical analysis of a scientific article.

Prerequisites

The students following this course are expected to have knowledge in organic, inorganic and general chemistry with insights in photochemistry. It is expected that they have some basic knowledge in biology and biochemistry, even if main reminders will be given.

MHMCHIM323

M2	S1	Dynamics of Biological Processes	
		Keywords: Stochastic processes; conformational change; dynamic evolution of a biomolecule	
Coordinator		Guillaume Stirnemann (guillaume.stirnemann@ens.psl.eu)	
Instructor(s)		Fabien Ferrage; Charlie Gosse; Zoher Gueroui; Antoine Taly; Philippe Nghe	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Analytical and physical chemistry at all scales (P); Chemistry and life science (P); Theoretical chemistry and modelling (S)	
		Total teaching hours: 48 h - Lectures: 33 h - Tutorials: 10 h - Practicals: 5 h	**Grading:** - written exam: 50% - intermediate written exam: 15% - oral exam / presentation: 35 %

Course description and content

Concepts and theories
Master equations for the study of dynamical processes
Kinetic models for enzymatic catalysis
Chemistry of systems: kinetics and stoichiometry
Phase separation in biomolecular systems
Intracellular phase transitions and biomolecular condensates Markov models and single-molecule kinetics

Experimental tools
Biomolecular dynamics from microseconds to seconds from chemical exchange NMR
Overview of other techniques // cryoEM, FRET, etc.
Microfluidics for controlled environments, analytics tools for dynamical networks
Experimental approaches to study phase separation
Single-molecule manipulation and single-molecule fluorescence

Simulation tools
Overview of molecular simulations and computation studies of reactivity and dynamics in biological systems

Learning goals

The student should be able to:

- Appreciate the importance of dynamical aspects and processes (e.g. conformational dynamics, transport) in explaining the function of biological macromolecules;
- Gain a comprehensive overview of the relevant timescales, and of the available experimental and simulation techniques to probe such processes;
- Understand how the synergy between experiments, simulations and theory can lead to a comprehensive molecular picture of the involved mechanisms;
- Apply these concepts to practical cases, including examples from the literature and projects that will be led by the students.

Prerequisites

Notions of thermodynamics (energy, entropy, free-energy, first and second principle)
Notions of statistical mechanics (thermodynamic ensemble, thermodynamic average, Boltzmann statistics) Notions of chemical kinetics (elementary reactions, kinetic models, 0th/1st/2nd order reactions)

MHMCHIM324

M2	S1	Chemical Biology	
		Keywords: inhibitors, drugs, fluorescent probes, nanoparticles, small molecule probes, organelle-specific targeting	
Coordinators		Raphaël Rodriquez (Raphael.Rodriguez@curie.fr) Sebastian Müller (Sebastian.Muller@curie.fr)	
Instructor(s)		Raphaël Rodriquez; Sebastian Müller; Alice Balfourier; Arnaud Gautier; Paola B. Arimondo	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Chemistry and life science (P); Health (P); Nanotechnologies (S)	
		Total teaching hours: 48 h - Lectures : 26 h - Tutorials : 22 h	**Grading:** - written exam: 50 % - report / assignments: 25 % - oral exam / presentation: 25 %

Part 1: Controlling cellular processes

Small molecules to manipulate cell processes

In the first part of the class, we will show how small molecules can be designed and used to target cellular processes. We will define distinct classes of compounds targeting (1) a biomolecule (protein, nucleic acid, lipid…) or a metal (2) an organelle (3) a process; or (4) a biochemical reaction. We will discuss the concept of addressing where and how a small molecule finds its way in the cell (hence finding where drugs go and engage with their targets). A broad overview of inhibitors will be presented targeting the metabolism, the epigenome, inducing DNA damage, blocking transcription/replication/splicing, protein synthesis and degradation, as well as trafficking, autophagy and cell death. The challenges of targeting mutated kinases in the context of cancer will be discussed with the examples of BRaf and KRas. We will show alternative strategies such as drugs targeting metals, proteolysis-targeting chimeras (PROTAC) and lipid degraders.

Molecule delivery: tools and challenges

This section will present how molecules can be delivered to targets at different scales (organs, cells, and organelles), introducing the main classes of cargoes that are used and developed today. The main challenges of selectivity, membrane crossing, and kinetics control will be presented, along with innovative approaches to overcome current issues. Finally, basic pharmacokinetics concepts will be introduced in the specific case of nano- and micro-cargoes.

Part 2: Probes (small molecule) and fluorescent reporters (genetically engineered proteins) to dissect and quantify cell processes

Epigenetics

The full-day course will be divided in two parts: During the first session, fundamental concepts in Chemical Epigenetics will be presented, with a special emphasis on chemical probes. In the second session, students will be divided in small groups to analyse scientific articles focusing work the chemical targeting and probing of the Epigenetics and their application in human diseases. An evaluation will be conducted at the end of the day.

Chemogenetic probes to understand biological processes

In this part, we will present how combining molecular engineering and protein engineering can enable the development of powerful tools for elucidating and controlling cellular functions with high spatial and temporal resolution. In particular, this part will focus on various engineering approaches for creating novel proteins able to use non-natural ligands or substrates. Key developments in Chemical Biology, such as selective protein labeling, genetic code expansion or analog-sensitive chemical genetics, will be presented.

The class will be based on lectures, case studies and mini-projects.

MHMCHIM324

Learning goals

The student should be able to:
-to master the fundamental of Chemistry applied to Life Sciences and the concepts of Chemical Biology
-to be able to base the design of small molecules as drugs and chemical probes based on the knowledge of cellular processes
-to understand how molecular probes can be used to investigate cellular processes
-to design new drugs based on their cellular targets
-to understand and present research articles

Prerequisites

It is recommended to have followed or to follow in parallel the M1 class "Chemistry and Life Sciences"
Cellular biology: types of cells, organelles, dynamics of the cell, cell death
Molecular biology: biomolecules (proteins, nucleic acids, lipids, carbohydrates), biosynthesis of proteins and nucleic acids
Chemistry: understanding basic chemical reactivity and simple synthetic routes

MHMCHIM325

M2	S1	Fluorescent probes for advanced cell imaging	
		Keywords: Organic fluorophores, fluorescent proteins, fluorescent nanoparticles, molecular design, photophysics, fluorescence microscopy, super-resolution microscopy	
Coordinator		Agathe Espagne (agathe.espagne@ens.psl.eu)	
Instructor(s)		Jérôme Delacotte; Blaise Dumat; Agathe Espagne; Thomas Pons; Kévin Renault	
Language of instruction		English	
Specialties (P = primary ; S = secondary)		Chemistry and life science (P); Analytical and physical chemistry at all scales (S), Molecular design and synthetic tools (S); Smart materials (S); Health (P); Nanotechnologies (S)	
		Total teaching hours: 48 h - Lectures : 24 h - Tutorials : 4 h - Practicals : 12 h - Visits : 8 h	**Grading:** - written exam: 30 % - oral exam / presentation: 30 % - intermediate written exam: 20 % - report / assignments: 20 %

Course description and content

Fluorescence microscopy is used in all biology laboratories to unravel the inner workings of cells. It encompasses a variety of techniques, the most advanced of which can now image intracellular components with nanometric resolution. Chemists play a central role in these developments, providing fluorescent probes with ever-improving photophysics for labeling biological samples. This teaching unit covers the molecular design, photophysical properties and applications of the different categories of probes used in biological imaging: organic fluorophores, fluorescent proteins and fluorescent nanoparticles. It combines theoretical courses, practical workshops and laboratory visits to provide students with a comprehensive and up-to-date training in fluorescent probes and fluorescence imaging.

Theoretical course program :

1 - Fundamentals of molecular photophysics
2 - Organic fluorophores
- 2.1 - Introduction to organic fluorophores
- 2.2 - Fluorescent analogues of amino-acids and nucleobases
- 2.3 - Fluorescent indicators of biological analytes
- 2.4 - Probes for nucleic acids, proteins, lipids
- 2.5 - Probes for advanced imaging techniques
- 2.6 - Hybrid chemogenetic

probes 3 - Fluorescent proteins
- 3.1 - Introduction to fluorescent proteins
- 3.2 - Fluorescent protein

photochemistry 4 - Quantum dots
- 4.1 - Synthesis and photophysical properties
- 4.2 - Functionalization and applications

Practical workshops and laboratory visits :

1 - Synthesis and characterization of colloidal quantum dots
2 - How to use a wide-field fluorescence microscope
3 - Monitoring of an enzymatic reaction at the single-molecule level
4 - Visit to the CurieCoreTech cell and tissue imaging platform
5 - Visit to a super-resolution microscopy laboratory

MHMCHIM325

Learning goals

By the end of the course, students will:

- know the different types of fluorescent probes available, their properties and applications;
- understand the fundamental phenomena governing the fluorescence of probes;
- master the design, optimization and bioconjugation of the different types of probes;
- know the principle of diffraction-limited and super-resolved fluorescence imaging techniques;
- be able to read and critically analyze a scientific article in the field of fluorescent probes and imaging;
- know the different parts of a microscope and their roles and master the use of a wide-field fluorescence microscope;
- be able to choose or design a probe for a given application and use it in a controlled manner;
- have acquired basic image analysis skills.

Prerequisitess

Basics of organic chemistry (aromaticity, conjugation, delocalization, mesomeric effects, Friedel-Craft reaction, heterocyclic chemistry) and physical chemistry (optical spectroscopy, reactivity, kinetics).
Basics of molecular and cell biology (it is advisable to have taken the course offered in M1).

MHMCHIM326/327

M2	S1	Scientific communication	
		Keywords: scientific writing, articles, slides, and presentations	
Coordinator		Fabien Ferrage (Fabien.Ferrage@ens.psl.eu)	
Instructor(s)		Fabien Ferrage; Alice Balfourier; Mathilde Lepoitevin	
Language of instruction		English	
		Total teaching hours: 30 h - Lectures : 6 h - Tutorials : 24 h	**Grading:** • **Article evaluation: eq. 2 ECTS** • **Presentation: eq. 2 ECTS** • **Video presentation: eq. 2 ECTS**

Course description and content

Communicating the results of your work is essential. Why is a project important? What are the main results? What prospects do these results open up? Taking as an example two central communication activities for researchers: writing articles and designing oral presentations, we address a number of general communication principles. We study the structure of an article at several levels: its general organization, how to write an abstract, how to design the introduction, how to structure a paragraph. We also pay close attention to vocabulary and mistakes to avoid in English for non-English speakers. For oral presentations, we work on slide design, rhythm and expression.

All activities take place in groups of two or three students. In written form, we carry out a few exercises such as writing a summary of an article, then the heart of the work takes place around writing a short article based on unpublished results (usually an internship report). The groups work collectively, correcting each other, to produce a short but high-quality text in just a few sessions.

Oral communication involves a “pecha kucha” exercise, which forces participants to simplify their slides and organize their speech. Training by a drama teacher enables everyone to become an actor in their presentation. A 10-minute presentation is then prepared and rehearsed several times before a final session in front of a small audience of researchers and students.

In an optional project (2 ECTS), the students will adapt their presentations in video format. The best presentations will be made available online.

Learning goals

By the end of the course, students will:

- Know the general principles of scientific writing
- Have experience in writing collectively and iteratively
- Have learnt how to give and receive constructive feedback
- Know how to design an efficient slide
- Master the assertion-evidence style of presentation
- Have improved their presenting skills

Prerequisitess

Having written one report and given at least one presentation with slides before the class is helpful
Being able to use one writing software (word, LaTeX…) and one presentation software (powerpoint, keynote, beamer) is useful

MHMCHIM328

M2	S1	Research Design	
		Keywords: project design; scientific proposal; formal report, planning and drafting.	
Coordinator		Georges Mouchaham (georges.mouchaham@ens.psl.eu)	
Instructor(s)		Georges Mouchaham; Fabien Ferrage; Vanessa Pimenta; Kong Ooi Tan; Nicolas Delsuc	
Language of instruction		English	
		Total teaching hours: 18-24 h - Lectures: 6 h - Tutorials: 12-18 h	**Grading:** - **Terminal grading** - report: 50 % - oral exam / presentation: 50 %

Course description and content

This module aims to guide the students in developing a compelling research project starting from identifying a scientific hypothesis up to crafting a well-structured project proposal.
More specifically, the work consists of:
(i) defining a scientific question or problem in the field of chemistry and related fields at the interface with energy, environment, life sciences, analytical and computational methods;
(ii) writing a state-of-the-art review of the field; and
(iii) proposing a methodology to address and solve the identified question or problem.

Students will work in groups of 3 to 4 under the supervision of a tutor. Sessions will alternate between general guidance on grant applications and scientific writing, together with oral presentations on the progress of group projects. Students are expected to demonstrate a strong commitment and devote personal efforts to ensure the quality of their work.
At the end of the module, each group will provide:
(i) a written proposal that includes the research question and objectives, a state-of-the-art review, and the proposed methodology: and
(ii) a project presentation aiming to explain and defend the project to a general public audience.

Learning goals

The student will learn how to:

- identify a research problem, formulate the hypothesis and suggest possible solution pathways;
- craft a well-structured project proposal in a critical manner; and
- clearly and simply present the overall concept of the project proposal.

Prerequisites

Motivation to acquire basic and advanced skills in designing and defending projects/proposals.