Integrative Chemistry and Innovation
Master degree

Course syllabus - M1 level

2021-2022

SEMESTER 1	ECTS
Basic science courses	
Introductory Mathematics and Physics	3
Molecular Design and Synthetic Tools - Basic	3
Analytical and Physical Chemistry - Basics	3
Theoretical Chemistry and Modelling Basics	3
Smart Materials Chemistry - Basics	3
Advanced science courses	
Select 3 courses in the list below:	
Molecular Design and Synthetic Tools - Advanced	3
Analytical and Physical Chemisry - Advanced	3
Theoretical Chemistry and Modelling - Advanced	3
Smart Materials Chemistry - Advanced	3
Innovation and Soft Skills	
Innovative Transdisciplinary Project	2
Design Thinking	2
i-teams workshops	1
Language	1
SEMESTER 2	
Super advanced chemistry courses	
Select 3 courses in the list below:	
Chemical Biology	3
Advanced theoretical and computational chemistry	3
Electronic Properties of Solids	3
Soft matter and Development	3
Inorganic Materials (includes Inorganic assemblies + Chemistry for Functional Materials)	3
Bio-analytical Chemistry	3
Physical Chemistry for Bio-systems (includes Bio-interfaces + Colloids and Biomolecules)	3
Organometallic Chemistry (includes Bioinorganic Chemistry + Heteroelements and Applied Catalysis)	3
Innovation and Soft Skills	
Design Thinking	2
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Internship and seminars	
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SEMESTER 1

Basic science courses

C&I M1	S1	**Course Title: Introductory Mathematics and Physics** *Keywords: linear algebra, Hamiltonian, group theory, crystallography, applied statistics*

Instructor(s), Coordinator	Name(s) and e-mails : F. Labat (frederic.labat@chimieparistech.psl.eu), L. Binet (laurent.binet@chimieparistech.psl.eu), P. Loiseau (pascal.loiseau@chimieparistech.psl.eu), J. Vial (Jerome.Vial@espci.fr)

ECTS : 3	*Total hours* : 30 h	*rating: final exam: written (100%)*

Description

This module introduces the main concepts in mathematics and physics useful to follow the Chemistry & Innovation track of the Graduate Program in Chemistry.

The training is based on three main courses: applied statistics (9h), mathematics (6h) and physics (15h), which are each presented with illustrating examples and exercises in class.

The main concepts covered are: applied statistics, linear algebra, Hamiltonian and Fourier transform, along with quantum physics, group theory, symmetry, crystallography and diffraction.

Learning goals

The student should be able to:

- understand the notions of random variable, distribution, estimation, hypothesis formulation and testing
- know the basic concepts of quantum physics and chemistry, such as linear algebra, Hamiltonian, eigenspace, hermiticity and Fourier transform
- understand the main concepts of quantum physics, group theory, symmetry, crystallography and diffraction, along with their connections.

Pre-requisites

None

C&I M1	S1	**Course Title: Molecular Design and Synthetic Tools - Basics** **Synthetic Molecular Chemistry and Biochemistry** *Keywords: C-C bond formation, asymmetric synthesis, rearrangements, pericyclic reactions, organometallic catalysis, coordination chemistry, biochemistry*	
Instructor(s), Coordinator		Guillaume Lefèvre (guillaume.lefevre@chimieparistech psl.eu) Yann Verdier (yann.verdier@espci.psl.eu)	
ECTS : 3		*Total hours : 24h*	*rating: final written exam*

Description

This course will be divided into 3 units:

a) Basics in organic chemistry

Contents: 4 courses. (i) classical synthetic tools for C-C bond formations, reactivity of usual functional groups (carbonyls, iminiums, enamines, Mannich reaction and related transformations, Evans aldol reaction); (ii) asymmetric / diastereoselective synthesis involving main-group reagents; (iii) rearrangements and transpositions; (iv) pericyclic reactions.

b) Basics in organometallic chemistry

Contents: elementary steps in organometallic chemistry, reactivity of transition-metal complexes, electron counting in complexes, usual C-C bond formation or C=C hydrogenation catalytic cycles (hydrogenation, metathesis, cross-coupling, extension to industrial synthesis of fine chemicals (e.g.: L-DOPA) or to high-scale processes (eg: acetic acid in Cativa / Monsanto processes)).

c) Basics in biochemistry

Contents: the chemistry of life; 50 molecules to know: Nucleic acid, Amino acids and proteins, Carbohydrates & Lipids; DNA and the genetic code; RNA synthesis, Protein synthesis ; Enzymes.

Learning goals

The student should be able to:

- Give the mechanism of multistep transformations of complex targets involving carbonyls as well as carboxylic acids and derivatives, interpret the diastereoselectivity of transformations based on simple models, give the mechanism of multistep rearrangements and various pericyclic reactions, demonstrate that pericyclic reactions are allowed using adequate selection rules.
- Give a catalytic cycle for simple transformations in organometallic catalysis, and analyze the evolution of the oxidation state / electron number of the intermediates involved, as well as interpret the electronic effect of several ligands on the catalytic efficiency in some simple cases.
- Describe the structure and function of the major classes of biomolecules.
- Explain the mechanisms of DNA, RNA and protein synthesis and regulation.

Pre-requisites

Good knowledge of reactivity of classic functional groups. No pre-requisite for the organometallic and biochemistry courses.

C&I M1	S1	**Course Title: Analytical and Physical Chemistry – Basics** *Keywords: solution chemistry ; physical chemistry and interfaces, separation sciences, electrochemistry, molecular spectroscopy*	
Instructor(s), Coordinator		Name(s) and e-mails Fethi Bedioui (fethi.bedioui@chimieparistech.psl.eu), Jean-François Hochepied, Fanny d'Orlyé, Fabien Ferrage	
ECTS : 3		*Total hours : 24*	*rating: final written exam (75%), intermediate reports (25%)*

Description

The course is aimed at arming the student with fundamental concepts in solution thermodynamics and molecular spectroscopies enabling to understand and address experimental questions on how to characterize, analyze, separate molecular components in solutions or complex mixtures

(i) **Solution chemistry**: Brønsted & Lewis acids & bases; complexation; solubility & precipitation
(ii) **Physical chemistry and interface**: (a) focus on gases, ionic solutions and binary mixtures, emphasizing the notion of ideality and non-ideality and use of valid models for real behaviours (Van der Waals, Debye-Huckel models, regular solutions for example); (b) basics laws such as Laplace, Jurin, Kelvin, Young, Gibbs will be presented to describe the presence of bubbles, droplets, surfactants etc…. Finally, the Gibbs adsorption model will be introduced focusing on surfactant effect
(iii) **Separation Sciences**: basic principles of mechanical separation processes (such as sedimentation, decantation, centrifugation, membrane processes …) and diffusion separation processes (such as extraction, crystallization, chromatography …) and introducing the notions of sample pretreatment and multi-step analysis for the development of analytical strategies
(iv) **Electrochemistry**: fundamental principles of electrochemistry, in particular microelectrolysis and the current-potential characteristics i=f(E) to elaborate a basis for the approach in analysis. An overview of the effect of the size of the electrode and the chemical medium on i=f(E) curves will also presented
(v) **Molecular spectroscopy**: NMR: structure of NMR 1D spectra (energy levels. time-independent Schrödinger equation; angular momentum operators; nuclear spin Hamiltonian; energy levels and transition energies for a system of two coupled spins; principles of a 1D NMR experiment (the vector model. Nuclear Magnetization, Bloch Equations; radiofrequency pulses; Fourier transform). Optical spectroscopies: basics of absorption and emission, effects of structure and environment, lifetime of excited electronic states; quantum yield and non-radiative transitions; inhibition of fluorescence

Learning goals

The student should be able to:
- Predict acid-base, complexation or precipitation reactions in a system knowing its composition,
-Take into account non-ideality to describe the properties of mixtures (either in gas, solution, binary mixtures,..) and adapt the laws of thermodynamics to systems where the interface plays a predominant role,
- understand the fundamental aspects of electrochemistry, how to integrate the effect of the chemical medium (acidity, complexation, precipitation) and the size and shape of the electrode in the establishment and plot of i = f (E) curves,
- know the principal forces and interactions that control the performances of each separation method and evaluate these methods in terms of recovery rate, separation selectivity, concentration factor,
- Understand the physical principles of NMR and optical spectroscopies.
- Understand how a simple NMR experiment is performed.
- Describe the structure of these simple spectra.

Pre-requisites

Basics in thermochemistry, inorganic chemistry, organic chemistry, redox chemistry.
Mathematical basics applied to thermodynamics (integration, derivatives, exact total differentials, cross derivatives, differential equations)
Basics of quantum physics and chemistry (Schrödinger equation, energy levels). Descriptive 1D spectroscopy (1D proton NMR, absorption spectra in optical spectroscopies).

C&I M1	S1	**Course Title: Theoretical Chemistry and Modelling – Basics Fundamentals of Theoretical Chemistry** *Keywords: electronic structure, statistical mechanics, quantum chemistry, thermodynamics*	
Instructor(s), Coordinator		Name(s) and e-mails Ilaria Ciofini, François-Xavier Coudert	
ECTS : 3		*Total hours : 24*	*rating: final written exam (67%), intermediate reports (33%)*

Description

Part 1: Basic Electronic Structure Theory

The knowledge of the electronic structure of molecules and extended systems allows for the understanding of their reactivity and properties. Here we will provide a general introduction to the methods and concepts encountered when aiming at describing the electronic structure of single to multi electronic atoms and molecules.
After the introduction of Schrödinger equation and of the common approximations applied to solve it, we will be detailed the Hartree Fock method and define the concept of electronic correlation. Examples on how reactivity can be linked to frontier orbitals analysis will also be given in the case of molecular systems.

Part 2 : Fundamentals of Statistical Mechanics

Statistical mechanics is one of the pillars of modern physics, linking the laws of physics at the microscopic scale, at the quantum (Schrödinger's equation) or classical level (Newton's laws), with the properties of matter and its macroscopic behavior (the laws of thermodynamics). We introduce the fundamentals of statistical mechanics, and introduce the concepts of temperature, work, heat, and entropy, the postulates of statistical mechanics, the notion of statistical ensembles and their use in the calculation of average quantities. We will cover simple models that are widely found throughout physics and chemistry: harmonic oscillator, ideal and nonideal gases, phase transitions, mean field approximations.

Learning goals

The student should be able to:

- understand the meaning of the Schrödinger equation
- know the common approximations used to solve Schrödinger
- describe a multi-electronic atomic or molecular system using the Hartree-Fock method
- define the concept of electron correlation
- rationalize the reactivity of a molecular system on the basis of frontier orbitals analysis
- know the difference between classical and quantum models
- calculate the partition function of a given system
- determine the thermodynamic properties from the partition functions
- apply a mean field approximation
- use equations of state and phase diagrams

Pre-requisites

BSc level in physical chemistry, quantum chemistry, thermodynamics

C&I M1	S1	**Course Title: Smart Materials Chemistry – Basics** **Introduction to inorganic and soft materials** *Keywords: Inorganic and soft matter, hybrids materials, synthesis and characterization*	
Instructor(s), Coordinator		Bruno Viana (bruno.viana@chimieparistech.psl.eu) 12h, Michel Cloitre (michel.cloitre@espci.fr) 12h	
ECTS : 3		*Total hours : 24h*	*rating: final exam (written), intermediate exams, assignments, reports*

Description

This course aims at giving the rules of construction of all inorganic, organic and hybrid systems but also to show their richness and their applications in current problems (such as energy, environment, photonics, nanotechnologies …).

The first part will be an "Introduction to Inorganic Materials" presenting at first basics of the solidification, including symmetry properties, intrinsic and extrinsic defects in solids, thermodynamics stability. Focus materials will be ionic solids, ionocovalent and ionometallic solids. Basic concepts on the electronic band structures and structure-properties relationships will be envisioned. We will present the fundamental aspects in the synthesis of inorganic materials, including phase diagrams, concepts of growth of inorganic materials from nanocrystals to large size materials and their characterization methods.
Nanoparticles synthesis and functionalization will be presented. Materials synthesis using "Chimie douce", i.e. synthesis in solution at relatively low temperature of oxides (sol gel chemistry), organic-inorganic hybrids, molecular compounds, as well as carbon-based solids (graphene…) will be introduced.
Soft Matter encompasses very different materials that share in common weak cohesive forces and a great sensitivity to the environment: polymers, colloids, surfactants, liquid crystals. Behind this apparent diversity, they exhibit common features that can be understood in terms of unifying concepts borrowed from thermodynamic and statistical physics: entropy, enthalpy, phase separation, molecular forces.
The course "Introduction to Soft Matter" will provide the student with a global approach connecting molecular design, synthetic chemistry, mesoscopic and macroscopic structure, material properties, and applications. Selected topics will include an introduction to polymers in bulk and solutions, colloids, and self-assembled systems made of block copolymers, surfactants, and liquid crystals. We will show how transport, flow, mechanical, and optical properties are exploited in advanced functional materials and processes.

Learning goals

At the end of this course, the student will be able to acquire the following knowledge and skills:

- Appropriate the description of the main structural types characterizing solids.
- Be able to distinguish the different types of defects in a solid and be aware of the mechanism of the formation of defects in a solids and the remarkable properties associated with these defects.
- Understood the different existing synthesis routes for the development of inorganic materials. Can assess the pros and cons of these pathways.
- Mobilize a multidisciplinary background in chemistry and physics to rationalize important material behaviors in Soft Matter (i.e. solubility versus phase separation).
- Connect macroscopic behavior to microscopic phenomena (competition between entropy and enthalpy as a driven force for self-assembly)
- Draw analogies between different soft materials.
- Be ready to tackle more complex problems like the design of materials with tailored properties

Pre-requisites

Thermodynamics, Chemical bonding, Group theory,

SEMESTER 1

Advanced science courses

C&I M1	S1	**Course Title: Molecular Design and Synthetic Tools – Advanced Synthetic tools for health sciences** *Keywords: Retrosynthesis, Total Synthesis, Atom- and Step-Economy, transition-metal catalysis, mechanisms, ligand effects, non-noble metals*

Instructor(s), Coordinator	Kevin Cariou (kevin.cariou@chimieparistech.psl.eu), Guillaume Lefèvre (guillaume.lefevre@chimieparistech.psl.eu)	
ECTS	*Total hours: 24h*	*rating: final written exam*

Description

This course advanced course is divided into two units:

a) Retrosynthetic analysis and total synthesis of bioactive compounds (12 h, K. Cariou)
This course will introduce the principles of retrosynthetic analysis and their applications for the design of synthetic routes. Recent examples of syntheses of bioactive molecules (whether natural products or manufactured drugs) will serve as illustrations and a particular emphasis will be placed on atom- and step-economic synthetic strategies.
The course will be divided between classes and practical exercises that will take the form of team projects.

b) Advanced organometallic chemistry (12 h, G. Lefèvre)
This course follows the "basics in organometallic chemistry" course. Classic transition-metal-catalyzed processes (in particular cross-coupling, C-H activation, formation of C-C bonds involving radicals) will be discussed from a mechanistic standpoint (kinetics data, role of the ligand in the promotion of the elementary steps of the catalytic cycle). An overview of the state-of-the art in non-noble metal catalysis (e.g. with 3rd-row metal catalysts) will also be given.

Learning goals
The student should be able to:
- do the retrosynthetic analysis of a given molecule
- propose the key synthetic steps
- devise an efficient synthetic strategy
- solve a synthetic problem through teamwork
- extract the key data from a scientific publication
- rationalize the choice of a catalytic system (ligand, metal, conditions) for a given goal
- suggest a plausible catalytic cycle taking into account of experimental data

C&I M1	S1	**Course Title: Analytical and Physical Chemistry – Advanced** **Physical chemistry of detection, probing and imaging** *Keywords: sample treatment, separation, detection, trace or even ultra-trace analysis, process miniaturization, mesoscale and supramolecular characterizations and imaging*	
Instructor(s), Coordinator		Name(s) and e-mails Laure Trapiella (laura.trapiella@chimieparistech.psl.eu), Fethi Bedioui, Christophe Tribet, Fanny d'Orlyé, Anne Varenne, Bich-Thuy Doan	
ECTS : 3		*Total hours : 24h*	*rating: rating: final written exam (67%), intermediate reports (33%)*

Description

This course has two parts and it is aimed at presenting a journey of discovery of up-to-date techniques and design of molecular probes used to investigate molecular compositions of samples, and/or spatial organization and dynamics of molecules or assemblies. The objective is to become familiar with most common analytical methods, types of spectroscopy, and imaging practices. To complement fundamental presentations of the methods, a hands-on understanding will be provided by visiting experts in their laboratories.

(i) **Analytical physico-chemistry for environmental analysis**: the course will focus on detection techniques (i.e. spectroscopic, electrochemical) capable to reach very low detection limits of pollutants and the need for the development of portable, rapid, reliable and in-situ analysis, thus the need of the miniaturization, will be presented (Laura Trapiella; 6h)

(ii) **Analytical physico-chemistry for biotechnology and clinical diagnostics:** notion of biomarkers and sample matrix effects will be presented. Then the different kinds of biorecognition events and associated bioassay formats will be introduced. Also considering the whole analytical process the main processes on sample treatment, separation techniques and coupling with performant detection methods (i.e. spectroscopic and electrochemical) will be illustrated. Finally, the concept of method/test validation will be afforded in the view of the development of new analytical strategies that can arrive to the end-users (Laura Trapiella; 6h).

(iii) **Radiation-based analysis, from spectroscopy to imaging (part I):** basics of the chemical probes and probing methods at the molecular level will be presented in MRI, EPR, optical mono (IR, UV-Vis)/bi-photon fluorescence to characterize the structure and understand the properties of probes. Advanced applications in cellular diagnosis or for novel therapies will be detailed (including photoactivable biomolecules, NIR probes for image guided therapy, biphotonic and super resolution techniques) (Bich Thuy Doan; 6h).

(iv) **Radiation-based analysis, from spectroscopy to imaging (part II):** The course will cover a range of optical and scattering-based methods, used to characterize structures at the nanometer to micrometer length scalesThe theory of scattering (light, small angle X-ray) will be established. Models of scattering patterns will be presented to determine molecular weight, radii, shape, and impact of inter-molecular attraction/repulsion forces involved in molecular assemblies, macromolecules, colloids, up to spatial organization of biological matter. (Christophe Tribet; 6h).

Learning goals

The student should be able to:

- Identify the steps of an analytical process, know the principal processes and techniques for the sampling, sample treatment and analytical determination
- Know the more common formats and detection methods used for the environmental and biological analysis
- Understand the general principle of Magnetic Resonance methods and MR imagings.
- Understand optical methods for mesostructure characterization (microscopies, elastic static scattering, tracking)

Pre-requisites

Basics in atoms and molecules energy levels, molecules interactions, complexation, magnetic resonance and optical spectroscopy. Basics in physical and analytical chemistry, chemistry of solutions & molecular interactions. Basics in optics and interferences

C&I M1	S1	**Course Title: Theoretical Chemistry and Modelling – Advanced Modelling and simulation in chemistry** *Keywords:*	
Instructor(s), Coordinator		Name(s) and e-mails: Carlo Adamo (carlo.adamo@chimieparistech.psl.eu), Frédéric Labat (frederic.labat@chimieparistech.psl.eu), Damien Laage (damien.laage@ens.psl.eu)	
ECTS : 3		*Total hours : 24h*	*rating: final written exam (67%), intermediate reports (33%)*

Description

Advanced electronic structure methods enabling the treatment of electron correlation will be introduced focusing on Density Functional Theory. The coupling and extension of ab-initio approaches to describe condensed phases (solution, solids, interfaces and surfaces) will be detailed. Multi-layer methods combining Quantum and Classical approaches will be introduced for the simulation of complex environments.
Example of academic and industrial applications of these QM and mixed QM/MM methods to model i) chemical reactivity and catalysis (homogenous and heterogeneous) and ii) macroscopic properties of materials for energy production and storage and iii) biomolecules will be provided.

Based on the concepts of statistical physics and thermodynamics, molecular simulation has developed as a way to obtain information about the physical and chemical properties of a given complex system. We will introduce the students to the main classes of molecular modelling methods, molecular dynamics and Monte Carlo simulations. We will learn to study reactivity in condensed phases, both from the theoretical and computational points of view. We will contrast the approaches of quantum chemical and classical methods, and provide an introduction into mesoscale modeling methods, such as lattice-based simulations and kinetic Monte Carlo.

The course will use examples from a wide variety of fields, and demonstration applications of the methods and theories in the areas of chemistry in the liquid phase, at interfaces, for materials, and biological systems.

Learning goals

The student should be able to:

- understand the fundamentals of Density Functional Theory
- understand how one can simulate periodic systems
- understand the fundamentals of molecular simulation in chemistry, and their ties to statistical mechanics
- know differences between molecular simulation techniques
- choose an appropriate simulation technique for a given complex question
- read a computational chemistry article and understand the methodology and its limitations

Pre-requisites

BSc level in statistical physics, quantum chemistry, physical chemistry

C&I M1	S1	**Course Title: Smart Materials Chemistry – Advanced** ***Materials design and properties*** *Keywords:* Advanced functional materials. Hybrid materials. Energy storage and conversion. Batteries. Optical Materials. Metal Organic Frameworks, Stimuli-responsive materials
Instructor(s), Coordinator		A. Tissot 6h (antoine.tissot@ens.psl.eu), A. Grimaud 6h (alexis.grimaud@college-de-france.fr), B. Viana 6h (bruno.viana@chimieparistech.psl.eu), Y. Tran 6h (yvette.tran@espci.fr)
ECTS : 3	*Total hours : 24h*	*rating: final exam (written), intermediate exams, assignments, reports*

Description

This course will provide at first the necessary skills to design smart materials. The focus will be: how to start from these concepts to develop smart materials. The relevant applications of the advanced functional materials will be described as well as their fate and recycling issues.

- Description of basic concepts of coordination chemistry including geometry/reactivity/stability of coordination complexes.
- Ligand field theory, electronic properties of solids.
- Electronic transitions in rare-earths and transition metal doped materials.
- Diffusion properties in solids and quick recapitulative about electrochemistry and its application to solids and solid/liquid interfaces.
- Triggering of a stimulus such as temperature, pH, salt, light, electric and magnetic fields.
- Inducing changes of molecular conformation (surfactants, polymers) and/or changes of assembling (gels, colloids, emulsions).
- Control of macroscopic properties (rheological, mechanical, interfacial as wetting, adhesion, friction).

Toward applications

=> Synthesis, properties and applications of crystalline porous solids (Metal-Organic Frameworks).
=> New developments of batteries: which battery/chemistry for which application? Current research trends in battery performances and chemistry: tradeoff between energy/power density and scalability. Recycling issues
=> Materials for lasers, scintillation, photovoltaics and imaging
=> Materials and biotechnologies (encapsulation, microfluidics, injectable gels, photonic crystals…)

Furthermore, materials sustainability will be envisioned: can smart materials be sustainable and what are the bottlenecks to tackle?

Learning goals

At the end of this course, the student will be able to acquire the following knowledge and skills in the various fields:

- Structure and reactivity of coordination compounds
- Description of the properties of porous solids
- Photon, electron and phonon properties relationships. Radiative and non-radiative relaxations.
- Color and luminescence
- Redox properties of solids and alkali-cation diffusion properties in solids
- Charge transfer at solid/liquid interface
- Concept of stimuli-responsiveness
- To pilot molecular changes for microscopic/mesoscopic/macroscopic changes

Pre-requisites

Basics of inorganic and organic chemistry, coordination chemistry. Basics of soft matter. Thermodynamics. Basics courses of the Graduate Program.

SEMESTER 1

Innovation and soft skills

C&I M1	S1	**Course Title: Innovative Transdisciplinary Project** *Keywords: innovation, scientific project*
Instructor(s), Coordinator		Name(s) and e-mails : Fethi Bedioui (fethi.bedioui@chimieparistech psl.eu), Guillaume Lefèvre (guillaume.lefevre@chimieparistech psl.eu)
ECTS : 3	*Total hours : 54h*	*rating: final report and oral presentation*

Description

The students must design a scientific and innovative project based on research topics developed in PSL laboratories in order to gain awareness of the transformation of research results into innovative applications. Their projects will be carried out in strong interaction with these laboratories.

Learning goals

The student will become familiar with project design and planning, group work and multi-partner interaction.

Pre-requisites

none

Entrepreneurship and Soft Skills

C&I M1	S1	**Course Title: Design Thinking** *Keywords: design, innovation*	
Instructor(s), Coordinator		Name(s) and e-mails: Faustine Vanhulle, Damien Ziakovic, Marc Dolger, Corinne Soulié, Hélène Montès	
ECTS : 2		*Total hours : 35h*	*rating: written exam (30%), intermediate assessments (35%), oral presentation (35%)*

Description

This course aims at showing how to imagine a material / innovate for a specific object by interacting with other actors such as designer, marketing manager, etc…

In this course, the "Design Thinking" approach is presented and applied to a real innovation issue. In 2019, the theme was "personalised care" proposed by LVMH Research.

The course is articulated between courses and workshops given by innovation advisors, designers and scientific researchers. It takes place over one quarter, with a dedicated week in November and a few isolated sessions of 2 or 3 hours upstream and downstream.

The initial problem is first analysed (example of the existing situation, surveys, tests) and then repositioned in an innovative approach (responding to a real identified need). The analysis and repositioning methods are based on ideation sessions, the preparation of a trend book, tests and surveys.
Intermediary presentation sessions allow to iterate the process, to refine the positioning, to define the technical feasibility and the business model and to check the sustainability of the proposed solution.

The solutions selected for their innovative potential are developed during a dedicated week at the end of January, preceded by a presentation session at the beginning of January.

Learning goals

- identify innovation in a specific field (do not confuse innovation and invention…)
- mobilize design thinking tools to generate innovative ideas, test them, etc.
- mobilise the designer's tools to position his ideas in relation to the existing market (trend book)
- confronting one's ideas with existing or implementable technical feasibility
- take into account the development of its ideas (marketing, target audiences, sustainability by industry)

Pre-requisites

none

C&I M1	S1	**Course Title: PSL I-teams workshops** *Keywords: innovation, entrepreneurship*	
Instructor(s), Coordinator		Name(s) and e-mails : Nadine-Eva Jeanne (nadine-eva.jeanne@psl.eu), Karla Balaa (karla.balaa@psl.eu)	
ECTS : 1		*Total hours : 16h*	*rating: validation*

Description

This course aims at developping entrepreneurship skills and exposing to the challenges of innovation. It will provide students with hands-on introduction to the valorisation of research results and the creation of companies.

Learning goals

The student will become familiar with idea conceptualization, go-to-market strategy, market study, project developpement, management, law and financial aspect of companies.

Pre-requisites

none

C&I M1	S1	**Course Title: Language** *Keywords:*
Instructor(s), Coordinator		Name(s) and e-mails : Daria Moreau (daria.moreau@chimieparistech.psl.eu)
ECTS : 1	*Total hours :*	*rating: intermediate assessments*
Description Students are offered courses in various languages (French for foreigners, English,…)		
Learning goals Develop student's proficiency in foreign language		
Pre-requisites none		

SEMESTER 2

SUPER-ADVANCED CHEMISTRY COURSES

Chemical Biology

C&I M1	S2	**Course Title: Chemical Biology** *Keywords: Nucleic acids, Modified-Nucleic acids, Synthesis, Biochemistry, Chemical Biology Applications, peptide, protein, solid phase synthesis, biotechnology, fluorescence spectroscopy, fluorophores, fluorescence imaging; biomolecules*	
Instructor(s), Coordinator		Name(s) and e-mails Daniela Verga (daniela.verga@curie.fr), Nicolas Delsuc (nicolas.delsuc@ens.psl.eu), Anton Granzhan (anton.granzhan@curie.fr), Blaise Dumat (blaise.dumat@ens.psl.eu)	
ECTS : 3	*Total hours : 24h*		*rating: final written exam*

Description

1) Chemical Biology of modified –Nucleotides and –Nucleic Acids (6h, D. Verga)

In this section, we will focused our attention on the methods for obtaining modified and native nucleic acids and their biological applications. Several specific topics will be faced during the class:

- Chemical synthesis of modified nucleosides, nucleotides, and oligonucleotides concerning both DNA and RNA;
- Expansion of the genetic alphabet in nucleic acids by creating new synthetic nucleobases and as a consequence new base-pairs;
- The concept of chemical biology applied to DNA replication, by probing DNA polymerase selectivity mechanisms with modified nucleic-acid-template chemistry;
- The interactions of small synthetic molecules with DNA and effects produced on biological processes, and more specifically on replication and transcription;
- At last, DNA methylation as epigenetic mechanism involving the transfer of methyl groups on DNA nucleobases and effects produced on gene expression.
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2) Peptides and Proteins synthesis, application to peptide biological activity (8h, N. Delsuc)

This section aims at giving an overview of the different approaches used to synthesize peptides and proteins. This will include chemical synthesis in solution and on solid support and chemical reactions to perform ligation enabling the synthesis of long sequences. The chemical part will include the reactions required to form efficiently amide bonds while preserving the enantio-purity of amino acids as well as protecting group management.

The course will also deal with the synthesis of proteins using new biotechnological tools involving bacteria as well as procedures to ensure an appropriate folding of the proteins. In particular, the controlled formation of disulfide bridges will be discussed. Several examples of biological active peptides and proteins already on the market will be shown to illustrate these strategies.

3) Molecular design strategies for fluorescent probes (12h, A. Granzhan, B. Dumat)

Due to its versatility, ease of implementation and high spatial and temporal resolution, fluorescence has become a ubiquitous tool in chemical biology to monitor biological processes *in vitro* or *in vivo*. Fluorescent reporters, or probes, can be used for very diverse applications, ranging from *in vitro* analytical applications to *in vivo* imaging, which call for very different requirements in terms of photophysical and biochemical properties. The goal of his course is to present the different molecular design strategies currently used to elaborate and tailor fluorescent probes for various applications. After a presentation of the underlying phenomenon of molecular fluorescence, we will cover different classes of fluorophores (from the classically used ones to the newest additions to the field), photophysical principles governing the operation of different types of fluorescent reporters, and consider various examples of the probes used for the detection, labeling and imaging of biomolecules (such as nucleic acids, proteins, enzymes…) and biologically relevant analytes (metal ions, anions, reactive species, etc.).

Learning goals

The student should be able to:

- Present the synthetic pathways employed for the preparation of both modified and native nucleic acid;
- Describe the applications of modified nucleotides and oligonucleotides
- Describe the synthesis of new synthetic nucleobases and their biological applications;
- Explain the mechanisms that allow specific DNA polymerases to incorporate modified-nucleotides and recognized modified DNA templates;
- Mention the structural characteristics allowing small molecules to interact with specific DNA structures and explain the exploitation of such interactions;
- Explain the natural DNA modifications why they occur and explain their effects in gene expressions.

- Master the different steps of the chemical synthesis of peptides and proteins and the requirements to produce enantiopure peptides and the different steps to produce recombinant proteins using bacteria
- Propose strategies to synthesize proteins
- Understand the principles of molecular fluorescence
- Know various applications of fluorescence in chemistry and biology such as structural or analyte sensing, imaging
- Know the most widely used classes of fluorophores and their characteristics, be able to identify the fluorescent scaffolds;
- Understand the photophysical and supramolecular principles governing the operation of fluorescent probes and requirements for a given application
- Tailor a fluorescent probe for a given application by combining the proper fluorescent scaffold with the adequate functional groups while taking into account the synthetic feasibility

Pre-requisites

Knowledge in organic chemistry and basic knowledge in biochemistry, organic synthesis: (orthogonal reactions, protecting groups), basics in cellular biology (protein expression), heterocyclic chemistry, physical chemistry

Advanced theoretical and computational chemistry

C&I M1	S2	**Course Title: Advanced theoretical and computational chemistry** *Keywords:*
Instructor(s), Coordinator	Name(s) and e-mails Ilaria Ciofini (ilaria.ciofini@chimieparistech.psl.eu); François-Xavier Coudert (fx.coudert@chimieparistech.spl.eu)	
ECTS : 3	*Total hours : 24h*	*rating: final written exam (67%), intermediate reports (33%)*

Description

The course will provide an advanced perspective both on theoretical models and simulation techniques treating several among the topics detailed below. Regarding numerical simulations, building o
n the introduction given in the advanced class, this course will address a range of modern techniques, including first-principle methods, extended statistical ensembles, description of nuclear quantum effects via path-integral simulations, multi-scale strategies, and the combination with machine learning approaches. Various applications of these techniques to condensed phase chemistry will be studied. This course will also present advanced theoretical models to describe chemical reactivity; starting from Transition State Theory, the course will introduce the concept of friction on barrier-crossing, its formal description via stochastic approaches and will finally address the complex case of non-adiabatic chemical reactions.
Concerning electronic structure methods, the course will explicitly address state of the art methods enabling the first-principle simulation of spectroscopic properties of molecules and extended systems. Perturbative and variational methods allowing to obtain accurate vibrational spectra will be introduced and compared to approaches based on dynamical approaches. Linear response –in the framework of the Time Dependent DFT approach- will be introduced and the simulation of the photophysical properties of molecular and extended (3D, 2D, 1D) systems will be discussed.
The accuracy and the limit of these methods (coupled with embedding techniques and/or multi-layer approaches to simulate the environment) will be illustrated through selected examples.

Learning goals

The student should be able to:

- understand the main concepts related to the modeling of spectroscopic properties of molecules and extended systems
- list the tradeoffs involved in different molecular simulation techniques
- write up a work plan for a multi-scale simulation strategy
- compare experimental data, computational results, and theoretical models of reactivity
- understand articles on machine learning techniques applied to chemistry

Pre-requisites

BSc level in statistical physics, quantum chemistry, physical chemistry

Electronic Properties of Solids

C&I M1	S2	**Course Title: Electronic Properties of Solids : from Concepts to Devices** *Keywords: band structures, optical and electrical properties, semiconductors, devices*
Instructor(s), Coordinator	Name(s) and e-mails: Laurent Binet, Pascal Loiseau, Frédéric Wiame Laurent Binet (laurent.binet@chimieparistech.psl.eu)	
ECTS: 3	*Total hours : 22,5h*	*rating: final written exam*

Description

The aim of this course is to describe the electronic structure of solids and the main properties and applications resulting from them, with an overview of current technological developments.

In the first part the course introduces the basic concepts and models (free electron gas, tight-binding) for the electronic band structures of solids and shows how these models explain the main classes of properties, electrical, optical and chemical of solids.

In the second part, the course focuses on an important class of materials, semiconductors, and describes in details the phenomena that occur in a p-n junction. The applications of such junctions are described, in particular solar cells, photodiodes and light-emitting diodes.

Learning goals

The student must be able to do:

- to define the characteristics of the two main models of electronic structure of solids and to know in which context to apply them,
- explain the main parameters that govern the electrical and optical properties of materials and the factors that have a positive or negative effect on these properties,
- interpret a band structure diagram of a solid and deduce its electrical and optical behaviour,
- describe in detail the electronic processes occurring in the main semiconductor devices and explain the factors controlling their performance
- to establish a structure-property relationship for a given application.

Pre-requisites

quantum mechanics (Hamiltonian, operators, Dirac notation, model quantum systems), electronic structure of atoms and molecules (atomic orbitals, molecular orbitals, bonding/antibonding orbital), crystallography (crystal systems, normal lattice, reciprocal lattice), general physics (classical mechanics, electrostatics, waves), maths (integrals, partial derivatives, differential, laplacian, gradient, divergence)

Soft Matter and Developpement

C&I M1	S2	**Course SuperAdvanced : Soft matter and Development** *Keywords: soft matter, polymers, liquid crystals, colloids, formulations*
Instructor(s), Coordinator	Name(s) and e-mails: Michel Cloître (michel.cloitre@espci.fr)	
ECTS : 3	*Total hours : 26h*	*rating: final written exam*

Description

The Soft Matter and Development course, designed for physicists, chemists and physico-chemists, illustrates how a good knowledge of basic concepts in Soft Matter, with an interdisciplinary approach, allows you to design and develop innovative materials and processes.

Course's content.

1- Macromolecular engineering : polymer blends, block copolymers, microphase separation of block copolymers, thermoplastic elastomers, nanostructured materials, analogy with surfactants phases

2- Molecular engineering : phases of liquid crystals (nematic, smectic, chiral), defects and textures, liquid crystal displays and other display devices

3- Colloidal engineering : hard spheres suspensions, glasses and colloidal crystals, development of photonic materials, deformable colloids (emulsions, microgels, micelles…), jamming transition

4- Formulations in solution: polymers in diluted and semi-diluted solutions, physical and chemical gels, stimuli-responsive polymers, gels and biomaterials, polyelectrolytes, associative polymers

Course support:

- Richard A.L. Jones, Soft Condensed Matter, Oxford University Press
- Masao Doi, Soft Matter Physics, Oxford University Press

Learning goals

The student must be able to:

- mobilize knowledge to solve a complex problem
- critically analyze a scientific article
- interpret experimental data and modelize them
- relate macroscopic behavior to microscopic phenomena
- draw analogies between different issues
- use English scientific and technical vocabulary

Pre-requisites

Basics of thermodynamic and statistical physics: entropy, enthalpy, phase separation, molecular forces. Basic knowledge of rheology. Basic knowledge of the structure of materials

Inorganic Materials
includes the “Inorganic Assemblies” course and the “Synthesis of Inorganic and Hybrid Materials course” (next page)

C&I M1	S2	**Course Title: Inorganic assemblies** *Keywords:*	
Instructor(s), Coordinator		Name(s) and e-mails: Philippe Barboux (philippe.barboux@chimieparistech.psl.eu)	
ECTS :		*Total hours : 15h*	*rating: final written exam*

Description

The objective of this course is to give the rules of construction of all inorganic and mineral systems but also to show how much this inorganic chemistry is alive and has many applications in current problems (energy, environment, information storage, nanotechnologies…). An introduction to the industrial mineral chemistry industry completes the course (cements, glasses, aquatic chemistry, batteries). The theoretical part focuses on transition metal and lanthanide complexes and describes in particular their optical and magnetic properties.

Learning goals

At the end of the course,

- The student knows the periodic table and the trends of the different elements (ionization, complexation, orbital levels).
- He can describe a mineral system and choose between two simples approaches to describe inorganic complexes according to two-ion binding or covalent-binding models.
- He can explain the stability and reactivity of inorganic molecules based mainly on transition elements or elements of the p-block
- He can have a view of the applications in various domains such as energy, environment, information storage, nanotechnologies.

Pre-requisites

Atomistic, Chemical bonding, electronic structure of atoms and molecules (atomic orbitals, molecular orbitals, bonding/antibonding orbital, crystal field), crystallography (crystal systems, normal lattice, reciprocal lattice), general physics.

C&I M1	S2	**Course Title: Synthesis of Inorganic and Hybrid Materials** *Keywords: Inorganic materials, porous solids, synthesis, challenges*	
Instructor(s), Coordinator		Name(s) and e-mails: Sandrine Ithurria, Thomas Pons, Vanessa Pimenta, Christian Serre (sandrine.ithurria@espci.fr)	
ECTS :		*Total hours : 14h*	*rating: final written exam*

Description

The « Chemistry for Functional Materials » course is dedicated to chemists who wish to develop a broader view on the synthesis and characterization of inorganic materials and functional hybrids.
The course contains two (equal) parts: crystallized inorganic materials (7 hours) and crystallized porous materials (7 hours). For both classes of materials, the methods of synthesis and the challenges related to their characterization will be addressed, as well as their potential applications in various fields (health, energy, environment, optoelectronics). Few hours of tutorial will complement this course.

Course's content.
1. Introduction to porous crystalline solids (zeolites, clays, LDH, MOFs, hybrid cages)
2. Methods of synthesis and modulation of porosity (exfoliation, composites…)
3. The challenges of characterizing porous networks (BET, in-situ IR, solid NMR, MET, modeling)
4. Potential applications of porous solids (environment, energy, health)
5. Outlook – scaling up, shaping and industrialization (marketing, proven applications)
6. Introduction to advanced inorganic materials
7. Methods for the synthesis of inorganic materials
8. Characterization methods
9. Applications of advanced inorganic materials

To deepen your knowledge:
F. Schüth, K. S. W. Sing, J. Weitkamp, Handbook of Porous Solids, Wiley
Print ISBN:9783527302468 |Online ISBN:9783527618286
|DOI:10.1002/9783527618286

Learning goals

The student must be able to:
- identify the different classes of inorganic and hybrid crystalline materials…
- describe the different modes of synthesis of functional materials
- relate structural characteristics to material properties
- discuss the characterization methods
- consider the potential applications of crystalline functional materials
- analyze and identify important results of scientific publications
- explain concepts and ideas in a short presentation
- use English scientific and technical vocabulary

Pre-requisites

Basics of structural and solid state chemistry
Basics of coordination chemistry

Bio-analytical Chemistry

C&I M1	S2	**Course Title: Bio-analytical Chemistry** *Keywords: analytical systems, engineering, process miniaturization, innovation, engineering*
Instructor(s), Coordinator		Name(s) and e-mails : Fanny d'Orlyé (fanny.dorlye@chimieparistech.psl.eu)
ECTS : 3	*Total hours : 24h*	*rating: final written exam + intermediate rating*

Description

Developments and trends in modern analytical chemistry point in the direction of simplification, automation and miniaturization of processes while preserving the performance and reliability of the analytical results. The opportunities and challenges inherent in miniaturization at each stage of an analysis processes are very different and need to be addressed. The main objective of this course is therefore to provide a comprehensive overview of current innovations in the field of analytical systems. The final objective is the development of micro(nano)sensors and total analysis microsystems (µTAS) for the biotechnology and clinical diagnostic applications.

Learning goals

The course will focus on new analytical and bioanalytical tools for downscaling several laboratory operations (sample introduction, processing, separation, detection) in order to process extremely small volumes of fluids and also to integrate the above-mentioned processes on a device miniaturized of a few square centimetres allowing for high-speed automation and processing of analysis.
The main competences to be acquired by the students will concern:
1) new nanomaterials functionalized for diagnostics: (nanosupports, nanoparticles, nanotubes, monoliths, molecular printed materials, etc.), selective agents (antibodies/proteins, aptamers, chelating agents...) and procedures for conjugation;
2) the development of miniaturized separation methods (chromatographic or electrokinetics) mainly based on molecular recognition to purify, concentrate and isolate analytes of interest;
3) the detection in miniaturized analytical systems (optical, electrochemical, mass spectrometry);
4) The analytical processes ranging from standard bioassays to micro(nano)sensors and total analysis microsystems for biotechnology and clinical diagnostic applications.

Pre-requisites

basic notion in solutions thermodynamics, non-covalent interactions, colloïds, electrochemistry and separation methods

Physical Chemistry for Bio-systems
includes the "Bio-interfaces" course and the "Colloids and biomolecules" course (next page)

C&I M1	S2	**Course Title: Bio-interfaces** *Keywords: surface, composition, reactions, techniques, biomolecules*
Instructor(s), Coordinator		Name(s) and e-mails : Anouk Galtayries (anouk.galtayries@chimieparistech.psl.eu)
ECTS :	*Total hours : 15h*	*rating: final written exam*

Description

This lecture aims at showing that the key role played by the surface of materials in the issues related to the interfaces between solids and biological environment (biointerfaces). These issues are mainly in the biomedical context but also, more widely, for any innovative systems implying surfaces and biomolecules (biosensors, biofilms in food industry, biocorrosion…).

This course implies the following items:

- Introduction: the surface = a complex material (structure, composition, model surfaces, real surfaces
- Biointerfaces; where all biological processes occur
- Dedicated physico-chemical characterization techniques: in situ real time ones, UHV techniques, combination of techniques morphology and composition…
- Different examples of surface reactivities from amine acid reactions to protein non specific and specific interactions

Interactivity on specific topics: understanding the quantitative approach

Learning goals

- The student will take into account the outermost layers in a material issue.
- The student will know the principles, advantages and drawbacks of some characterization techniques of solid surfaces/materials
- The students should be able to propose quantification and qualitative approaches when discussing a biointerface characterization strategy
- The students should be able to identify the properties of biomolecules adsorption, and impact on further reactions, and to model an experiment to understand surface reaction mechanisms in the frame of biomaterials.

Pre-requisites

none

C&I M1	S2	**Course Title: Colloids and Biomolecules** *Keywords:*
Instructor(s), Coordinator		Name(s) and e-mails : Jérôme Bibette (jerome.bibette@espci.psl.eu)
ECTS :	*Total hours : 10h*	*rating: final written exam*

Description

The key topics addressed in this course are :

• How do collids diffuse in their environement via brownian motion?

• How do colloids and biomolecules react and associate in a complex medium? How to model ligand-receptor interactions on cell membranes?

• What is the dissociation dynamics of bio-complexes and how to studt the properties of these associations?

• How to apply colloidal science to medical diagnostic?

Learning goals

The student should be able to:

- explain and predict the diffusion of colloids in a complex medium
- explain and model interactions at stake between colloids and biomolecules
- explain and predict the association/dissociation dynamics
- relate the associations and their dynamics to the properties of the macroscopic systems
- propose medical diagnostic

Pre-requisites

Organometallic Chemistry
includes the « Bio-inorganic chemistry course" and the "Heteroelements and applied catalysis" course (next page)

C&I M1	S2	**Course Title: Bioinorganic chemistry** *Keywords: bioorganometallic chemistry, enzymes, inorganic chemical biology, medicinal inorganic chemistry, metal complexes*	
Instructor(s), Coordinator		Gilles Gasser gilles.gasser@chimieparistech.psl.eu	
ECTS		*Total hours: 15h*	*rating: final written exam*

Description

The vast majority of drugs used today are purely "organic" compounds – they do not contain any metal atoms. However, due to their different kinetic, geometric and electronic properties, metal complexes can undergo reactions which are not possible with organic 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.

Learning goals

This course will cover 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 mechanism of action of the metal-based drugs will be presented in detail.

Pre-requisites

This course requires basic knowledge of inorganic chemistry and biochemistry.

Teaching language: english
Lecture notes: yes
URL:

C&I M1	S2	**Course Title: Heteroelements and Applied Catalysis** *Keywords: catalysis, transitions metals, coupling reactions, heteroelements*
Instructor(s), Coordinator		Name(s) and e-mails : Phannarath Phansavath (phannarath.phansavath@chimieparistech.psl.eu)
ECTS :	*Total hours : 12h*	*rating: final written exam*

Description

The course Heteroelement Chemistry aims at introducing the various methode for preparing phosphorus, sulfur and silicon reactants. The main transformations achieved with these compounds are given with applications in total synthesis. The goal of the course Applied Catalysis is to provide with the bases of organometallic chemistry involving transition metals (palladium, rhodium and ruthenium), as a tool for the developpement of synthetic processes. Coupling reactions and other major applications in homogeneous catalysis are introduced with a focus not only on reaction mechanisms and but also on applications, both at industriel level and for the synthesis of natural molecules or molecules of biological interest.

Learning goals

At the end of the course, the students should be able to master the methods to perform the main transformations achieved with phosphorus, sulfur or silicon derivatives and to explain the corresponding reaction mechanisms. They should be able to use the organometallic complexes suitable for the main coupling reactions and other major reactions used in homogeneous catalysis.

Pre-requisites

Good knowledge of basic reactions in organic chemistry and goog understanding of classical reaction mechanisms.

SEMESTER 2

Innovation and soft skills

Entrepreneurship and Soft Skills

C&I M1	S2	**Course Title: Design Thinking** *Keywords: design, innovation*	
Instructor(s), Coordinator		Name(s) and e-mails: Faustine Vanhulle, Damien Ziakovic, Marc Dolger, Corinne Soulié, Hélène Montès	
ECTS : 3		*Total hours : 35h*	*rating: written exam (30%), intermediate assessments (35%), oral presentation (35%)*

Description

This course aims at showing how to imagine a material / innovate for a specific object by interacting with other actors such as designer, marketing manager, etc…

In this course, the "Design Thinking" approach is presented and applied to a real innovation issue. In 2019, the theme was "personalised care" proposed by LVMH Research.

The course is articulated between courses and workshops given by innovation advisors, designers and scientific researchers. It takes place over one quarter, with a dedicated week in November and a few isolated sessions of 2 or 3 hours upstream and downstream.

The initial problem is first analysed (example of the existing situation, surveys, tests) and then repositioned in an innovative approach (responding to a real identified need). The analysis and repositioning methods are based on ideation sessions, the preparation of a trend book, tests and surveys.
Intermediary presentation sessions allow to iterate the process, to refine the positioning, to define the technical feasibility and the business model and to check the sustainability of the proposed solution.

The solutions selected for their innovative potential are developed during a dedicated week at the end of January, preceded by a presentation session at the beginning of January.

Learning goals

- identify innovation in a specific field (do not confuse innovation and invention…)
- mobilize design thinking tools to generate innovative ideas, test them, etc.
- mobilise the designer's tools to position his ideas in relation to the existing market (trend book)
- confronting one's ideas with existing or implementable technical feasibility
- take into account the development of its ideas (marketing, target audiences, sustainability by industry)

Pre-requisites

none

C&I M1	S2	**Course Title: PSL I-teams workshops** *Keywords: innovation, entrepreneurship*	
Instructor(s), Coordinator		Name(s) and e-mails : Nadine-Eva Jeanne (nadine-eva.jeanne@psl.eu), Karla Balaa (karla.balaa@psl.eu)	
ECTS : 1		*Total hours : 16h*	*rating: validation*

Description

This course aims at developping entrepreneurship skills and exposing to the challenges of innovation. It will provide students with hands-on introduction to the valorisation of research results and the creation of companies.

Learning goals

The student will become familiar with idea conceptualization, go-to-market strategy, market study, project developpement, management, law and financial aspect of companies.

Pre-requisites

none

C&I M1	S2	**Course Title: Language** *Keywords:*
Instructor(s), Coordinator	Name(s) and e-mails : Daria Moreau (daria.moreau@chimieparistech.psl.eu)	
ECTS : 3	*Total hours :*	*rating: intermediate assessments*
Description Students are offered courses in various languages (French for foreigners, English,…)		
Learning goals Develop student's proficiency in foreign language		
Pre-requisites none		

SEMESTER 2

Internship and seminars

Internship

C&I M1	S2	**Course Title: Pre-internship Project and Seminars** *Keywords:*
Instructor(s), Coordinator		Name(s) and e-mails :
ECTS : 3	*Total hours :*	*rating: written report and oral presentation*

Description
The pre-internship project consists in a bibliographic study in connection with the internship research topic. The students should become aware of the state of the art of the topic and gain a deep understanding of the principles of the techniques to be used during the laboratory work.
The seminar work consists in a short written summary of selected seminars attended during the academic year.

Learning goals
The aim of this activity is to extend the scientific knowledge of the students and to make them aware of up-to-date research topics.
The student should then be able to read and understand scientific academic literature to get into an unknown topic.

Pre-requisites
none

C&I M1	S2	**Course Title: Laboratory Internship** *Keywords:*
Instructor(s), Coordinator		Name(s) and e-mails :
ECTS : 15	*Total hours : minimum 3 months*	*rating: written report and oral presentation*

Description
The internship should take place in a research laboratory either academic or in private company.

Learning goals
The student shoulb be able to conduct a small research project, to plan and carry out experiments, to understand the theoretical bases of his/her project, to interact with other researchers and staff members, to make written and oral reports of his/her results.

Pre-requisites
none

Syllabi of the new M2 track

Integrative Chemistry and Innovation, ICI

to open in September 2021

Course 1: Flow chemistry

Course title: Flow chemistry, an emerging technology for organic synthesis

Pedagogical objectives: the objective of this teaching unit is to raise awareness and train students to flow chemistry for the synthesis of molecules of interests. Flow chemistry will be instrumented to decipher the fundamental reactivity and mechanisms of classical and new activation modes in organic synthesis. At the end of this course, the students will be able to:

- Understand the principles of flow chemistry: the theoritical concepts and the advantages associated with this technique versus classical batch methods
- Know the existing equipments and their utilisations
- Predict the reactivity and the reaction mechanisms of given species when submitted to various activation conditions
- Propose solutions in flow chemistry to existing problems in batch systems based on critical literature survey

Prerequisites: The student should possess a good background in organic chemistry and be aware of the classical reactivity profiles of important functional groups. He should have some basics in redox reactions and reactivity of radical species.

Course structure :

Part 1. Introduction, processes, reactors (8h)

a. General introduction (2h, **B. Laroche**)
This lecture will consist in an introduction of the technology, the description of relevant parameters and comparisons of batch vs. flow systems for organic synthesis. The different types of flow reactions will be depicted as well as the different reactors associated. This lecture will also introduce the different activation modes and chemical reactivity that will be further studied in part 2.

b. An upgrade on energy and matter transfers in continuous-flow reactors: (6h, **S. Ognier**)
At first, the influence of hydrodynamic and heat/mass transfers on reaction rate and selectivity will be illustrated by concrete examples. Then, the different physical values and associated tools enabling to characterize the chemical reactors in terms of hydrodynamic and transfer efficiency will be introduced and explained. Finally, the characteristics of different types of flow reactors (commercials or not) will be exposed as well as their utilizations.

Part 2. Flow chemistry in organic synthesis (20h)

a. Flow chemistry for organic synthesis: classical reactions and transpositions from batch to flow (2h, **C. Len**).
Examples of organic reactions: oxidation, reduction, halogenation, nitration, diazotation in batch and continuous flow processes. Integration of inline, online, atline

and offline analysis. Continuous flow production of active pharmaceutical ingredients; Continuous flow production of bio-based chemicals.

b. Flow photochemistry (4h, **B. Laroche**)
This lecture will emphasize the chemical reactions promoted by the absorption of light through the prism of flow chemistry. At first, the principles of photochemistry will be explained (absorption and emission of radiation), as well as the light irradiation effect in flow systems. This will lead to study the chemical reactivity of molecules at the excited state via direct photochemistry and photocatalysis. Finally, case studies in flow and batch systems will be analyzed.

c. Flow electrochemistry: (4h, **F. Bedioui**)
(i) basics on electrochemistry and more specifically how to integrate the characterization of redox species byelectrochemistry in the implementation of quantitative electrolysis
(ii) application in continuous process: how to design electrodes and implement them in flow cells

d. Highly reactive intermediates in flow (4h, **C. Lescot**)
(i) reactions with gases as reagents, products or by-products, high pressure reactions, in-situ formation of gazeous intermediates, in continuous flow/ reactions with toxic/explosive reagents or intermediates (ii) basics of organometallic catalysis, specificities in continuous flow and advantages of heterogeneous catalysis with the different types of reactors (packed bed reactors, surface functionalization)

e. Plasmas (2h, **M. Tatoulian**)
Basics on plasma processing of materials– Plasma technology to engineer chemical reactions in microreactors

f. Other integrated technologies (4h, **C. Len**)
Ultra-sound, microwave, ball-milling and application in biomass valorization. Description of different innovative technologies and their integrations in continuous flow varying different parameters such as residence time, reactor design, source, temperature, pressure... Choice of the innovative technologies in function of the organic reactions/catalysis. Examples of organic reactions/catalysis applied to biomass and bio-based chemicals.

Part 3. Applications (10h)

a. TD 1: energy and matter transfers in flow systems (1h30, M. Zhang)
TD 2: transposition of classical reactions from batch to flow (1h30, M. Zhang)
TD 3: photoredox catalysis and applications to flow chemistry (1h30, B. Laroche)
TD 4: electrochemistry and applications to flow chemistry (1h30, F. Bedioui)

b. Presentation, visit and demonstration of flow reactions at ParisFlowTech platform (Presentation: **M. Tatoulian** (2h); demonstration: **S. Ognier** or **M. Zhang** or **R. Radjagobalou** (2h)).

Part 4. Conferences (6h) *not submitted to examination*

a. Industrial lecture: flow chemistry for pharmaceuticals (2h, **C. Mallia**, AstraZeneca, UK)
b. Application lecture: inorganic colloidal physical chemistry under flow (2h, **A. Abou-Hassan**, SU)
c. Academic lecture: flow photochemistry (2h, **T. Noël**, U. Amsterdam, NL)

Timing and speakers (total : 44h)

Teachers: B. Laroche (ESPCI, 7h30), S. Ognier (Chimie Paris, 6h), C. Len (Chimie Paris, 6h), F. Bedioui (Chimie Paris, 5h30), M. Zhang (Chimie Paris, 3h), C. Lescot (Chimie Paris, 4h), M. Tatoulian (Chimie Paris, 4h).

Extra: Demonstration at the platform (2h: S. Ognier or M. Zhang or R. Radjagobalou).

External speakers: C. Mallia (AstraZeneca, UK, 2h), T. Noël (U. Amsterdam, NL, 2h), A. Abou-Hassan (SU, 2h).

Assessment methods : final exam (70%) – continuous (30%)
1) Final exam will consist of questions and exercises related to part 1 (30 min) and part 2 (1h30) of the module.
2) Continuous assessment will consist in the analysis of 2 publications related to themes 2a-f (the student will choose the publications that he wants to report between the different activation methods a-f).

Course 2 : Valorization of Small molecules

Objectives

This set of courses ambitions to give the students a general overview about the state of the art and current challenges in the field of small molecules, from their capture to their catalytic transformation. The vast majority of existing courses focus either on sole gas storage or separation issues or alternatively discuss only their catalytic conversion (e.g. H_2 production, CO_2 reduction). To our knowledge, there is no master level formation that gathers both approaches. Both point of views are strongly related and complementary and most likely any major future breakthrough that will come out shall rely on such integrated approaches. In addition, instead of typically focusing on a specific catalytic transformation (e.g. electrochemical or photocatalytic, homogenous) or relying on a given class of catalysts (homogenous or heterogeneous, dense or porous materials, inorganic, hybrid or organic), a global overview of the field within pros and cons for each class of materials is proposed in order to enable students to possess a comprehensive and fair vision of this domain of major importance for the energy transition.

Teachers :

-Chimie Paris Tech : G. Lefèvre (CR CNRS)

-Collège de France : A. Grimaud (CR CNRS), C. Mellot-Draznieks (DR CNRS), M. Fontecave (PR)

-ESPCI/ENS : G. Mouchaham (CR CNRS), C. Serre (DR CNRS)

Prerequisites

Kinetics, electronic properties of solids, introduction to electrochemistry (redox reactions, Nernst potential, Tafel slopes etc.), basic organic chemistry knowledge, basics in coordination and organometallic chemistry (electronic structure of transition metal complexes, elementary steps in organometallic chemistry), basics on porous materials and their sorption properties.

Course structure :

General considerations (4h)

- CO_2 cycle (2h) GM : A general introduction about the CO_2 cycle will be given from emission to the capture, transport and utilization of CO_2, including a brief techno-economic point of view.

- H_2 production : (2h) AG : A general introduction about hydrogen will be given from production, to transport and utilization, including a techno-economic stand-point.

Basics (4h):

(i) Materials synthesis, stability: give a brief introduction for each class of materials (2h each for inorganics, MOFs, complexes/organics) AG/CS/GL

(ii) Electrocatalysis, photocatalysis (e.g. interfaces (charge transfer, separation) (2h each) AG, CM

Adsorption/separation (10h)

- Gas storage (H_2, CH_4…) : a general introduction about gas storage and its related applications will be first given. One will then deciphers the different mechanisms of interactions (chemisorption, physisorption) and analyse the advantages and limitations of each class of inorganic, hybrid or carboneous, dense of porous materials and related composites (2h) CS

- CO_2 capture (CO_2/N_2, CO_2/CH_4) (3h) GM : following the general introduction about CO_2 capture, students will be given an overview about the different chemical and structural strategies to capture CO_2 from air (direct air capture) and flue gases (pre- and post-combustion) based on MOFs, in comparison with benchmark sorbents (zeolites, carbons, amine grafted solids). The basics on separation mechanisms will be discussed together with the existing and emerging separation processes. A particular attention will be also given to highlight the different parameters (stability, shaping, heat transfer…) that impact the performances of a sorbent during utilization.

- Other separations (3h) CS : Students will be given representative examples of utilization of MOFs for strategic separations (e.g. purification of biogas, H_2 production, C_2/C_3, C_6, xylene…), including a short introduction about the importance of each of these separations in industry.

- Proton conductivity (2h) (CS) : A general overview of the different strategies (functionalization with acidic groups, open metal sites, encapsulation, pore size…) to optimize the transport properties of protons within the pores of MOFs will be given.

Chemical transformation (22h)

(i) Hydrogen production, water oxidation

- **Inorganic materials** (oxides, intermetallic, nitrides) **for an electrochemical production of H_2** through water splitting (electrochemistry) (4h) : the Bronsted-Evans-Polaniy (BEP) relationship that links physical properties of solid's surfaces to the kinetics for electrocatalyzed reactions such as the HER or the OER will be discussed. Based on this relationship, students will be given the tools to select and design the best catalysts for a given reaction. As well, the principles of coupled proton electron transfer (PCET) steps during which protons and electrons are simultaneously exchanged and that are the heart of OER, HER and CO_2 reduction reactions will be discussed for adsorbates on the surface of heterogeneous electrocatalysts. Finally, the impact of weak interactions such as hydrogen bonding networks or cation-water interactions at the solid/liquid interface on the kinetics of the OER and HER will be given, providing a molecular picture for interfacial reactions that is complementary to the one based on the sole physical properties of heterogeneous electrocatalysts.

- **MOFs for water splitting or O_2 oxidation :** (4h) CS + CM : the class of metal-organic frameworks will be introduced in the context of photocatalytic applications of OER and HER, with a specific emphasis on MOFs and related composites capable of capturing light in the visible. This course will cover the interest of using (i) selected MOFs intrinsic photoactive character and (ii) how take full benefit from their inherent porosity for the immobilization of catalysts (molecular species, nanoparticles, metal doping…) for water oxidation purposes, providing stable heterogeneous photocatalysts, highlighting the various synthetic strategies (one-pot-synthesis, encapsulation, covalent grafting), while discussing issues related to their solid-state characterizations and computational chemistry, their stability/recyclability, their interfacing (heterojunctions, 2D materials…), and finally pointing to their specificity in terms of reactions mechanisms when compared to their homogenous analogues.

(ii) CO_2 reduction

- **Molecular complexes, organic catalysis** (3h) GL : Molecular systems allowing the activation of CO_2 and H_2 under homogeneous catalytic conditions will be discussed. An overview of the state of-the art will be given, covering both transition-metal-based catalysts (with a particular focus on non-noble-metals such as Fe, Ni, Cu) and organocatalysts (e.g. N-Heterocyclic Carbenes (NHCs), Frustrated Lewis Pairs (FLPs)). Several transformations will thus be presented, e.g. the reduction-functionalization of CO_2 into valuable chemicals, the use of CO_2 as a C_1 building-block in fine chemical synthesis, as well as catalytic hydrogenation of organic compounds using either H_2 or one of its surrogates (formic acid, Hantzsch esters, …). An important focus will also be put on the different strategies available to promote the interconversion of CO_2 with related C_1-building blocks such as formic acid or methanol.

- **MOFs (and composites)** (4h) CM + GM : This part will focus on the progress of MOFs and related composites for the CO_2 conversion encompassing the photocatalytic reduction, with a specific emphasis on robust high valence MOF capable of capturing light in the visible, as well the electrochemical or hydrogenation assisted CO_2 reduction. The different strategies to produce photoactive MOFs together with the different routes encompassing MOFs as versatile platforms for the heterogenisation of molecular or nanoparticulate species will be described (co-catalysts, promotors, photosensitizers, etc.), with the pros and cons of this family of materials to be systematically discussed. The specificities of porphyrinic MOFs will also be covered together with mechanistic aspects through computational approaches. Finally this course will end with short overviews about more recent concepts such as of the FLP-based strategies into MOF chemistry for the conversion of small molecules or (ii) the global concept of “capture & conversion”.

- **Nanostructured inorganic materials** (3h) MF : the importance of CO_2 conversion with respect to the new energy technologies will be discussed to illustrate its impact on CO_2 mitigation, energy storage and carbon utilization, as well as the fundamental aspects of CO_2 reduction. Currently the most efficient catalysts for the electroreduction of CO_2 are solid materials. The different metals will be compared in terms of their reaction mechanisms and their resulting selectivity. A specific focus will be made on copper-based materials as they are unique in catalyzing CO_2 conversion to multicarbon compounds such as ethylene or ethanol, two key products of the chemical industry. Various strategies aiming at tuning the efficiency and selectivity of

heterogeneous catalysts, in particular copper-based ones, will be presented: (i) nanostructuration of surfaces; (ii) activation of surfaces with small ligands; (iii) surfaces with isolated metal sites; (iii) heterogeneized molecular catalysts etc. Finally part of the class will be devoted to the description of technological devices (electrolyzers, flow cells, membrane electrode assemblies) which are specifically designed for CO_2 reduction and of some examples of such cells coupled to solar panels in order to achieve artificial photosynthesis.

- Introduction to the activation of other small molecules (e.g. alkanes, N_2, NO_x…) (2h) GL : a short overview of the principles and strategies enabling the activation of N_2 and of "inert" C-H bonds from small hydrocarbons (methane, ethane, …) will be discussed. Classic transition-metal-based systems will be presented. A focus will be put on the correlation between the electronic structures of those complexes and their activity towards the targeted molecules. This course will be complemented by an overview of the current strategies to utilise MOFs (e.g. with open metal sites, immobilization of nanoparticles…) and related composites in order to activate small molecules. GM (2h)

Practical courses (4 h) (to be confirmed)

(iii) Photocatalytic production of H_2 from solar light simulator and water (ENS)

(iv) Electrochemical reduction of CO_2 or H_2 production (ENSCP)

Seminars (2 h)

Seminar given by an expert in N_2 transformation or in CO_2 capture / conversion.

Course 3 : Dynamic and Reconfigurable Polymers and Soft Materials

Objectives:

The objective of this course is to give students an overview of the engineering of dynamic and reconfigurable polymers in materials and biomimicry. We offer an interdisciplinary approach to soft matter and polymers: from molecular / macromolecular chemistry to physicochemical and mechanical properties.

The following systems and/or concepts will be covered:

- Synthesis, characterization and specific properties of dynamic covalent polymer networks
- Sequence-controlled and semi-crystalline polymers: organization, interfaces, specific properties
- Impact of the presence and spatial organization of dynamic bonds onto the properties and processing of dynamic covalent polymer networks
- Responsive polymers: gels and interfaces
- Light-responsive assemblies
- Soft materials based on thermotropic and lyotropic liquid crystal polymers

Prerequisites:

Basics in polymer and soft matter: chemistry, physicochemical and mechanical properties, thermodynamics.

Content of the class:

Part 1: Synthesis, chemistry and characterization of dynamic covalent polymer networks (10 hrs, RN)

In this part, we will discuss the different synthetic routes that can be followed to prepare dynamic covalent networks, including the direct polymerization of functional monomers, the crosslinking of functional thermoplastics and the reactive processing of conventional (un-functional) thermoplastics. Both fundamental and practical aspects will be covered. The fundamentals of dynamic covalent chemistry (kinetics, thermodynamics, stimuli) will be presented in the context of polymer networks. The characterization of dynamic covalent polymer networks will be presented and the specific properties of these materials, such as reshapeability, recyclability, self-healing ability, will be illustrated.

Part 2: Sequence-controlled and semi-crystalline polymers: organization, interfaces, specific properties (8 hrs, FT)

In this part, we will discuss systems where the regularity of the polymer chains induces cooperative assembly mechanisms. While providing a high degree of cohesion, promoter of macroscopic properties such as rigidity, resistance to creep, low solubility, low diffusivity to molecules and gases, these interactions remain essentially non-covalent and reversible. Another of their characteristics is to be specific without however requiring any particular chemical function. They are also found at work both in polyethylene, the simplest polymer imaginable, and in complex sequences composed exclusively of functional monomers such as collagen.

Two main families of systems will be covered:

1 - semi-crystalline polymers and vitrimers

2 - sequence-controlled synthetic polymers (“precision polymerization)

Part 3: Dynamic bonds: from the molecule to processing and final material properties (8 hrs, CC)

The objective of this part is to acquire the basic vocabulary and notions to understand how the properties and processing of materials are affected by the presence and spatial organization of dynamic bonds. The idea is to connect molecular concepts like bond energy, entropic elasticity, bond lifetime and force-activated scission, with macroscopic properties such as viscoelasticity and viscosity, fracture toughness, energy dissipation upon cyclic loading. Special effort will be made to introduce two advanced topics:

1 - the notion of non-linear properties: from finite chain extensibility to macroscopic strain stiffening. Role of the network architecture on the macroscopic properties.

2 - the incorporation of mechano-sensitive molecules in networks to detect and quantify forces on bonds and bond scission with optical signals.

Part 4: Responsive polymers: gels and interfaces (8 hrs, YT)

The objective of this part is to provide an overview of responsive polymers. We will discuss how to drive molecular interactions to induce reversible macroscopic change in structure and properties. We will focus on responsive gels and interfaces and will address some innovations for soft materials and biotechnologies.

1 - Responsive properties

How does change of conformation at molecular scale induce change of macroscopic properties (in solutions or at interfaces)?

Which stimuli? Temperature, pH, salt, light, electric or magnetic field…

Which polymers? How to play with weak interactions? Dynamic bonds. Reversibility. Intermolecular interactions with weak energy (hydrogen bond, electrostatic, hydrophobic).

Responsive polymers. Good/Bad solvent. LCST/UCST. Polyelectrolyte, counterions, osmotic pressure.

2 - Responsive hydrogels

Architecture of hydrogels. From molecules to polymer networks. Simple and more complex networks. Physical and chemical crosslinks. Applications to injectable hydrogels

3- Responsive interfaces

Polymer thin layers. Hydrogel films. Synthesis and characterization. Physico-chemical properties. Applications to sensors and actuators

Part 5: Light-responsive assemblies (6 hrs, CT)

Light-responsive organic assemblies have important developments in the biomedical field (optogenetics, phototherapies) and in material science (nanomotors, optical devices). The control of complex, dynamic systems by light offers a remote, non-invasive trigger, that can easily be applied with high spatial and temporal resolution. This part will cover up-to-date methods and design strategies of light-switchable surfactant-based and polymer-based systems. Lectures and (a few representative) case studies will review:

- the main classes of molecular switches, i.e. photoconversion of light-sensitive groups (photochromes, photocages) and use of nanoparticules to generate photothermal or photocatalytic reactions;

- the principles and practical constraints to achieve amplification from molecular up to macroscopic scale via perturbation of interfacial assemblies, phases separation, sol-gel transitions, with application in actuation;

- recent illustrations of out-of equilibrium dynamics (microflow, microswimmers), emphasizing the fundamental difference between quasi-equilibrium evolution between (photo)stationary states and dissipative systems.

Part 6: Smart soft materials based on thermotropic and lyotropic liquid crystal polymers (8 hrs, M-H L)

In this part, we will treat liquid crystal (LC) systems of polymers, which exhibit exciting potential as smart soft materials.

Two main families of systems will be covered:

1 - Thermotropic LC polymers and elastomers as soft actuators and sensors

Thermotropic liquid crystals are typically fluids made of relatively stiff and rod-like molecules (called mesogens) with long-range orientational order. The simplest LC phase is the nematic phase, in which the mean ordering direction of the mesogens is uniform. Long polymer chains incorporating mesogens in their chemical structures can also form a nematic phase (nematic polymers). The anisotropic characters (self-organization) of LC polymers and their conformational changes (entropic elasticity) upon external stimuli are the key to the exceptional properties of materials made of LC polymers and elastomers. We will discuss in detail some examples of actuators and sensors made of LC polymers and elastomers.

2 - Lyotropic LC polymers: amphiphilic block copolymers self-assembled in water

In this part we will focus on polymer micelles and vesicles, which belong to the normal (oil-in-water) self-assembled nanostructures, and polymer cubosomes and hexosomes, which belong to the inverted (water-in-oil) self-assembled nanostructures. These polymer colloids have diameters, membrane thicknesses or lattice sizes of up to one order of magnitude higher than small molecular colloids. More interestingly, the colloidal properties can be adjusted by the almost unlimited possibilities offered by polymer chemistry that allow to synthesize polymers with many different chemical structures. Stimuli-responsive properties of these polymer colloids will be highlighted for potential application in controlled delivery.

Faculty:

Costantino Creton (Part 3, 8 hrs); Min-Hui Li (Part 6, 8 hrs); Renaud Nicolaÿ (Part 1, 10 hrs, coordinator), François Tournilhac (Part 2, 8 hrs), Christophe Tribet (part 5, 6 hrs); Yvette Tran (Part 4, 8 hrs, coordinator)

Evaluation:

Project of students

Analysis and discussion of research articles and/or experimental data

Course 4 : Coupling analytical techniques for *in operando* monitoring of local events

Educational goals

The development of analytical methods is closely related to advances of complementary in-situ microscopies, spectroscopies, spectrometric techniques etc…. Their combination provides a wealth of new information on structure changes, reaction pathways and local events determining and/or taking place during chemical or biological reactions. This course will gather contributions highlighting recent methodological and topical developments in the field and those predicted to be important in the near future. It will be composed of 4 parts of 12 h each, including one session of application (TD; 1,5 h) and one seminar (1,5h)

Positioning (compared to the existing offer in the M2 Chemistry Paris Centre and the other PSL masters)

Prerequisite

It is necessary to know the basics and principles of the techniques that will be discussed and deepened. Also, general culture in the field of analytical techniques in chemistry, physics and chemistry, spectroscopy will be a plus. In particular:

- Know the basics of thermodynamics and electrochemical kinetics: electrode potential, current-tension curves, load transfer, material transport

- Know the principal forces and interactions that control the performances of separation method and how to evaluate these methods in terms of recovery rate, separation selectivity, concentration factor,

- Know the physical principles of NMR and optical spectroscopies.

- Know how a simple NMR experiment is performed.

Course structure

- coupling electrochemical microscopy SECM and AFM/STM for in situ monitoring of substrate morphological changes and reactivity (Fethi Bedioui, Chimie ParisTech)

In order to enrich and complete its capacities for local electrochemical reactivity characterization, and to further increase its role in the development of nanosciences, electrochemistry has had to associate itself with, high-performance surface analysis techniques allowing, if possible simultaneously, local physico-chemical analysis in situ, with optimal spatial resolution. It is in this context that the techniques known as "probe scanning" have gradually become essential in the study of interfacial electrochemical processes, initially at the micrometer scale, and then at the nanometer or even atomic scale. Considerable efforts have been made to bring

together the electrochemistry of the two scanning probe techniques (SPM), which are only slightly older than scanning electrochemical miscroscopy SECM, namely scanning tunneling microscopy (STM) and atomic force microscopy (AFM) . These efforts have consisted in showing how these two techniques have made it possible to multiply tenfold the contributions of electrochemistry in the field of nanosciences by providing it with the means to generate, modify and above all very widely characterize nanostructured or nanofunctionalized electrochemical interfaces as well as electrogenerated nanoobjects, no longer globally but very locally with nanometric or even atomic resolution depending on the working conditions and the technique used. This course introduces precisely the AFM/electrochemistry and STM/electrochemistry couplings and their most developed applications.

- coupling of electrochemical techniques with ICP emission spectrometry, on-line volumetric measurements, gravimetric measurements for in situ investigation of interfacial reaction kinetics(corrosion/dissolution of metals and alloys) (Kevin Ogle, Chimie ParisTech)

The characterization of interfacial processes at the metal / electrolyte interface are of paramount importance for research in many fields such as corrosion, energy storage and electrocatalysis. Electrochemical measurements provide rich and meaningful kinetic information on the underlying faradaic processes but are often insufficient to identify the chemical mechanisms of these processes, limiting their utility as predictive tools. As a complement to conventional electrochemical information, we would like to know how the individual elemental constituents of a material react with the environment? What are the stoichiometries of dissolution, film formation, and electron exchange? Do alloy components dissolve selectively, leaving behind other components in the form of oxide films or dealloyed metallic layers? Can non-faradaic corrosion processes such as oxide dissolution or the release of intermetallic particles or metallic grains be detected and quantified? To this end, it is necessary to couple the electrochemical techniques with other real time analytical methods so as to quantify the elementary reactions and processes that contribute to an electrochemical response. The focus of this course will be on the coupling of spectroscopic solution analysis with electrochemistry (spectroelectrochemistry) in which the solution composition is monitored as a function of time during transient electrochemical measurements. Spectroscopic techniques such as UV-Visible, ICP atomic emission spectrometry, and ICP – mass spectrometry will be described. Significant applications will be reviewed, and the basic theory of quantification, time resolution, and transfer functions will be developed. Frequency resolved methods may also be discussed such as electrochemical impedance spectroscopy. In addition, non-spectroscopic measurements such as gravimetric techniques with a quartz crystal microbalance or real time volumetric gas measurements will be presented.

- coupling optical techniques (IR, Fluorescence) and NMR imagery (and electrochemistry) for in situ monitoring of biological events (Bich Thuy Doan, Chimie ParisTech & Laurent Thouin, ENS)

In the context of development of nanosciences in biology and medicine, spectroscopy and imagings with Optics or Magnetic Resonance are widely used as non-invasive technologies with their high specific performance to investigate

biological phenomena in living tissues. Optics provides high sensitivity to investigate the dynamic behavior of fluorescently labelled moieties and their interactions in biological environment, solutions, cells and tissues. Magnetic Resonance technologies provide structural and chemical information of organic molecules with spectroscopy and, exceptional images contrast and high 3D spatial resolution with imaging. Electrochemical commands aimed at modulating the fluorescence of molecules are also particularly exploited in this field, considering that many analytes are redox-active and can be detected/mapped with high sensitivity through fluorescence. These techniques require optical or MR probes to be grafted on molecular or nanoparticular scaffolds or can count on natural signal of intrinsic biological molecules.

In order to study with precision, the biological information investigated, couplings of the optical and MR techniques, or coupling of optical and electrochemical techniques, in spectroscopy and/or imaging via the multimodality of probes or signals, as well as multiscale couplings (photonic microscopy) will improve the diagnosis. Coupling with optics with other in vivo imaging modalities is also of interest. This course introduces Optical / Magnetic Resonance spectroscopies and imaging couplings via multimodal chemical molecular or nanoparticular probes design and presents their most developed applications in the biomedical field for biological investigation diagnosis and evaluation of innovative therapies in vitro to in vivo. The electrochemically-promoted fluorescence modulation of organic fluorescent or fluorogenic probes will also be addressed to investigate important biological mechanisms and to monitor biological events.

- coupling multidimensional separations and detections (optical, electrochemical detection, mass spectrometry) towards integrated microfluidic devices (Fanny d'Orlyé, Chimie ParisTech)

In order to address the issue of analyzing always more complex samples, and to further increase their role in environmental and health sciences, separation methods (chromatographic or electrokinetic) must move towards multi-dimensional strategies as well as coupling with specific detection technologies to monitor the separation process but also consider complementary aspects, such as speciation, based on molecular (mass spectroscopy MS), functional (UV/Vis, Fluorescence, Electrochemistry) or elementary (ICP-MS) characterizations. Coupling two separation dimensions and separation to detection techniques is a real challenge, both from theoretical and technical points of view. To do so, analytical conditions must be optimized with regards to each operatory unit while being compatible with one another and coupling interfaces must preserve the overall analysis stability et performance at each step. In this context, perspectives offered by the miniaturization of analytical systems and the development of multiparametric microfluidic devices may enable to overcome several afore-mentioned challenges. Resulting multi-dimensional mapping are unprecedent with regards to the very high resolving power of multi-dimensional analysis. Nevertheless, it addresses the topic of data analysis, which is a critical component of any 2D-separation workflow.

Course 5 : Dynamics of molecular processes in biological systems

Goals

- 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.

Pre-requisites

(essential)

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

(recommended - some bibliographic references can be suggested)

Vector model of NMR
Classical mechanics (Hamiltonian, Lagrangian)
Basic notions of molecular biology (biomolecules, structure)

Syllabus

General introduction, overview of the class (GS - 1h)

1. *Key concepts, experimental and simulation techniques (34 h - CM 28h, TD 6h)*

<u>Concepts and theories</u>
Master equations for the study of dynamical processes (GS - CM 4h, TD 2h)
Kinetic models for enzymatic catalysis (DL - CM 2h, TD 1h)
Conformational motions, allostery, importance of transport and transfers in the cell (AT - CM 2h)
Chemistry of systems: kinetics and stoichiometry (PN - CM 3h)
Phase separation in biomolecular systems (FF - CM 1h)

Experimental tools
Biomolecular dynamics from microseconds to seconds from chemical exchange NMR (FF - CM 4h, TD 1h)
Overview of other techniques // cryoEM, FRET, etc. (FF - CM 1h)
Microfluidics for controlled environments, analytics tools for dynamical networks (PN - CM 1h)

Simulation tools
Enhanced sampling techniques (EDD - CM 4h, TD 2h)
Tools for reactivity, EVB, QM/MM (DL - CM 4h)
Indirect dynamic techniques, NMA, PCA (AT - CM 2h)

2. Practical cases from the literature, key questions and challenges (5h)

5x1h devoted to 1 topic (FF, PN, DL, GS, EDD - 1h each), may include (TBD):

- Dynamical effects in enzymatic catalysis;
- Allostery: positive, negative allostery, long-range effects of mutations (lac operon?);
- Transport across the membranes: water, ions, NMs, nuclear pores;
- Networks of genetic regulations.

3. Hands-on sessions: basic simulations, projects (7h)

- Basic simulations and illustration the class' concepts: potential of mean force, kinetics of barrier crossing, NMA, clustering, Markov models, interpretation of NMR data (DL 2h, GS 2h, EDD 1h, FF 1h)

- Mini-projects based on literature and/or PI's work, each project includes some numerical analysis or very basic simulations. Max 6 groups/projects (1 per PI), 1-hr tutoring along the way. Short report and 2-hr poster session (GS - 2h)

Faculty

- Élise Duboué-Dijon, IBPC (CNRS) (8h)
- Fabien Ferrage (Assoc. Prof. ENS) (8h)
- Damien Laage (Assoc. Prof. ENS) (10h)
- Philippe Nghe (Assoc. Prof. ESPCI) (6h)
- Guillaume Stirnemann, IBPC (CNRS) (12h) - coordinator
- Antoine Taly, IBPC (CNRS) (4h)

Exams

Final exam (50%)
Mini-project (30%)
Continuous evaluation (20%)

Course 6 : Modeling and understanding of reaction processes

Contributors :

Theory : Ilaria Ciofini (i-CLeHS, ChimieParisTech), Frédéric Labat (i-CLeHS, ChimieParisTech),

Experimental approaches : Guillaume Lefèvre (i-CLeHS, ChimieParisTech), Laurence Grimaud (LBM-ENS), Maxime Vitale (LBM-ENS)

Objectives:

The aim of this module is to provide, through a limited number of key reactions in organometallic catalysis (cross-couplings catalyzed by Pd, Fe or Ni, Cu-catalyzed hydroamination of unsaturated derivatives), an overview of the experimental and theoretical approaches that can be used and combined to untangle complex reaction mechanisms.

From an experimental point of view, we propose to address different analytical techniques (spectroscopies, multinuclear NMR, cyclic voltammetry...) allowing to access structural, functional or kinetic data in order to propose structures of reaction intermediates or reaction mechanisms which are then compared and completed by theoretical predictions in order to rationalize a given catalytic process. Several examples will also be provided to present the experimental approaches adopted to rationalize a reaction mechanism on the basis of kinetic data (in particular determination of kinetically determining steps, use of Hammett correlations). Reminders of formal kinetics will also be given at the beginning of the course.

From a theoretical point of view, ab-initio approaches (DFT and post-HF) and their coupling with methods to describe the environment (solvation models, QM/MM approaches) will be illustrated by considering the reactions in homogeneous phase (solution) previously mentioned as an example. The possible extension of these methods to the description of the reactivity in confined or supported environment (heterogeneous catalysis) will also be briefly illustrated. Particular attention will be paid to the modeling of photo-activated reactions (photocatalysis) and to the methods allowing to describe the reactivity in the excited state.

Each student will also develop a bibliographic project on recent systems from the literature (8h).

A series of 4 seminars, given by invited researchers, will be organized in order to illustrate the state of the art and challenges in current research (4x2h).

Course structure : 8 h bibliographic project; 8 h seminars; 16 h experimental approaches; 16 h theoretical approaches

Prerequisites: Basic Organic and organometallic chemistry course (M1)

Evaluation : Written exam (70%), bibliographic project restitution (30%).

Course 7 : Optical Materials, from Design to Devices

Objectives: Inorganics and hybrids materials for optical applications such as photovoltaic, lighting, quantum information, imaging, sensor, etc. are developed under various shapes and sizes. These lectures will focus on the design; modelling preparation and practical use of these materials.

Detailed content:

Part 1: Photovoltaic materials and technologies: Introduction to semiconductors and to semiconductor junctions; fabrication of photovoltaic devices and panels; emerging technologies (Th. Pauporté, CNRS, Chimie Paristech) (9h including one seminar and one practical course) **and Modelling for photovoltaic**: electronic structure of semiconductors (bulk and interfaces; effect of defects); modelling of hybrid systems and properties (Frédéric Labat, Chimie Paristech) (3h)

Part 2: Engineering of colloidal optical inorganic nanomaterials. Semiconductor and metal nanocrystals, synthesis, surface and interface, functionalization and applications (T. Pons, INSERM, S. Ithurria, ESPCI) (12h including one seminar and one practical course).

Part 3: Color and colorimetry, LED and Laser chemistry and technologies, strategies and mechanisms of luminescence stimulation; (mechanoluminescence, OSL, thermoluminescence); (B. Viana, CNRS, Prof Attaché, Chimie Paristech) (12h including one seminar and one/two practical course)

Part 4: Switchable hybrid materials: spin crossover, photomagnetism, porosity, chemosensing (A. Tissot, CNRS, Prof Attaché, ENS) (6h) **Materials for optical quantum technologies**: 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) (6h)

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

Evaluation : Written exam and oral for retaken exam

Course 8 : Databases and statistical learning for chemical discovery

Objectifs pédagogiques :

- Repérer les types de données produites au cours d'une activité de recherche, les métadonnées associées et les enjeux de leur conservation
- Connaître les principales bases de données existantes en chimie
- Comprendre la méthode d'apprentissage statistique utilisée dans des travaux publiés, son mode de fonctionnement et ses limitations
- Mettre en œuvre une méthode d'apprentissage statistique sur des données de chimie

Positionnement (par rapport à l'offre existante dans le M2 Chimie Paris Centre et les autres masters de PSL) : pas d'UE spécifique sur les données, bases de données et apprentissage statistiques dans le M2 Chimie Paris Centre. Dans les autres masters, l'offre est essentiellement soit disciplinaire (physique, pharma, etc), soit très théorique (maths appliquées, informatique).

Prérequis : mathématiques de premier cycle (algèbre linéaire), formation M1 de chimie physique ; pas de prérequis stricts sur la chimie théorique, mais une formation M1 sera un plus.

Structure du cours :

- Bases théoriques (16 h)
  - Les données en chimie : métadonnées, stockage et curation, API
  - Les bases de données existantes : matériaux, molécules ; théoriques, expérimentales ; structures, propriétés
  - Fondamentaux de l'apprentissage statistique : machine learning, deep learning
  - Données et reproductibilité, démarche open science
- Cours-conférences sur les applications (16 h)
  - Relations structure/propriété, structures/activité ; méthodes QSAR/QSPR
  - Machine learning pour la chimie théorique : fonctionnelles, champs de forces réactifs, exploration et variables collectives, etc
  - Criblage à large échelle pour applications pharma, docking et méthodes avancées
- Projets par binôme (16 h)

Intervenants : François-Xavier Coudert, Carlo Adamo, Damien Laage, Jérôme Hénin, Maximilien Levesque / Aqemia

Modalités d'évaluation :

- 50% sur un examen écrit, portant sur les bases et les applications
- 50% sur la présentation des résultats de leurs projets

Course 9: Magnetic Resonance

Objectives:

- Give chemists the foundations to understand magnetic resonance (MR) spectroscopies and how MR can be used in many fields in chemistry, physics, and biology.
- Introduce MR spectroscopies (NMR and EPR) using a theoretical quantum mechanical framework
- Give chemists a link between the observables of magnetic resonance and molecular structure, dynamics, molecular orbitals and other chemical properties.
- Introduce the use of MR in various fields of research, ranging from materials, biological systems, cultural heritage, etc.

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

Contents of the class:

Part 1: Fundamentals of Magnetic Resonance (8 hrs)
Vector model; quantum description; tensors notation; Hamiltonians of spin interactions (chemical shift; *J* coupling; dipolar couplings; quadrupolar interaction; *g* tensor; hyperfine interaction); General instrumentation aspect (magnet / rf / console)

Part 2: Dynamics and Relaxation (7 hrs)
Chemical exchange; Wangsness-Bloch-Redfield theory of nuclear spin relaxation; Overhauser effect; Effects of dynamics in solution EPR; Overhauser DNP

Part 3: Continuous wave EPR (8 hrs)
Relevant systems and examples of applications; Instrumental and practical aspects; Physical interactions and spin Hamiltonian; EPR in fluids and isotropic interactions; EPR in solids and anisotropic interactions; Systems with spin >½; CW Electron Nuclear Double Resonance

Part 4: Time Domain Magnetic Resonance (16 hrs)
Product operators; coherence transfer; 2D NMR; Magic angle spinning; cross polarization; MQMAS; average Hamiltonian theory: Recoupling techniques; Pulsed EPR (Davies/Mims ENDOR/Hyscore)

Part 5: Hyperpolarization Techniques (6 hrs)
Dynamic nuclear polarization; optical pumping; ferromagnetic resonance

3 hours will be devoted to presentations by students and invited speakers (not included in syllabus)

Faculty:
Laurent Binet (8 hrs); Jean-Baptiste d'Espinose (10 hrs); Fabien Ferrage (coordinator; 12 hrs); Kong Ooi Tan (*future* coordinator, 15 hrs)

Evaluation:
Project (40 %)
Mid-term exam after part 3 (20 %)
Final Exam (40 %)

Course 10 : Entrepreneurship and Innovation (60h)

PSL's transverse innovation and impact entrepreneurship training program is a high-level program that combines classroom and distance learning courses. It is designed for master's, doctoral and post-doctoral students who want to learn the fundamentals of innovative design methods and the challenges of designing entrepreneurial projects in the field of scientific research. Combining a theoretical approach and design workshops in small groups, it allows students to work on concrete cases of invention development or impact entrepreneurship projects.

OBJECTIVES OF THE TRAINING

The objective of this cross-disciplinary training is to enable students to acquire the skills that will allow them to think about an innovation project and to design a business model strategy

- **Thinking an innovation project:** by acquiring the methods of innovative design applied to a scientific entrepreneurship framework;
- **Designing a business model strategy:** by studying the main business models and knowing how to apply them to concrete situations;

ORGANIZATION OF THE COURSE

With the exception of the course "Reasoning and acting in the unknown" which takes place in person during PSL week, the courses have been designed in blended learning: alternating asynchronous learning sessions at the student's own pace, and synchronous sessions in the presence of the teacher. The 60-hour cross-disciplinary training is organized around 2 main courses:

- **The unknown:** introduction to theories and methods of design and innovation (3 ECTS, 30h in-class)
- **Business model thinking for impact entrepreneurship** (3 ECTS, 17h synchronous, 13h asynchronous)

CALENDAR

Période	Titre	Enseignants	Établissement	Rythme	Volume horaire	ECTS
22/11/2021 - 26/11/2021	Reasoning and acting in the unknown: introduction to theories and methods of design and innovation	Pascal Le Masson Benoit Weil	Mines Paris-PSL	Full week (9h-17h)	30h	3
3/12/2021 - 21/01/2022	Business model thinking for impact entrepreneurship	Lionel Garreau	Dauphine Paris-PSL	3h par per week for six weeks (Fridays 9h-12h)	30h	3

PROGRAM

1. **Reasoning and acting in the unknown: introduction to theories and methods of design and innovation** (3 ECTS)

This 30-hour face-to-face course, organized during PSL Week in November 2021, is an in-depth introduction to the foundations of CK theory and innovation management methods for learners wishing to enter innovation and scientific entrepreneurship programs. Alternating theoretical classes in the morning and application workshops in the afternoon, it will begin with a presentation of design theory and the challenges of thinking in the unknown, then will provide a history of the place of RID (research, innovation and development) in companies. He will then present the principles and functioning of the CK theory, to lead the learners to implement the CK method of innovation management applied to concrete cases. The course will continue on the links between design and science, and will then address the subject of the mission-based company in the context of the governance of the innovative company.

2. **Business model thinking for impact entrepreneurship** (3 ECTS)

This course is structured around 6 synchronous sessions of one to three hours, and asynchronous work sessions using selected readings and videos produced by the teachers. It will start with a definition of the business model concept, and then present the four main business model analysis models: the Business Model Canvas, the RCOV, the Causal Loop and the Triple Layer Business model Canvas. These models will be used to analyze practical cases of impact businesses. The course will continue with a presentation of ESG factors (environmental, social and governance) which will lead to the production of a wiki by the learners on the links between business model and impact entrepreneurship. Based on role-playing, analysis of practical business cases and interviews with entrepreneurs, learners will then be led to articulate the business model strategy in a business ecosystem and to anticipate the dynamics of business model development.

EVALUATION

Students are evaluated on:

- Attendance and participation during classes (15%)
- The completion of knowledge control quizzes (25%)
- The realization and the defense of a project in team or individual (60%)

TRAINING LOCATIONS

Mines Paris-PSL
Dauphine Paris-PSL
PSL-Lab