Chemistry

Master degree

Integrative Chemistry and Innovation

Course syllabus - M1 level

2023-2024

Course list

	ECTS	Hours	Grading coefficient
Semester 1	**30**	**245**	
Basics	**19**	**171**	
IMP-Basics : Introductory Mathematics and Physics	3	27	1
MDST-Basics : Molecular Design and Synthetic Tools	4	36	1,25
APC-Basics : Analytical and Physical Chemistry	4	36	1,25
TCM-Basics : Theoretical Chemistry and Modelling	4	36	1,25
SMC-Basics : Smart Materials Chemistry	4	36	1,25
Innovation & Soft skills	**11**	**74**	
Transdisciplinary & innovative project	4		1,25
Innovation & entrepreuneurship	4	50	1,25
Design Thinking	*3*		*1,25*
i-Teams	*1*		*validation*
Language	3	24	1
Semester 2	**30**	**208**	
Chemistry Advanced – Common Courses	**5**	**60**	
MDST-Advanced : Molecular Design and Synthetic Tools	1	12	0,5
APC-Advanced : Analytical and Physical Chemistry	1	12	0,5
TCM-Advanced : Theoretical Chemistry and Modelling	1	12	0,5
SMC-Advanced : Smart Materials Chemistry	1	12	0,5
ICM-Advanced : Introduction to chemometrics	1	12	0,5
Chemistry - Advanced - Elective Courses (3 courses to be selected)	**9**	**approx. 72**	
Inorganic Materials	3	29	1
Inorganic chemistry: from molecules to materials MH24OP.NOR			*0,5*
Synthesis of Inorganic and Hybrid Materials (ESPCI)			*0,5*
Soft Matter and Development (ESPCI)	3	26	1
Electronic Properties of Solids MH24OP.PES	3	22,5	1
Physical Chemistry for Bio-systems	3	25	1
Biointerfaces MH24OP.BIF			*0,5*
Colloids and Biomolecules (ESPCI)			*0,5*
Bio-Analytical Chemistry MH24OP.BIA	3	24	1
Chemical Biology	3	26	1
Organometallic Chemistry	3	27	1
Heteroelements MH24OP.HC			0,5
Bioinorganic chemistry MH24OP.CBI			0,5
Advanced Theoretical and Computational Chemistry	3	24	1

Innovation & soft skills	**6**	**76**	
Innovation & entrepreuneurship : Desing Thinking & i-Teams	4	58	1
Design project	*3*		*1*
i-Teams	*1*		*validation*
Language	2	18	0,75

Introduction to research	**10**		
Pre-internship project & seminars	1		0,75
Internship	9	≥ 3 months	3

SEMESTER 1

Basic science courses

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S1</td><td colspan="2">Course Title: Introductory Mathematics and Physics - Basics</td></tr>
<tr><td colspan="2">Keywords: mathematics, quantum physics, crystallography</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">F. Labat (frederic.labat@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">L. Binet (laurent.binet@chimieparistech.psl.eu), F. Labat (frederic.labat@chimieparistech.psl.eu), P. Loiseau (pascal.loiseau@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 3</td><td>Total teaching hours : 27 h</td><td>Grading: final written exam (100%)</td></tr>
<tr><td colspan="4">Course description and content

This module introduces the main concepts in mathematics, quantum physics and crystallography necessary to follow the Integrative Chemistry and Innovation track of the Graduate Program in Chemistry.
The training is based on three main courses: mathematics (9h), quantum physics (12h) and crystallography (6h), which are each presented with illustrating examples and exercises in class.
The main concepts covered are:
- in mathematics: linear algebra, Hilbert spaces and Fourier transform
- in quantum physics: postulates, potential wells and barriers, harmonic oscillator, angular momenta
- in crystallography: crystal lattice, point symmetry, space groups, international tables for crystallography</td></tr>
<tr><td colspan="4">Learning goals
The student should be able to:
- know the basic concepts of quantum physics and chemistry, such as linear algebra, Hilbert spaces, eigenfunctions, hermiticity and Fourier transform
- understand the main concepts of quantum physics and calculate the properties of simple quantum systems
- describe the symmetries of crystals and their structures using the international tables for crystallography.</td></tr>
<tr><td colspan="4">Pre-requisites
- basics of linear algebra (matrices and operations on matrices, matrix diagonalization, vector spaces, scalar product), 1^{st} and 2^{nd} order linear differential equations.
- basics of classical physics: momentum and angular momentum, kinetic and potential energies, conservation laws, elementary electrostatics and magnetostatics, electromagnetic waves
- basics of Euclidian geometry: scalar and vector products, equation of plane and line</td></tr>
</table>

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S1</td><td colspan="2">Course Title: Molecular Design and Synthetic Tools – Basics
Subtitle: Synthetic Molecular Chemistry and Biochemistry</td></tr>
<tr><td colspan="2">Keywords: C-C bond formation, asymmetric synthesis, organometallic chemistry, biochemistry</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Guillaume Lefèvre (guillaume.lefevre@chimieparistech psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Yann Verdier (yann.verdier@espci.psl.eu), Guillaume Lefèvre (guillaume.lefevre@chimieparistech psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 4</td><td>Total teaching hours : 36 h</td><td>Grading: final written exam (100%)</td></tr>
</table>

Course description and content

This course is divided into 3 units:

a) Basics in organic chemistry (13h)

Contents: 2 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.

b) Basics in organometallic chemistry (12h30)

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 (10h30)

Contents: the chemistry of life; Nucleic acids; Amino acids and proteins; Carbohydrates; Lipids and cell membranes

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 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 biochemistry / organometallic courses.

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S1</td><td colspan="2">Course Title: Analytical and Physical Chemistry – Basics</td></tr>
<tr><td colspan="2">Keywords: solution chemistry, separation sciences, electrochemistry, molecular spectroscopy, analytical methods</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Fethi Bedioui (fethi.bedioui@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Fethi Bedioui (fethi.bedioui@chimieparistech.psl.eu), Anne Varenne (anne.varenne@chimieparistech.psl.eu), Fanny d'Orlyé (fanny.dorlye@chimieparistech.psl.eu), Laura Trapiella-Alfonso (laura.trapiella@@chimieparistech.psl.eu), Fabien Ferrage (fabien.ferrage@ens.psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 4</td><td>Total teaching hours : 36 h</td><td>Grading: final exam (written)+ intermediate exam (75% and 25%, respectively)</td></tr>
</table>

Course description and content

The course aims at arming the student with fundamental concepts in solution chemistry, separation sciences, electrochemistry, and molecular spectroscopies enabling to understand and address experimental questions on how to characterize, analyze, separate molecular components in solutions or complex mixtures towards the building up of an efficient analytical method.

(i) **Solution chemistry**: Basic principles of solution chemistry: aqueous solutions (from diluted to concentrated), activity coefficient, acid/base and complexation equilibria. Control of the chemical separations (solubilisation, precipitation, liquid/liquid extraction, liquid/solide extraction) through the understanding of the reactions involved in solution. Introduction to non-aqueous solutions (micelles, molecular solvants, ionic liquids, supercritical fluids) (Anne Varenne; 6h)

(ii) **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 (Fanny d'Orlyé; 6h)

(iii) **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 (Fethi Bedioui; 6h).

(iv) **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). <u>Optical spectroscopies</u>: basics of absorption and emission, effects of structure and environment, lifetime of excited electronic states; quantum yield and non-radiative transitions; inhibition of fluorescence (Fabien Ferrage; 6h)

(v) **Building up analytical methods**: The strategies and techniques used for the construction of the whole analytical process (sampling, sample treatment, separation techniques and coupling with performant detection methods) adapted for the analysis of complex samples will be presented. Concepts such as biomarker, interferents, standard, sample matrix effects, speciation, bioassays formats, screening test and/or quantitative analysis (internal and external calibrations) will be illustrated. Finally, the concept of method/test validation and analytical quality parameters (sensitivity, LOD, LOQ, precision, trueness, etc.) will be afforded in the view of the development of new analytical strategies. (Laura Trapiella; 9h)

(iv) **Tutoring** (all instructors: 3h)

Learning goals

The student should be able to:
- Predict acid-base, complexation or precipitation reactions in a system knowing its composition,
-Control the reactions involved in solution to develop efficient chemical separations in complex mixtures
-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.
- Know the more common formats and detection methods used for the environmental and biological analysis
- Built up an adapted and efficient analytical method regarding the sampling, sample treatment and analytical determination of a given molecule/compound.

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).

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S1</td><td colspan="2">Course Title: Theoretical Chemistry and Modelling – Basics</td></tr>
<tr><td colspan="2">Keywords: electronic structure, statistical mechanics, quantum chemistry, density functional theory, thermodynamics</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Ilaria Ciofini (ilaria.ciofini@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Ilaria Ciofini (ilaria.ciofini@chimieparistech.psl.eu), Carlo Adamo (carlo.adamo@chimieparistech.psl.eu), Frédéric Labat (frederic.labat@chimieparistech.psl.eu), François-Xavier Coudert (francois-xavier.coudert@psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 4</td><td>Total teaching hours : 36 h</td><td>Grading: final written exam (67%), intermediate reports (33%)</td></tr>
<tr><td colspan="4">Course description and content

Part 1: Electronic Structure Theory (24h)
The knowledge of the electronic structure of molecules and extended systems allows for the understanding of their reactivity and properties. Here we will first 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.
Next, 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.

Part 2: Fundamentals of Statistical Mechanics (12h)
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.</td></tr>
<tr><td colspan="4">Learning goals
The student should be able to:
- understand the meaning of the Schrödinger equation
- know the common approximations used to solve the Schrödinger equation
- 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 based on frontier orbitals analysis
- know the difference between classical and quantum models
- understand the fundamentals of Density Functional Theory
- understand how one can simulate periodic systems
- 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</td></tr>
<tr><td colspan="4">Pre-requisites
BSc level in physical chemistry, quantum chemistry, thermodynamics</td></tr>
</table>

<table>
<tr><td rowspan="3">M1</td><td rowspan="3">S1</td><td colspan="2">Course Title: Smart Materials Chemistry – Basics</td></tr>
<tr><td colspan="2">Introduction to inorganic and soft materials
Keywords: : Inorganic and soft matter, hybrid materials, synthesis and characterizations</td></tr>
<tr></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Yvette Tran (yvette.tran@espci.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Bruno Viana (bruno.viana@chimieparistech.psl.eu)
Michel Cloître (michel.cloitre@espci.psl.eu)
Yvette Tran (yvette.tran@espci.psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 4</td><td>Total teaching hours : 36 h</td><td>Grading: final exam (written)</td></tr>
</table>

Course description and content

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 …).

One part of the lectures deals with "Inorganic Materials" presenting at first; basics of the solidification and material stability. Materials presented 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 including glass, ceramics and vitroceramics as well as single crystals elaboration. Their respective properties and characterization methods will be studied.
Intrinsic and extrinsic defects in solids with formation and stabilization mechanisms will be presented as well as the remarkable properties associated with these defects. Overview of the optical, electrical and magnetic properties in the inorganic materials will be presented.

"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 "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. We will also tackle the concept of stimuli-responsiveness: how to induce changes of molecular conformation (surfactants, polymers) and/or changes of assembling (gels, colloids, emulsions) and to control macroscopic properties (rheological, mechanical, interfacial as wetting, adhesion, friction) by triggering a stimulus such as temperature, pH, salt, light, electric and magnetic fields.

Learning goals

The student should be able to:
The student should be able to:
- Appropriate the description of the main structural types characterizing solids.
- Understand the different existing synthesis routes for the development of inorganic materials. Can assess the pros and cons of these pathways.
- Photon, electron and phonon properties relationships. Radiative and non-radiative relaxations. Applications to colors and luminescence
- Mobilize a multidisciplinary background in chemistry and physics to rationalize important material behaviors in Soft Matter (i.e. solubility versus phase separation).
- Concept of stimuli-responsiveness: pilot molecular changes for microscopic/mesoscopic/macroscopic changes
- Draw analogies between different soft materials

Pre-requisites

Basics of inorganic and organic chemistry, coordination chemistry.
Thermodynamics, Chemical bonding, Group theory

SEMESTER 1

Innovation and soft skills

Entrepreneurship and Soft Skills

M1	S1	Course Title: Design Thinking – MAD-THINK *Keywords: design, innovation*	
Coordinator		Majooran Kanthiah (Majoorank@gmail.com)	
Instructor(s),		Faustine Vanhulle (faustine.vanhulle@feve-conseil.fr), Majooran Kanthiah (Majoorank@gmail.com)	
ECTS : 3		*Total hours : 28h*	*rating: report and oral presentation*

Description

During this course, we will introduce and apply the "Design Thinking" approach to a real issue proposed by a company (e.g. LVMH, Vicat …).
Design Thinking is a human-centered approach to innovation that draws from the designer's toolkit to integrate the needs of people, the possibilities of technology and the requirements for business success.
Hence, in the frame of the course, students will start from the initial formulation of the issue (challenge), observe and interact with stakeholders and potential users or customers in order to define their own "point of view". They will then find options to propose an innovative solution (MAD-THINK).
Intermediary sessions will be devoted to an iteration of the process, refinement of the positioning, definition of the technical feasibility and of the business model and control of the sustainability of the proposed solution.
The solution(s) selected for their innovative potential will be developed during the Design Project (MAD-DES), that will give the groups the opportunity to prototype and test their ideas, before presenting them.
This course is built on both lectures and practical workshop conducted by coaches in innovation, designers and scientists.

Learning goals

- Identify innovation in a given field (difference between innovation and invention)
- Use the tools of Design thinking to generate innovative ideas, prototype and test them, and confront them to the market
- Evaluate technical feasibility, and business viability

Pre-requisites

none

M1	S1	Course Title: PSL I-teams workshops *Keywords: innovation, entrepreneurship*	
Coordinator		Nadine-Eva Jeanne (nadine-eva.jeanne@psl.eu	
Instructor(s),		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

M1	S1	Course Title: Language *Keywords:*	
Coordinator		Daria Moreau (daria.moreau@chimieparistech.psl.eu)	
Instructor(s),		Name(s) and e-mails :	
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

M1	S1	**Course Title: Innovative Transdisciplinary Project** *Keywords:*	
Coordinator		Fethi Bedioui, Guillaume Lefèvre	
Instructor(s),		Name(s) and e-mails : fethi.bedioui@chimieparistech.psl.eu, guillaume.lefevre@chimieparistech psl.eu	
ECTS : 4		*Total hours : 50h*	*rating: report and oral presentations*

Description The project aims at training students to get aware of an unknown scientific or technological topic and to find out innovative approaches to address a scientific problem. Topics are proposed by laboratories either academic or from the private sector (start-ups).
Learning goals Develop student's ability to address new topics, to find out an innovative approach to a situation, and to present their conclusions in a written report and oral presentations.
Pre-requisites none

SEMESTER 2

ADVANCED CHEMISTRY COMMON COURSES

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S2</td><td colspan="2">Course Title: Molecular Design and Synthetic Tools – Advanced
Subtitle: Synthetic tools for health sciences</td></tr>
<tr><td colspan="2">Keywords: Retrosynthesis, Total Synthesis, Atom- and Step-Economy</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Guillaume Lefèvre (guillaume.lefevre@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Kevin Cariou (kevin.cariou@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 1</td><td>Total teaching hours : 12 h</td><td>Grading: continuous assessment (project) and final written exam</td></tr>
<tr><td colspan="4">Course description and content

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, relying on the synthetic methods studied during the “Basics” course. 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, which will be graded as part of the total grade for the course.</td></tr>
<tr><td colspan="4">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</td></tr>
<tr><td colspan="4">Pre-requisites</td></tr>
</table>

M1	S2	**Course Title: Analytical and Physical Chemistry – Advanced** **Subtitle: Radiation-based analysis: from spectroscopy to imaging**
		Keywords: Spectroscopy, Imaging, Optics, Magnetic Resonance, X-ray, scattering, diffraction, molecular and nanoparticular structure, biology, biomedical.
Coordinator		DOAN Bich-Thuy, bich-thuy.doan@chimieparistech.psl.eu
Instructor(s)		DOAN Bich-Thuy, bich-thuy.doan@chimieparistech.psl.eu TRIBET Christophe, christophe.tribet@ens.psl.eu
ECTS : 1		**Total teaching hours : 12 h** — **Grading:** *final exam (written* *+ coefficient for each rating modality ½ and ½.*

Course description and content

The objective of the course is to provide advanced knowledges from Optical and Magnetic Resonance spectroscopy to Imagings in order to probe the structure of chemical objects developed in the latest innovations and technological developments in chemistry and in biology.
The course prepares chemists or physicochemists students to the applications of basics concepts of spectroscopies for the understanding and work in cutting edge spectroscopic to imagings techniques in advanced theoretical, experimental and applied research performed in academic and industrial laboratories.
This course covers a range of experimental methods, and spectroscopy. Optical, Magnetic Resonance and scattering-based approaches, used to characterize structures at the nm to micrometer length scales, from molecules, nanoparticles to microsize organic objects.

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 MR, optical (NIR, UV-Vis) fluorescence methods to characterize the structure and understand the properties of probes for biology. 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, MRS/MRI basics applications) (Bich Thuy Doan; 6h).
Radiation-based analysis, from spectroscopy to imaging (part II): The course cover a range of optical and scattering-based methods, used to characterize structures at the nanometer to micrometer length scales. The 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 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:

- to understand the general principle of Magnetic Resonance methods (spectroscopy and imaging) as well as optical ones.
- discover the main imaging probes
- to understand the general principles of optical methods used to characterize the chemical functions and structure of molecules by IR, UV, NMR.
- to understand the general principles of optical methods used to characterize the size and shapes of nanoparticles, molecular or macromolecular assemblies by i) elastic static scattering, ii) high resolution microscopies, iii) dynamic light scattering and tracking of single particle/molecules.
- to understand cutting edge techniques in MR and optical spectroscopy to imaging in advanced experimental and theoretical research.

Pre-requisites

Basics (L2) in physical chemistry, Chemistry in solution, Atoms and molecules energy levels, molecules interactions, complexation
Basics (L2) in optics and interferences
Basics : mathematics

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S2</td><td colspan="2">Course Title: Theoretical Chemistry and Modelling – Advanced</td></tr>
<tr><td colspan="2">Keywords:</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Damien Laage</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Damien Laage</td></tr>
<tr><td colspan="2">ECTS : 1</td><td>Total teaching hours : 12 h</td><td>Grading: final written exam (67%), intermediate reports (33%)</td></tr>
<tr><td colspan="4">Course description and content
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.</td></tr>
<tr><td colspan="4">Learning goals
The student should be able to:
- 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</td></tr>
<tr><td colspan="4">Pre-requisites
BSc level in statistical physics, quantum chemistry, physical chemistry</td></tr>
</table>

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S2</td><td colspan="2">Course Title: Smart Materials Chemistry – Advanced</td></tr>
<tr><td colspan="2">Keywords: Advanced functional materials. Hybrid materials. Energy storage and conversion. Batteries. Metal Organic Frameworks</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">A. Tissot (antoine.tissot@ens.psl.eu), V. Pereira-Pimenta (vanessa.pereira-pimenta@espci.fr)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">A. Tissot (antoine.tissot@ens.psl.eu), V. Pereira-Pimenta (vanessa.pereira-pimenta@espci.fr)</td></tr>
<tr><td colspan="2">ECTS : 1</td><td>Total teaching hours : 12 h</td><td>Grading: Final written exam</td></tr>
</table>

Course description and content

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.
- Diffusion properties in solids and quick recapitulative about electrochemistry and its application to solids and solid/liquid interfaces.

Toward applications

=> Synthesis, properties and applications of crystalline porous solids (Metal-Organic Frameworks).

=> New developments of batteries: Current research trends in battery performances and chemistry: tradeoff between energy/power density and scalability. Recycling issues

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

Learning goals

The student should be able to:

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
- Redox properties of solids and alkali-cation diffusion properties in solids
- Charge transfer at solid/liquid interface

Pre-requisites

Basics of solid state and coordination chemistry. Thermodynamics. Basics courses of the Graduate Program

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S2</td><td colspan="2">Course Title: Introduction to Chemometrics</td></tr>
<tr><td colspan="2">Keywords: Distribution, Random Variable, Confidence Interval, Hypothesis testing, Linear Regression</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Jérôme VIAL (jerome.vial@espci.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s)</td><td colspan="2">Jérôme VIAL (jerome.vial@espci.psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 1</td><td>Total teaching hours : 12 h</td><td>Grading: 1h final exam: written (100%)</td></tr>
</table>

Course description and content

Chemometrics consist in the application of statistical and mathematical tools to problematics of chemistry.

After a brief description of the basic concepts of descriptive statistics, the main statistical distributions will be presented. Then the concept of random variable will be introduced and punctual and by interval estimations of the mean and of the variance of experimental chemical results will be detailed. Hypothesis testing will be exposed and applied to trueness evaluation and method comparison. Finally, the principle of linear regression will be exposed, and it will be explained how to apply this tool to the problematics of calibration.

Each theoretical concept presented will be illustrated by case studies issue from practical situation that an experimenter can be faced to in his laboratory.

Learning goals

The student should be able to:

- Present in an adapted graphical way its experimental results.
- Use the principal statistical distributions.
- Provide confidence intervals for the mean and the variance of a set of experimental results.
- Carry out tests of hypothesis to answer practical questioning usually raised in a lab (Is my method true? Can we consider two experimental results equal? Different?)
- Apply linear regression to calibration problematics.
- Adequately use the term significant

Pre-requisites

None

SEMESTER 2

SUPER-ADVANCED CHEMISTRY ELECTIVE COURSES

(3 courses to be selected in the list hereafter)

Chemical Biology

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*	
Coordinator		Anton Granzhan	
Instructor(s),		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 teaching hours :** *24h*	**Grading:** 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.
-

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

M1	S2	**Course Title: Advanced theoretical and computational chemistry** *Keywords:*	
Coordinator		Ilaria Ciofini (ilaria.ciofini@chimieparistech.psl.eu)	
Instructor(s),		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*	*grading: 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

M1	S2	**Course Title: Electronic Properties of Solids : from Concepts to Devices** *Keywords: band structures, optical and electrical properties, semiconductors, devices*

Coordinator	Laurent Binet (laurent.binet@chimieparistech.psl.eu)	
Instructor(s),	Name(s) and e-mails: Laurent Binet, Pascal Loiseau, Frédéric Wiame Laurent Binet (laurent.binet@chimieparistech.psl.eu)	
ECTS: 3	*Total hours : 22,5h*	*grading: final written exam*

Description

The objective of this course is to describe the electronic structure of solids, 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 (free electron gas and tight-binding models, dispersion curves, density of states) to describe the electronic band structures of solids and shows how these concepts explain the main classes of properties, namely electrical, optical and chemical of solids.

In the second part, the course focuses on an important class of materials, semiconductors. It thus introduces the specific crystal and electronic structures of the elemental, III-V and II-VI semiconductors, the n-type and p-type dopings and their electrical and optical behaviors. The course then describes in detail the phenomena that occur in a p-n junction. The applications of the p-n junction are described, in particular solar cells, photo-diodes and light-emitting diodes.

Learning goals

The student must be able:

- to define the characteristics of the two main models of electronic structure of solids and to know in which context to apply them,
- to 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,
- to interpret a band structure diagram of a solid and deduce its electrical and optical behaviour,
- to describe in details 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

- Classical mechanics: Newton's laws, momentum, force and potential energy, kinetic energy, work done by a force.
- Quantum physics: Schrödinger equation, De Broglie and Planck-Einstein relations, Dirac notation, eigenfunctions and eigenvalues and their physical meaning, scalar product in a Hilbert space, energies and wavefunctions of a free particle and a particle in a quantum well.
- Quantum chemistry: atomic and molecular orbitals, linear combinations of atomic orbitals, bonding and antibonding molecular orbitals, Born-Oppenheimer and single electron approximations.
- Crystallography: crystal systems, normal and reciprocal lattices, relation between basis vectors of these lattices.
- Electromagnetism: plane waves, wave vector, electrostatic potential, electric field, Poisson's equation.
- Themodynamics: Boltzmann and Fermi-Dirac statistics, Ficks' law.
- Mathematics: gradient, Laplacian, divergence, partial derivative, differential.

Soft Matter and Developpement

M1	S2	**Course SuperAdvanced : Soft matter and Development** *Keywords: soft matter, polymers, liquid crystals, colloids, formulations*
Coordinator		Michel Cloître (michel.cloitre@espci.fr)
Instructor(s),		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 both the "Inorganic Chemistry : from molecules to materials" course and the "Synthesis of Inorganic and Hybrid Materials course" (next page)

M1	**S2**	**Course Title: Inorganic Chemistry : from molecules to materials (MH24OP.NOR)** *Keywords:*
Coordinator		Domitille Giaume, domitille.giaume@chimieparistech.psl.eu
Instructor(s),		Name(s) and e-mails:

ECTS :	*Total hours : 18h*	*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 overview of the industrial mineral chemistry completes the introduction (cements, glasses, aqueous chemistry, batteries). The theoretical part focuses on:

- the formation of complexes around transition metal and lanthanide ions;
- the description in particular of their optical and magnetic properties (selection rules, intensity of colors, magnetism).

Learning goals

At the end of the course, the student should be able:

- to determine some trends of elements physicochemical properties depending on their position in the periodic table (ionization, complexation, orbital levels).
- to determine the stability of an inorganic complex following the 18 electron rule.
- to describe a mineral system and choose between two simple approaches to describe inorganic complexes according to ionic binding or covalent binding models: crystalline field theory or ligand field theory.
- to explain the reactivity of inorganic molecules based mainly on transition elements or elements of the p-block.
- to compare optical properties between complexes (color and intensity) based on transition selection rules and electronic configuration.
- to read and use Tanabe-Sugano diagram to determine the optical transitions of a complex.
- to determine the origin of luminescence properties of a material.

Pre-requisites

atomistics, chemical bonds, crystal field theory

M1	S2	**Course Title: Synthesis of Inorganic and Hybrid Materials** *Keywords: Inorganic materials, porous solids, synthesis, challenges*
Coordinator		Sandrine Ithurria
Instructor(s),		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

M1	S2	**Course Title: Bio-analytical Chemistry** *Keywords: analytical systems, process miniaturization, lab-on-chip, bio-sensors*

Coordinator	
Instructor(s),	Name(s) and e-mails : Fanny d'Orlyé (fanny.dorlye@chimieparistech.psl.eu)

ECTS : 3	*Total hours : 23.5h*	*rating: final written exam + intermediate rating*

Description

Developments and trends in modern analytical chemistry are moving towards the simplification, automation and miniaturization of processes, while maintaining the performance and reliability of analytical results. The opportunities and difficulties inherent in miniaturization at each stage of an analytical process are very different and need to be addressed. The main aim of this course is therefore to provide a comprehensive overview of current innovations in analytical systems. The ultimate goal is the development of micro(nano)sensors and total analysis microsystems (µTAS) for biotechnology and clinical diagnostic applications.
The course will focus on new analytical and bioanalytical tools enabling the downscaling of several laboratory operations (sample introduction, processing, separation, detection) to handle extremely small volumes of fluids, as well as integrating the above-mentioned processes on a miniaturized device of just a few square centimeters, enabling automation and high-throughput processing of analyses. The main knowledge imparted to students will concern 1) new functionalized nanomaterials for diagnostics: nanocarriers (nanoparticles, nanotubes, monoliths, molecularly printed materials, etc.), selective agents (antibodies/proteins, aptamers, chelating agents, etc.) and conjugation procedures.) and conjugation procedures; 2) the development of miniaturized separation methods (chromatographic or electrokinetic) mainly based on molecular recognition to purify, concentrate and isolate analytes of interest; 3) detection in miniaturized analytical systems (optical, electrochemical, mass spectrometry); 4) analytical processes ranging from standard bioassays to micro(nano)sensors and total analysis microsystems for applications in biotechnology and clinical diagnostics.

Learning goals

At the end of this course, students will be able to
- describe and explain the fundamental microscopic mechanisms underlying the selectivity of analytical separation methods and the sensitivity of coupled detection modes
- synthesize, interpret and report experimental results from the scientific literature
- mobilize their knowledge to propose an analytical and technological solution to a complex clinical diagnostic problem

Pre-requisites

basic notion in thermodynamics, solution chemistry, nano-materials, electrochemistry and separation methods

Physical Chemistry for Bio-systems

includes both the "Bio-interfaces" course and the "Colloids and biomolecules" course (next page)

<table>
<tr><td>C&I
M1</td><td>S2</td><td colspan="2">Course Title: Bio-interfaces
Keywords: surface, composition, reactions, techniques, biomolecules</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Anouk Galtayries (anouk.galtayries@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s),</td><td colspan="2">Name(s) and e-mails : Anouk Galtayries (anouk.galtayries@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">ECTS :</td><td>Total hours : 15h</td><td>rating: final written exam</td></tr>
</table>

Description

This lecture aims at showing the key role played by the surface of solid 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, biofouling, etc. …).

This course implies the following items:

- Introduction: the surface, a complex material (structure, composition, model surfaces, real surfaces, adsorption, tools for characterization)
- Biointerfaces: places where all biological processes occur
- Dedicated physico-chemical characterization techniques: in situ real time ones, UHV techniques, combination of techniques as morphology and composition…
- Different examples of surface reactivities from amine acid reactions to protein non specific and specific interactions with surfaces
- Interactivity on specific topics: understanding the quantitative approach, students presentations in small groups, questions from all the class.

Learning goals

- the student will take into account the outermost layers in a material's question
- the student will know the principles, advantages and drawbacks of a certain number of characterization techniques of solid surfaces,
- quantification and qualitative approaches will alternatively be proposed by the students when discussing a biointerface characterization strategy
- identifying the properties of biomolecules adsorption, and impact on further reactions, modelizing an experiment to understand surface reaction mechanisms in the frame of biomaterials.

Pre-requisites

analytical chemistry, chemical physics, knowledge about materials reactivity (passivation, corrosion, adsorption, functionalization…)

M1	S2	**Course Title: Colloids and Biomolecules** *Keywords:*
Coordinator		Jérôme Bibette (jerome.bibette@espci.psl.eu)
Instructor(s),		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: Medicinal Inorganic Chemistry, Bioorganometallic Chemistry, Bioinorganic Chemistry, Inorganic Chemical Biology.*
Coordinator		Gilles Gasser (gilles.gasser@chimieparistech.psl.eu)
Instructor(s),		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 organometallic compounds, 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.

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.

Learning goals

The course will be divided into two main sections. In the first section, the role of metal ions in a few key metalloproteins and biological processes will be explained. The second section will focus on the use of metal complexes to detect specific organelles/biomolecules, or a discussion to understand/modify biological processes. A large emphasis will be placed on experiments, which have been carried out in living cells or organisms.

Pre-requisites

This course requires basic knowledge of inorganic chemistry and biochemistry.

M1	S2	**Course Title: Heteroelements** *Keywords: catalysis, transitions metals, coupling reactions, heteroelements*
Coordinator		Phannarath Phansavath (phannarath.phansavath@chimieparistech.psl.eu)
Instructor(s),		Name(s) and e-mails : Phannarath Phansavath (phannarath.phansavath@chimieparistech.psl.eu)

ECTS :	*Total hours : 12h*	*rating: final written exam*

Description

The aim of the Heteroelement Chemistry course is to present the various methods for preparing phosphorus, sulfur and silicon reagents, which are important synthetic tools in organic synthesis. The main transformations carried out with these compounds are given, with applications in total synthesis. The aim of the Applied Catalysis course is to provide the basics of organometallic chemistry involving transition metals (palladium, rhodium, nickel, copper), as a tool for developing synthetic processes. Coupling reactions and other major applications in homogeneous catalysis are presented, with emphasis on catalyst types and reaction mechanisms, as well as industrial applications for the synthesis of natural molecules and pharmaceutical research. It should be noted that an introduction to Flow Chemistry is presented as part of this course (not graded).

Learning goals

At the end of the course, students will be able to identify and describe the methods used to carry out the main transformations involving phosphorus, sulfur and silicon derivatives, and explain the corresponding reaction mechanisms. They will be able to use suitable organometallic complexes to carry out the main coupling reactions and other major reactions used in homogeneous catalysis. They will be able to analyze simple multi-step syntheses and produce given molecules using the different approaches and methods seen in the course.

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

M1	S2	**Course Title: Design Thinking – MAD-DES** *Keywords: design, innovation*
Coordinator		Majooran Kanthiah (Majoorank@gmail.com)
Instructor(s),		Faustine Vanhulle (faustine.vanhulle@feve-conseil.fr), Majooran Kanthiah (Majoorank@gmail.com)
ECTS : 3	*Total hours : 26,5h*	*Rating : report and oral presentation*

Description
The solution(s) selected in the MAD-THINK course (1st semester) for their innovative potential will be developed during the Design Project (MAD-DES), that will give the groups the opportunity to prototype and test their ideas, before presenting them.
This course is built on both lectures and practical workshop conducted by coaches in innovation, designers and scientists.

Learning goals
- Identify innovation in a given field (difference between innovation and invention)
- Use the tools of Design thinking to generate innovative ideas, prototype and test them, and confront them to the market
- Evaluate technical feasibility, and business viability

Pre-requisites
none

M1	S2	**Course Title: PSL I-teams workshops** *Keywords: innovation, entrepreneurship*
Coordinator		Nadine-Eva Jeanne (nadine-eva.jeanne@psl.eu
Instructor(s),		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

M1	S2	**Course Title: Language** *Keywords:*
Coordinator		Daria Moreau (daria.moreau@chimieparistech.psl.eu)
Instructor(s),		Name(s) and e-mails :
ECTS : 2	*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

<table>
<tr><td>C&I
M1</td><td>S2</td><td colspan="2">Course Title: Pre-internship Project and Seminars
Keywords:</td></tr>
<tr><td colspan="2">Instructor(s),
Coordinator</td><td colspan="2">Name(s) and e-mails : Bruno Viana (bruno.viana@chimieparistech.psl.eu), Laurent Binet (laurent.binet@chimiueparistech.psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 2</td><td>Total hours :</td><td>rating: oral presentation</td></tr>
<tr><td colspan="4">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 poster presentation about one of the seminars attended during the academic year.</td></tr>
<tr><td colspan="4">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.</td></tr>
<tr><td colspan="4">Pre-requisites
none</td></tr>
</table>

<table>
<tr><td>C&I
M1</td><td>S2</td><td colspan="2">Course Title: Laboratory Internship
Keywords:</td></tr>
<tr><td colspan="2">Coordinator</td><td colspan="2">Laurent Binet (laurent.binet@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">Instructor(s),</td><td colspan="2">Name(s) and e-mails : Laurent Binet (laurent.binet@chimieparistech.psl.eu)</td></tr>
<tr><td colspan="2">ECTS : 9</td><td>Total hours : minimum 3 months</td><td>rating: written report and oral presentation</td></tr>
<tr><td colspan="4">Description
The internship should take place in a research laboratory either academic or in private company.</td></tr>
<tr><td colspan="4">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.</td></tr>
<tr><td colspan="4">Pre-requisites
none</td></tr>
</table>