Chimie

PSL UNIVERSITÉ PARIS

Integrative Chemistry and Innovation (ICI)

M2 - Course description

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Semester 1 (30 ECTS): A choice of 5 courses (6 ECTS/course) among the following:

Course 1: Flow chemistry

Course 2 : Valorization of Small molecules

Course 3 : Dynamic and Reconfigurable Polymers and Soft Materials

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

Course 5 : Dynamics of molecular processes in biological systems

Course 6 : Modeling and understanding of reaction processes

Course 7 : Optical Materials, from Design to Devices

Course 8 : Databases and statistical learning for chemical discovery

Course 9 : Magnetic Resonance

Course 10 : Scientific innnovation and entrepreneurship

Semester 2 (30 ECTS): 5 to 6 month Research internship

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Course 1: Flow chemistry
Flow chemistry, an emerging technology for organic synthesis

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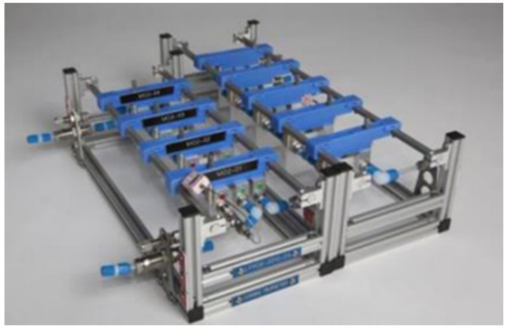
Objectives

*Flow chemistry for the synthesis of molecules of interest

*Decipher the fundamental reactivity and mechanisms of classical and new activation modes in organic synthesis

Understanding the principles of flow chemistry (theoretical concepts and advantages)

Existing equipments and their utilizations



Predicting the reactivity and the reaction mechanisms

Propose solutions in flow chemistry to existing problems in batch

Teachers

B. Laroche, S. Ognier, C. Len, F. Bedioui, M. Zhang, C. Lescot, M. Tatoulian
C. Mallia (AstraZeneca, UK), T. Noël (U. Amsterdam, NL), A. Abou-Hassan (SU).

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Course 1: Flow chemistry
Flow chemistry, an emerging technology for organic synthesis

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

General introduction
An upgrade on energy and matter transfers in continuous-flow reactors

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

Flow chemistry for organic synthesis
Flow & photochemistry
Flow & electrochemistry
Highly reactive intermediates in flow chemistry
Plasmas in flow
Other integrated technologies

Part 3. Applications(10h) :

TD and visit of the flow chemistry pla**tform ParisFlowTech**

Part 4. Conferences (6h)

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Course 2 : Valorization of Small molecules

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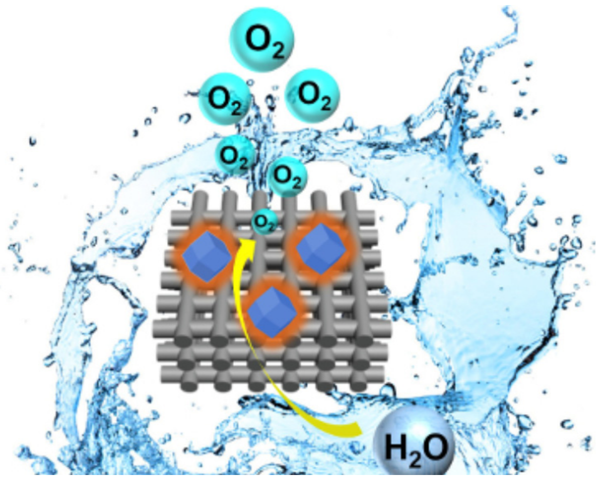
Objectives

*Small molecules, from their capture to their catalytic transformation
*Integrated approach : from gas storage to separation issues and catalytic conversion
*Comprehensive and fair vision of the various catalytic transformations and materials



Teachers

G. Lefèvre, A. Grimaud, C. Mellot-Draznieks, M. Fontecave, G. Mouchaham, C. Serre

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Course 2 : Valorization of Small molecules

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General considerations (4h)
CO_2 cycle
H_2 production

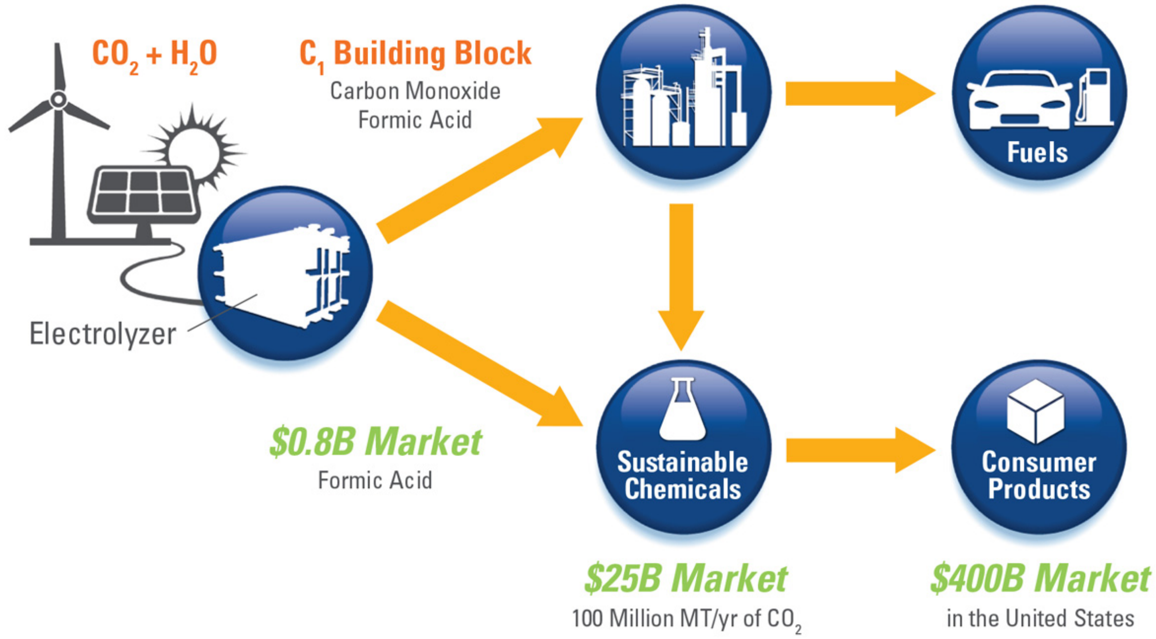
Basics (4h)
Materials synthesis, stability
Electrocatalysis, photocatalysis

Adsorption/separation (10h)
Gas storage (H_2, CH_4…)
CO_2 capture (CO_2/N_2, CO_2/CH_4)
Other separations
Proton conductivity

Chemical transformation (22h)
Hydrogen production, water oxidation
CO_2 reduction

Practical courses (4 h)

Seminars (2 h)



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Course 3 : Dynamic and Reconfigurable Polymers and Soft Materials

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Objectives

*Engineering of dynamic and reconfigurable polymers in materials and biomimicry
* An interdisciplinary approach to soft matter and polymers
* From molecular / macromolecular chemistry to physicochemical and mechanical properties.

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**

Teachers

Costantino Creton, Min-Hui Li, Renaud Nicolaÿ, François Tournilhac, Christophe Tribet, Yvette Tran

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Course 3 : Dynamic and Reconfigurable Polymers and Soft Materials

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Part 1: Synthesis, chemistry and characterization of dynamic covalent polymer networks

Part 2: Sequence-controlled and semi-crystalline polymers: organization, interfaces, specific properties

Part 3: Dynamic bonds: from the molecule to processing and final material properties

Part 4: Responsive polymers: gels and interfaces

Part 5: Light-responsive assemblies

Part 6: Smart soft materials based on thermotropic and lyotropic liquid crystal polymers

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

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Objective

Obtain pertinent information on structure changes, reaction pathways and local events determining and/or taking place during chemical or biological reactions

How to reach it?

Explore the basics of analytical methodologies with high coupling potential an

Appreciate through examples the contribution of coupling to solve issues not easily solved until now

Teachers

Fethi Bedioui, Kevin Ogle, Bich-Thuy Doan, Laurent Thoiun, Fanny d'Orlyé

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

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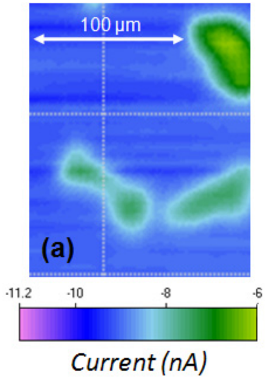
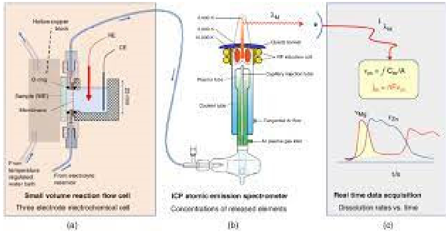
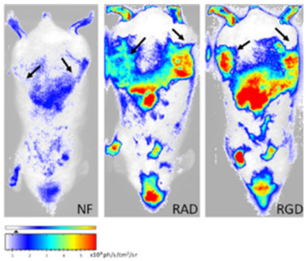


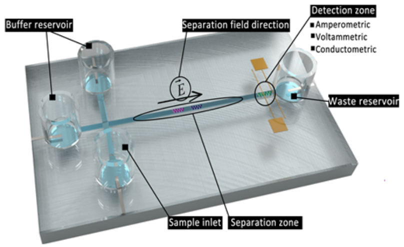
Coupling electrochemical microscopy SECM and AFM/STM for in situ monitoring of substrate morphological changes and reactivity



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)



Coupling optical techniques (IR, Fluorescence) and NMR imagery (and electrochemistry) for in situ monitoring of biological events



Coupling multidimensional separations and detections (optical, electrochemical detection, mass spectrometry) towards integrated microfluidic devices

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Course 5 : Dynamics of molecular processes in biological systems

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Objectives

*Dynamical aspects and processes (e.g. conformational dynamics, transport) in explaining the function of biological macromolecules

*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.

Teachers

Élise Duboué-Dijon, Fabien Ferrage, Damien Laage, Philippe Nghe, Guillaume Stirnemann, Antoine Taly

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Course 5 : Dynamics of molecular processes in biological systems

Key concepts, experimental and simulation techniques (34 h - CM 28h, TD 6h)
Concepts and theories
Experimental tools
Simulation tools

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

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

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Course 6 : Modeling and understanding of reaction processes

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Objectives

* Get knowledge of experimental and theoretical approaches that can be used and combined to untangle complex reaction mechanisms.

* Analyze examples from organometallic catalysis (ex. cross-couplings catalyzed by Pd, Fe or Ni, Cu-catalyzed hydroamination of unsaturated derivatives)

Structural, functional or kinetic data : structures of reaction intermediates and mechanisms

Theoretical **rationalization of a given catalytic process**

Ab-initio approaches (DFT and post-HF) and their coupling with methods to describe the environment

Description of the reactivity in **confined or supported environment** (heterogeneous catalysis)

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

Teachers

Ilaria Ciofini, Frédéric Labat, Guillaume Lefevre, Laurence Grimaud, Maxime Vitale

Course 7 : Optical Materials, from Design to Devices

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Objectives

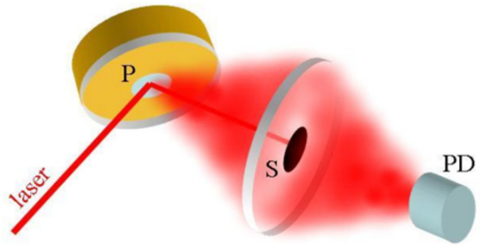
* Inorganics and hybrids materials
* Optical applications such as photovoltaic, lighting, quantum information, imaging, sensor, etc.
* Under various shapes and sizes from nanoparticles to large crystals.

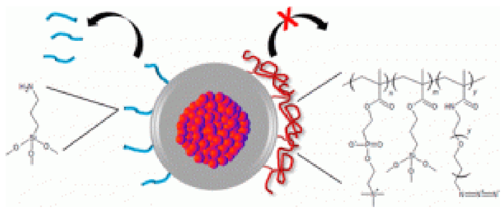
Design

Modelling

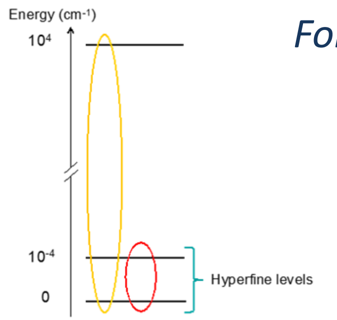
Preparation

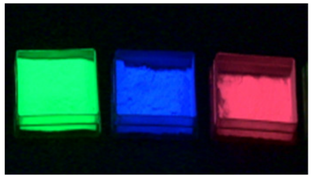
Practical use

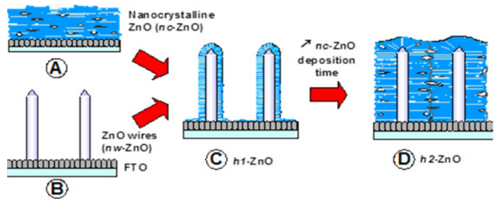




For quantum information, sensors, lighting







Teachers

Thierry Pauporté, Frédéric Labat, T. Pons, S. Ithurria, B. Viana, A. Tissot, Ph. Goldner

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Course 7 : Optical Materials, from Design to Devices

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Part 1 (12h): Photovoltaic materials and technologies: Introduction to semiconductors and to semiconductor junctions; fabrication of photovoltaic devices and panels; emerging technologies
Modelling for photovoltaic: electronic structure of semiconductors (bulk and interfaces; effect of defects); modelling of hybrid systems and properties

Part 2 (12h): Engineering of colloidal optical inorganic nanomaterials. Semiconductor and metal nanocrystals, synthesis, surface and interface, functionalization and applications

Part 3 (12h): Color and colorimetry, LED and Laser chemistry and technologies, strategies and mechanisms of luminescence stimulation; (mechanoluminescence, OSL, thermoluminescence)

Part 4 (12h): Switchable hybrid materials: spin crossover, photomagnetism, porosity, chemosensing
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.

Course 8 : Databases and statistical learning for chemical discovery

Objectives

* Identify the types of data produced in the course of a research activity, the associated metadata and the challenges of their conservation
* Get a knowledge of the main existing databases in chemistry
* Understand statistical learning methods used in published works (mode of operation and limitations)
*Implement a statistical learning method on chemistry data

Teachers

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

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Course 8 : Databases and statistical learning for chemical discovery

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Theoretical (16 h)
Data in chemistry: metadata, storage and curation, API
Existing databases: materials, molecules; theoretical, experimental; structures, properties
Fundamentals of statistical learning: machine learning, deep learning
Data and reproducibility, open science approach

Applications (16 h)
Structure/property, structure/activity relationships; QSAR/QSPR methods
Machine learning for theoretical chemistry: functionals, reactive force fields, exploration and collective variables, etc
Large-scale screening for pharma applications, docking and advanced methods

Group projects (16 h)

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Course 9 : Magnetic Resonance

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Objectives:

* Provide with the theoretical grounds of magnetic resonance spectroscopies
* Show how MR can be used in any field of chemistry

Introduce magnetic resonance spectroscopies (NMR and EPR) with a consistent theoretical quantum mechanical framework

Give chemists a keen sense of the link between the observables of magnetic resonance and **molecular structure, dynamics, molecular orbitals and other chemical properties**

Illustrate the use of magnetic resonance in a diversity of fields, from the investigation of **materials, biological systems, cultural heritage**, etc.

Teachers

Laurent Binet, Jean-Baptiste d’Espinose, Fabien Ferrage, Kong Ooi

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Course 9 : Magnetic Resonance

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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

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Course 10 : Scientific innovation and entrepreneurship

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Thinking and acting in the unknown: design theory and innovation methods (21h)

Business model and impact entrepreneurship (21h)

Other optionals such as :
Corporate finance, business plan (15 h)

In the framework of PSL Innovation and Entrepreneurship

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The ICI M2 track in a nutshell:

- **Broad and transdisciplinary training in chemistry through a unique a la carte offer of original tranversal courses**
- **Entirely taught in English**
- **Individualized program (free choice of courses + possibility to incorporate courses from other M2 tracks upon validation)**
- **5 to 6 month research laboratory in academic or private sector**
- **Strong integration in the graduate program (Master and PhD students, teachers, researchers)**
- **A broad offers of seminars within the graduate program**