Welcome Day of the Doctoral School 406: Program 2021

Wednesday, March 3rd, 2021 at 2 pm

Zoom meeting – Sorbonne University, Pierre et Marie Curie Campus

Schedule	Speaker	Title	Moderator
14h-14h30	***Welcome and introduction: Doctoral School 406 Management***		Dr Cyril OLLIVIER Doctoral School Director
14h30	Ludivine K/BIDI	*C-H activation by Polyoxometalates*	Pr Fethi BEDIOUI PSL Doctoral School Deputy Director
	Edwyn REMADNA	*Synthèse d'une nouvelle génération de complexes organométalliques d'or(III): de l'optimisation du squelette à la bio-conjugaison.*	
	JinGe CAO	*Nickel encapsulated inside NHC-capped Cyclodextrins: Cavity-controlled selective reactions*	
	Elodie DAVID	*Design and pharmacological evaluation of neuropsin (Kallikrein 8) inhibitors as therapeutics and potential diagnosis tools for Alzheimer's Disease and associated dementias*	
	Kevin MALL HAIDARALY	*Mesomorph PolyOxometalate(POM)-based hybrid materials for photonics*	
	Sonia KHEMAISSA	*Ionpair-π interactions and mechanisms of membrane interaction and cellular penetration of cell-penetrating peptides*	
	Lyna BOUREHIL	*Measurement of electronic effects of ligands on organometallic complexes*	
	Zihua YANG	*Plasmonic nanoparticles for biosensing and therapy*	
	Salwa Simona JAMIL	*Nouveaux assemblages de coordination panchromatique à base de ligands pyridilidènes π-étendus*	
	Federico BANCHINI	*Gem-Binucleophilic Linchpins for Orthogonal Multicomponent Asymmetric Reactions*	
	Vincent WOWK	*New iron complexes with low oxidation states and C-H activation*	Dr Vincent CORCÉ
	Lisa GOURDON	*Copper Complexes for Light-Initiated Catalysis Inside Cells*	
	Gaoyu LIU	*Artificial butterfly wing with stimuli-responsive structural colors*	
	Amélie AUVIGNE	*Design of a new Microwave-Assisted Continuous Flow equipment for selective catalysis*	
	Alessandro PERAZIO	*Carbon dioxide conversion to ethanol: towards selective heterogeneous catalysts*	
	Ivanna AMARSY	*Selective Delivery of Ruthenium Complexes into Cancer Cells*	
	Thomas DEIS	*New-Silicon Based Lewis Acids: Reactivity & Applications in Asymmetric Catalysis*	
	Youchao WANG	*Bimetallic Complexes as Photosensitizers for Photodynamic Therapy*	
	Yutong LI	*Functional Micro and Nanoparticles: Preparation and Biological Applications*	
	Juba SALHI	*Isolated switchable polyoxometalates (POMs) on a nanoporous highly organized carbon substrate.*	
	Lucie GUILLAUME	*Smart multi-catalytic systems for the production of biobased polymers*	Dr Cyril OLLIVIER Doctoral School Director
	Jean BOUVET	*Superoxide dismutase mimics: an integrated approach from chemical design to bio-activity in cells*	
	Steffi SEWSURN	*Bioengineering of metabolic pathways of pyrrocidines, derived from a fungal PKS-NRPS, for the study and generation of chemical diversity in this family of compounds.*	
	Diana MELIS	*Development of water-soluble Re-chelating ligands for ^{188}Re-based radiopharmaceuticals.*	
	Mae ROBIN	*New non-innocent ligands for C–H bond activation catalysis by iron complexes*	
	Ichrak EL HAJ BRAHIM	*Stereoselective preparation of 2-alkynylaminoalcohols-1,3 for an approach synthetic (-) – stemoamide*	
	Maria Dalla POZZA	*Selective photo-cleavage of DNA for gene therapy*	
	Xueyan ZHANG	*Novel Catalytic Silylation Reactions with Silyldiazenes*	
	Marco DI MATTEO	*Development of selective C-H Activations on terpenes: application to the synthesis of cannabinoid natural products and analogs*	
	Hong-Phong DUONG	*Carbon monooxide conversion to multicarbon products: towards selective catalysts*	
17h00	**End**		

Liste des résumés

Ludivine K/BIDI

C-H activation by Polyoxometalates

PhD advisor: Geoffroy GUILLEMOT

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The PhD work aims to explore C-H activation in the context of the conversion of alkane into high value-added synthons. Our approach is based on the dehydrogenation of alkane through two pathways: an oxidative dehydrogenation and a photochemical dehydrogenation of alkanes. To reach this objective, we will design original and stable molecular complexes based on earth-abundant metal centers (Fe, Co) onto polyoxometalate ligands. These robust catalysts provide well-defined active sites in an unconventional coordination environment and redox-active polyoxotungstic fragments that can play the role of photocatalysts.

Edwyn REMADNA

Synthèse d'une nouvelle génération de complexes organométalliques d'or(III): de l'optimisation du squelette à la bio-conjugaison.

PhD advisor: Serge THORIMBERT, Patricia FORGEZ, Benoit BERTRAND

Laboratory: Institut Parisien de Chimie Moléculaire (IPCM)-ChemBio

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Conventional chemotherapy uses platinum (II). However, these treatments have limitations in terms of resistance or significant side effects. An alternative to platinum(II) is envisaged, it is in this context that my thesis is part of . The aim of this is to develop a new family of gold(III) organometallic complexes by replacing C^C^N or NHC ligands with biphenyl C^C ligands or pyridinyl-NHC ligands (C^N). These complexes would have redox stability via C^C ligands and some hemi-lability via pyridinyl -NHC ligands. This structure would provide the possibility of coordination of gold(III) to biomolecules via the grafting of a biological vector to enable the targeting of cancer cells.

Jinge CAO

Nickel encapsulated inside NHC-capped Cyclodextrins: Cavity-controlled selective reactions

PhD advisor: Prof. Matthieu Sollogoub, Dr. Yongmin Zhang, Dr. Sylvain Roland

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Encapsulated metal complexes show distinctive behaviors resulting from the confinement of the metal. The cavity plays the role of second coordination sphere, which impacts reactivity and selectivity. In the framework of our studies on cyclodextrin(CD)-based metal catalysts, our group has developed NHC-capped CD complexes, called (ICyD)M, where the metal is literally wrapped by the CD scaffold. The position of an appended metal inside this cavity forces external

ligands to be influenced by its shape to interact with the metal center. Thus, these particular structures were found to induce shape-dependent enantio- and regioselectivities.

Many recent publications report the catalytic characteristics of nickel-NHC complexes, which can make reaction processes more efficient under milder conditions and catalyze numerous novel reactions. This project will first study the synthesis of complexes then their reactivity also in a context of enantio- and regioselectivity.

Elodie DAVID

Design and pharmacological evaluation of neuropsin (Kallikrein 8) inhibitors as therapeutics and potential diagnosis tools for Alzheimer's Disease and associated dementias

PhD advisor: Candice BOTUHA, Chahrazade EL AMRI, Vincent CORCE

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In France about 1.9 million people suffer from Alzheimer's type dementia, and 35 million patients worldwide. The challenges of Alzheimer's disease (AD) research are to diagnose the disease before the onset of irreversible brain damage services. A new physiopathological hypothesis is that a serine protease called Kallikrein 8 (KLK8) is involved in Alzheimer's disease. My project consists in designing and identifying the first organic inhibitors of KLK8 and characterizing their mechanism of inhibition. By doing so, the purpose of the project is to provide evidence that pharmacologic inhibition of KLK8 reduces clinical features of AD and to contribute to a better understanding of the role of KLK8 in AD. Recent results obtained by the supervisors exhibited two promising hit compounds to inhibit KLK8 with low-micromolar IC_{50}. These two hits are structurally different: the first is deferasirox (DFX) and the second compound belongs to the family of 4H-pyrido[e] [1,3]oxazin-4-ones (PyrOx). Following these results, by modulating these compounds we should be able to have better organic inhibitors of KLK8 in order to proceed to a biological evaluation.

Kevin MALL HAIDARALY

Mesomorph PolyOxometalate(POM)-based hybrid materials for photonics

Guillaume IZZET, Fabrice MATHEVET

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Highly nanostructured semiconducting materials displaying efficient charge transfer properties hold great promise in optoelectronics. MESOMORPHICS proposes to develop a new type of photoactive and semiconducting mesomorphic materials combining donor pi-conjugated mesogenic moieties and acceptor polyoxometalates, a class of discrete nanosized oxoclusters, within a unique molecular architecture. The antagonistic chemical nature of the charged polyoxometalate and hydrophobic donors will allow the nanosegregation of the donor/acceptor sub-units thus favouring charge transport properties. The structure-property relationship in these self-organized hybrid materials will be explored with a peculiar focus on their charge transfer ability. Combining the elaboration of original multifunctional mesomorphic systems with advanced spectroscopic experiments and analysis should open a path for exploring the influence of long-range order on exciton and hole/electron diffusion pathways.

Sonia KHEMAISSA

Ionpair-π interactions and mechanisms of membrane interaction and cellular penetration of cell-penetrating peptides

PhD advisor : Sandrine Sagan, Astrid Walrant

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Cell Penetrating Peptides (CPPs) are small peptides able to cross the membrane in a receptor-independent way. They are mostly cationic which lead them to interact with negatively-charged partners such as lipids and glycosaminoglycans (GAGs) at the level of the plasma membrane. Their internalization can occur according to two mechanisms: endocytosis, which is energy dependent and direct translocation which is a passive mechanism. In both mechanisms, the first step involves an interaction between peptide and GAGs or lipids. Many CPPs contain arginine residues, which are able to create electrostatic interactions and hydrogen bonds with lipids and GAGs. Sometimes, aromatic residues such as tryptophan can also be found in CPP sequences. This particular residue, provided its unique structure, could be implicated in various interactions including hydrophobic contacts, hydrogen bonds, cation-π interaction. Recently, ionpair-π interactions involving tryptophan have also been identified.

The aim of this project is to synthetize peptide sequences composed of a GAG-recognition sequence linked with a penetrating sequence, study their penetration properties and characterize their interactions with lipids and GAGs. In particular, the role of the linker between the two moieties is investigated. Then, a special attention will be given to the role of tryptophan residues in order to better understand ionpair-π interactions.

Lyna BOUREHIL

Measurement of electronic effects of ligands on organometallic complexes

PhD advisor: Heloise DOSSMANN, Gustavo GARCIA

Laboratory: IPCM organic and biological structural chemistry team

Synchrotron SOLEIL, line of light DESIRS

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In homogenous organometallic catalysis, a detailed focus is required on the organometallic complex in order to access a fine understanding of the catalytic reaction mechanism. This concerns in particular ligands bound to the metal center which play a crucial role as they influence the metal reactivity through their steric and electronic effects. This thesis work focuses on the use and the development of experimental methods to evaluate the electronic effects of various ligands bound to iron (Fe) and gold (Au(III)) metal (accessed through collaboration with chemists). To this end, two gas-phase approaches are applied. The first one is based on mass spectrometry which will allow us to measure the bond-dissociation energies of the complexes and derive thus the metal-Ligand or metal-CO bond strength (depending of the nature of the studied complex). The second one is photoelectron spectroscopy which provides access to ionization energies and the complex electronic structure, related to the energy levels of orbitals.

Zihua YANG

Plasmonic nanoparticles for biosensing and therapy

PhD advisor: Michèle Salmain; Souhir Boujday

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Noble metal nanoparticles display fascinating properties mainly owing to their optical features resulting from the localized surface plasmon resonance (LSPR) effect. They absorb and / or scatter light in the visible to the NIR spectral region, depending on their size, shape, composition and state of surface.

Herein, the shift of the LSPR band induced by nanoparticle growth (Au) or etching (core-shell Au-Ag) will be first used to set up a colorimetric assay of phenylalanine. The principle of the assay is that oxidation of phenylalanine catalyzed by L-aminoacid oxidase (LAAO) will an produce equimolar quantity of H_2O_2 that, in turn, will reduce $AuCl_4^-$ in the presence of AuNP resulting in NP growth. Alternatively, H_2O_2 will oxidize the silver shell of Au@AgNP. Both reactions will result in a red shift of the LSPR band position whose magnitude will be correlated to the concentration of phenylalanine. In a second part, multimodal therapeutic agents will be designed from core-shell gold-silica nanorods ($Au@SiO_2NR$). As such, $Au@SiO_2NR$ have a plasmonic core whose optical properties can be finely tuned in the red to the NIR spectral region by adjustment of their aspect ratio and a biocompatible mesoporous silica shell where therapeutic agents can be trapped and delivered at will and whose surface can be decorated with targeting ligands like antibodies.

Salwa Simona JAMIL

Nouveaux assemblages de coordination panchromatique à base de ligands py ridilidènes p-étendus

PhD advisor: Christopher DESMARETS

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My PhD project deals with the development of synthetic methodologies for the synthesis of new platinum coordination assemblies based on π-extended pyridylidene ligands, little-described in the literature and recently developed by the group. This type of ligands exhibit important luminescence properties. Therefore, a part of this project will be devoted to the synthesis of the π-extended ligands by varying topology (*meta* and *para*-substitution of the aromatic core) and subsequently by introducing the pyridylidene function. Then their coordination to platinum molecular bricks will be realized leading to luminescent bimetallic and polymeric architectures. The optical properties in particular luminescence will be deeply investigated, the main objective is the preparation of white-light emitting compounds.

Federico Banchini

Gem-Binucleophilic Linchpins for Orthogonal Multicomponent Asymmetric Reactions

PhD advisor: Prof. Fabrice Chemla, Dr. Olivier Jackowski and Dr. Alejandro Perez-Luna

Laboratory: Institut Parisien de Chimie Moléculaire – Team ROCS - Sorbonne Université - Faculté de Sciences et Ingénierie Tour 32-42 - 4 place Jussieu | 75005 Paris

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Multicomponent reactions (MCRs) represent an important trend in the development of more eco-compatible synthetic procedures because the assembly of at least three substrates in a single step allows the preparation of functionalized backbones in a straightforward manner and with high atom economy. Historically, the development of MCRs has been closely related to the use of specific synthetic linchpins enabling the course of domino processes, and these reagents behave either as electrophile/nucleophile or as bielectrophiles. In this context, the use of geminal binucleophilic carbon species has received much less attention and the field is dominated by reagents exhibiting two equivalent pro-nucleophilic geminal functions (e.g. malonates or, more recently, dibora species). In addition, asymmetric MCRs (AMCRs) remain so far largely underexplored. The present project aims at introducing Zn-containing geminal binucleophilic linchpins in the elaboration of AMCRs.

Vincent Wowk

New iron complexes with low oxidation states and C-H activation

PhD advisor: Guillaume Lefèvre

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My PhD project concerns the development of new catalytic methods of C-C bonds formation by functionalization of C-H bonds promoted by original iron complexes with low oxidation states, stabilized by a participatory ligand type LnZ.

The objective of this project is to promote, within the same catalytic system, the activation of C-H bonds of various substrates (arenes, alkanes) in order to generate a reactive C-Fe bond, which is reused *in-situ* in presence of an organic electrophile to lead to the formation of a coupling product (formation of a C-C bond). Particular interest will be brought to the elucidation of the links uniting the electronic structure of the complexes involved (oxidation states, spin states) to the observed reactivity. The development of the axes of this project calls for the overlap of several themes, at the border between organometallic chemistry, catalysis and mechanistic studies.

Lisa GOURDON

Copper Complexes for Light-Initiated Catalysis Inside Cells

PhD advisor: Gilles GASSER, Kevin CARIOU

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The aim of this PhD is to synthesize and study a series of copper(I) hexanuclear complexes, to evaluate them as photoactivatable catalytic therapeutic agents. The copper compounds can be photoactivated by light – a benign means of targeting specific cells – and then oxidized by biomolecules such as O_2, to produce radicals and a Cu(II) complex which can reduce thiols. A particularly relevant biothiol is glutathione (GSH), which intracellular regulation could be targeted for anticancer therapeutic applications. So far, a few Cu(I) hexanuclear clusters were synthesized and showed promising GSH oxidation under irradiation – while remaining inactive in the dark. However, their cytotoxicity could not yet be determined due to poor water solubility. Once an efficient and water-soluble Cu(I) cluster is synthesized, its phototoxicity on cancer cells and multicellular tumor spheroids will be assessed, as well as the evolution of GSH concentration and oxygen consumption rates inside cells.

Gaoyu LIU

Artificial butterfly wing with stimuli-responsive structural colors

PhD advisor: Min-hui LI

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In this PhD project, we propose to use a soft lithography technique to replicate the wings of Morpho butterflies. The materials for the replica will be home-designed liquid crystal elastomers (LCE). These LCE are thermo-responsive or photo-responsive artificial muscles. When patterned as nano-actuators with Morpho wing nanostructures, these LCE artificial wings will present structural colors tunable by external stimuli (temperature variation, light illumination, etc.). This bio-inspired functional material can find applications in photoelectrical devices, optical sensors, photonic crystals and photonic integrated circuits etc. I will be trained in organic chemistry and polymer chemistry, and gain knowledge in liquid crystals and their characterization, as well as in micro-fabrication (clean room techniques).

Amélie AUVIGNE

Design of a new Microwave-Assisted Continuous Flow equipment for selective catalysis

Christophe LEN, Bertrand Gerfault

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The aim of this thesis is to design a new equipment for chemistry synthesis and catalysis, using continuous flow chemistry under micro-wave irradiation. The goal is to optimize the production of glycerol oligomers and glycerol derivatives using organic chemistry and catalysis. The choice of the reactor material and its geometry will be defined,

electromagnetic sources layout will be determined and performances of power generating systems will be evaluated. In order to optimize those parameters and to design a new equipment, a multiphysics software will be used.

Alessandro PERAZIO

Carbon dioxide conversion to ethanol: towards selective heterogeneous catalysts

PhD advisor: Prof. Marc Fontecave

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With an atmospheric concentration of over 400 ppm, carbon dioxide represents an increasing threat for the environment due to its strong greenhouse effect. A way to mitigate this problem could be the conversion of CO_2 to useful products like fuels and carbon building blocks. This PhD project aims to electrochemically convert CO_2 to ethanol, a high energy density chemical that can be used as fuel in combustion engines and as a precursor in the synthesis of various compounds. One of the main hardships concerns the selectivity of the reaction. Ethylene is always produced together with ethanol due to very similar reaction pathways, hence it is troublesome to selectively obtain the desired molecule. Metallic copper is the selected catalyst for this project and it will be coupled with other materials (doped carbon, different metals, organic molecules, metal oxides) in the effort to design a catalytic system able to operate at industrially relevant performances.

Ivanna Amarsy

Selective Delivery of Ruthenium Complexes into Cancer Cells

PhD advisor: Gilles Gasser and Sebastien Papot

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In chemotherapy, metals represent a large domain in full exploitation, especially since the discovery of cisplatin. Since then, metal complexes have been used both in therapy and diagnostics due to their high efficiency. However, high levels of activity promotes the presence of significant side effects and, like many drugs, these complexes see the appearance of resistance. In order to reduce these effects, increase their solubility and overcome resistance, prodrugs based on metal complexes have been appearing since the 2000s. In this regard, the goal of my PhD project is to synthesis and evaluate novel Ru(II)-based compounds that can be selectively delivered into cancer cells.

Thomas DEIS

New-Silicon Based Lewis Acids: Reactivity & Applications in Asymmetric Catalysis

PhD advisors: Dr Gilles Lemière & Pr. Louis Fensterbank

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Over the last few years, the reactivity of silicon Lewis acids and more especially the Martin'spirosilane has been investigated within the MACO team. Owing to its spirosilane framework and the rigidity provided by the C,O-bidentate ligands, the Martin's spirosilane opens prospects to devise new silicon-centered chiral pentacoordinate silicates. In contrast to tetracoordinate silanes that display a very high configurational stability, pentacoordinate silicates undergo non-dissociative racemization through fast substituent sites interchange (Berry pseudorotation). Therefore, the PhD project aims to study and to increase the intrinsic chiral stability of these new pentacoordinate silicates in order to achieve first examples of asymmetric (organo)catalysis with pentacoordinated silicon species. Furthermore, recent work at MACO has established primary elements of frustrated Lewis pairs (FLP) reactivity with the Martin'spirosilane. Another strand of research aims to explore further their FLP reactivity by the steric and electronic modulations of substituents around the silicon center.

Youchao WANG

Bimetallic Complexes as Photosensitizers for Photodynamic Therapy

PhD advisor: Gilles Gasser

Laboratory: Chimie Paris Tech, PSL University, CNRS Institute of Chemistry for Life and Health Sciences Laboratory for Inorganic Chemical Biology 11, rue Pierre et Marie Curie F-75005 Paris, France

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The development of new anticancer drugs is a fast-developing field of research. In this work, we aim at developing new bimetallic complexes to act as a photosensitizer (PS) for photodynamic therapy (PDT). Polymetallic complexes can overcome the drawbacks of the currently established PDT PSs, such as low efficiency and poor body clearance rate. The combination of two metals is offering the possibility to overcome these drawbacks.

Yutong LI

Functional Micro and Nanoparticles: Preparation and Biological Applications

PhD advisor: Jean-Maurice MALLET

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In cancer therapies, many effective drugs will have many serious side effects (such as vomiting, aplasia, neurotoxicity) after being taken. These severe side effects are due to the absorption of chemotherapeutic agents by both healthy and cancerous cells. Targeting tumor cells, therefore, appears to be a critical point in reducing the toxicity for surrounding healthy cells. Thus, the challenge is to bring the drug to the right place and to release it locally at a therapeutic concentration. The objective of the thesis is to prepare and evaluate bioactive and biodegradable nanoparticles to deliver

drugs to a specific type of cell. This shuttle will have a reservoir that will contain the active drug, a decorated surface targeting the right type of cell (using specific peptides or carbohydrates), and an optimized delayed or controlled release mechanism. The biological activity will be evaluated in cell culture using different cell lines (for the treatment of cancer) and with various bacteria (for the antibiotic effect). The optimized construction will be evaluated in an in vivo model, in the topical treatment of cutaneous and mucous pathologies.

Juba SALHI

Isolated switchable polyoxometalates (POMs) on a nanoporous highly organized carbon substrate.

PhD advisor : Florence Volatron

Laboratory : Institut parisien de chimie moléculaire (IPCM)

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The aim of this research project is to develop a new material constituted of polyoxometalates deposited onto a substrate composed of highly oriented pyrolytic graphite (HOPG) nanostructured by self-assembled tristilbene based 2D network. In this system, POMs will be isolated from each other and it will be possible to address them individually, which will open the way for data information storage in single molecules. Indeed, POMs display remarkable switchable properties like photoreduction, magnetion…etc. To achieve this aim, several challenges have to be addressed, starting by the synthesis of the POMs, their functionalization with an organic tether to control their adsorption on the substrate, the imaging of the POMs/2D network assembly by STM before probing their physical properties with an STM tip.

Lucie GUILLAUME

Smart multi-catalytic systems for the production of biobased polymers

Dr Régis Gauvin, Pr Christophe Thomas

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Nowadays, most of the starting materials for the production of polymers such as polyesters come from fossil fuels. Because these resources are limited, the development of versatile processes for the conversion of bioresources to a large range of monomers is a crucial goal. In this context, organometallic catalysis is instrumental, thanks to its outstanding ability to achieve high degree of both stereoselectivity and mass control. Because a conventional synthesis of these polymers can be tedious, a smart approach such as tandem catalysis can be groundbreaking. Indeed, combining several complementary systems is a unique opportunity to perform series of chemical reactions with higher efficiency. Our approach will rely on the concept of metal-ligand cooperativity: with a single catalyst in a one pot reaction, diesters will be reduced to their corresponding diols and then will be polymerized via an acceptorless dehydrogenative coupling, leading to the targeted polymer. A major focus will be put on the initiating system design at the molecular level, to achieve efficient selectivity transfer during the polymerization process.

Jean BOUVET

Superoxide dismutase mimics: an integrated approach from chemical design to bio-activity in cells

PhD advisor: Clotilde Policar & Sylvie Demignot

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Crohn's disease is a type of inflammatory bowel disease (**IBD**). This lifelong affliction has no cure and heavily impacts life quality of patients. Previous researches have shown that, in this case, inflammatory response goes hand in hand with oxidative stress. Superoxide dismustase (**SOD**) is a metalloenzyme which catalyses the dismutation of the superoxide ion, belonging to reactive oxygen species (**ROS**), into dioxygen and hydrogen peroxyde: $2O_2^{\bullet -} + 2H^+ \Rightarrow O_2 + H_2O_2$. **ROS** are natural by-products of the metabolism and are known to have important functions in cell signalling and homeostasis. As **SOD** is an important part of cell antioxidant defenses, our lab hypothesized that supplementing cells with a mimic of this enzyme (**SODm**) could diminish oxidative stress as well as the inflammatory response. **Mn1** is the **SODm** designed by the lab and the team probed the anti-inflammatory effect. Thesis goal is to evaluate anti-oxidant activity and anti-inflammatory properties of several **SODm**, previously designed, on cellular model. Probing **Mn1** as well as **SODm** anti-inflammatory and anti-oxidant properties is not only a step for a possible **IBD** cure. Designing redox-active therapeutic agents opens up new perspectives for all diseases related, near or far, to oxidative stress: Parkinson, Alzheimer, atherosclerosis, ADHD, cancer and many more...

Steffi SEWSURN

Bioengineering of metabolic pathways of pyrrocidines, derived from a fungal PKS-NRPS, for the study and generation of chemical diversity in this family of compounds.

PhD advisor: Didier BUISSON[1], Stéphane MANN[2]

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Laboratory: Laboratoire Molécules de Communication et Adaptation des Micro-organismes (MCAM) du Muséum National d'Histoire Naturelle. 63 Rue Buffon 75005 Paris

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The filamentous fungus Acremonium zeae, an endophyte of maize, is capable of producing pyrrocidines. These metabolites have antifungal properties and antibiotics against phytopathogens in maize, thus conferring a protective role on the endophyte on maize against phytopathogens. The biosynthesis of these compounds involves a hybrid PKS-NRPS mega enzyme assisted by various auxiliary enzymes. A cluster of genes encoding these enzymes has been identified in the laboratory. The objective of this project is based on the bioengineering of the metabolic pathways of pyrrocidines, for the study and generation of chemical diversity in this family of compounds.

Diana MELIS

Development of water-soluble Re-chelating ligands for ^{188}Re-based radiopharmaceuticals.

PhD advisor: Gilles Gasser (PSL), Andrew Burgoyne (SCK CEN) and Maarten Ooms (SCK CEN)

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Current first-line treatments for cancer, such as chemotherapy and external beam radiation therapy, come with major side effects which often damage healthy cells. The focus of cancer treatment is therefore shifting towards more personalized, targeted therapies such as Targeted Radionuclide Therapy (TRNT). Over the past few years, several therapeutic radionuclides have been evaluated for their potential application in TRNT and, among them, ^{188}Re has emerged as one of the more promising radionuclides. It emits β^--particles with a maximum range of about 11 mm in soft tissue, making it well-suited for radiotherapy when effective deep tissue penetration is required. To avoid the off-target accumulation of the radiometal, conjugation of ^{188}Re to a vector is crucial. This is typically achieved using a bifunctional chelator which has both a strong metal-binding moiety and a chemically reactive functional group for the covalent attachment of a targeting biomolecule. Aqueous solubility and stability of these complexes is often an issue; therefore, the aim of this project is to develop new and novel water-soluble bifunctional chelators for ^{188}Re. This should help achieve the overall objective of improving the current practice in radiolabelling radiopharmaceuticals using ^{188}Re.

Mae Féo Robin

New non-innocent ligands for C─H bond activation catalysis by iron complexes

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The project aims to develop new catalytic methods for the formation of C─C bonds through functionalization of C─H bonds using unusual iron complexes featuring low oxidation states, stabilized by participative Fe=Z (Z = O, S, NR) ligand, in the presence of organic electrophiles. Links between the electronic structure of the involved complexes (redox state, spin state) and the observed reactivity will be closely investigated. Such a project naturally covers several chemistry areas, from organometallic chemistry to catalysis, including mechanistic investigations (using NMR, EPR and Mössbauer spectroscopies, as well as theoretical modelisation).

Ichrak EL HAJ BRAHIM

Thesis Title: Stereoselective preparation of 2-alkynylaminoalcohols-1,3 for an approach synthetic (-) – stemoamide.

PhD advisor: Dr Olivier Jackowski and Pr Franck Ferreira (thesis co-supervisor)

Laboratory: Sorbonne University, Faculty of Sciences and Engineering, Parisian Institute of Molecular Chemistry (UMR CNRS 8232) "Organometallic Reactivity and Catalysis for Synthesis" team 4 place Jussieu. 75 252 Paris Cedex 05, France

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The subject of the thesis is part of access to 2-alcynylaminoalcohols-1,3. Two complementary approaches will be considered. the first will be based on the extension of the previous methodology to the stereoselective reaction of 4-hydroxy-1- allenylborane with imines to give 2-alcynylaminoalcohols-1,3. In the second approach, the first step will be to study the reaction of diastereoselective silylborylation of acetylene aziridins to access 4-amino-1-allenylborane. the use of the latter for the stereoselective preparation of 2-alcynylamininoalcools-1,3 by reaction with aldehydes will then be considered.

Maria Dalla Pozza

Selective photo-cleavage of DNA for gene therapy

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Gene therapy is a medical field focused on inserting normal genes into the genome, replacing or altering mutated genes that cause disease. The manipulation of nucleic acids is of main importance for gene therapy and different methodologies of genetic engineering have been developed in the last decades. One of these strategies is the use of triplex forming oligonucleotides (TFOs) to target DNA in a specific site. This PhD project proposes to use novel Ru(II)-polypyridyl compounds, already known to be photoactive DNA binders, that can be linked to artificial TFOs and can act as selective nucleic acid photo-nucleases for gene therapy. The aim of the project is to develop new breakthrough methods for gene editing, obtaining inorganic materials for targeting DNA cleavage triggered by light (photo-cleavage).

Xueyan Zhang

Novel Catalytic Silylation Reactions with Silyldiazenes

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The last twenty years have witnessed growing interest in the direct functionalization of unactivated C–H bonds that allows the introduction of functional groups without substrate pre-activation. In particular, the direct silylation of C–H bonds is an especially attractive transformation because organosilanes are stable compounds used in various applied fields. Fundamentally, most of these C–H functionalization reactions rest on a C–H metalation elementary step, which is challenging both in terms of reactivity and selectivity. The latter challenges have traditionally been overcome either by using stoichiometric amounts of highly reactive Grignard or organolithium reagents or catalytic amounts of expensive transition metal-based complexes. The present doctoral project aims at providing and studying a novel molecular

platform, namely silyldiazenes, which are able to generate under mild conditions potent s-block metalation agents that could be catalytically regenerated upon C–H silylation of organic substrates.

Marco DI MATTEO

Development of selective C-H Activations on terpenes: application to the synthesis of cannabinoid natural products and analogs

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The project is part of the European Consortium "C-H Activation for Industrial Renewal" and concerns the valorisation of terpenes via C-H activation. It is therefore a project focused on industrial development. In particular, it aims at developing new protocols that allow selective and predictable oxidations on terpenes, with a special focus in allylic oxidations. Acyloxylation and aminations will be firstly studied *via* homogeneous catalysis with Pd, Ni, Cu, Fe or Mn salts. We wish then to apply the developed selective methods to the total synthesis of cannabinoid natural products such as cannabidiol (CBD) as well as analogues.

Hong-Phong DUONG

Carbon monooxide conversion to multicarbon products: towards selective catalysts

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Electrocatalytic conversion of carbon dioxide (CO_2) has attracted much attention owing to its ability to convert the greenhouse gas into multicarbon products such as ethanol and ethylene without requiring high pressure and temperature. Considering the mechanism of CO_2 reduction, carbon monoxide (CO) is the first intermediate generated before reaching further products. In addition, the use of CO in an aqueous alkaline electrolyte could alleviate the proton reduction, which occurs with the use of CO_2, thus reducing the efficiency of the target reactions. In this research, several home-made copper based electrocatalysts will be studied and coupled with a customized flow cell reactor to achieve a high faradaic yield of CO conversion into ethylene and other multicarbon products.