– Journée de Rentrée 2022 de l'ED406 –

Mercredi 23 mars 2022 à 9h30

Amphithéâtre Moissan – PSL, Chimie ParisTech

Livre des résumés

Alice AM

Development, characterization and in vitro to in vivo evaluation of a novel theranostic peptide-based nanostructures for cancer therapy

PhD advisor: Anne Varenne, Bich-thuy Doan

Laboratory: UMR 8060 Institute of Chemistry for Life and Health Sciences, 11 Rue Pierre et Marie Curie, 75005 PARIS

alice.am@chimieparistech.psl.eu

The PhD project presents an innovative approach to design and validate novel theranostic agents based on self-assembled biocompatible multifunctional nanopeptides. The use of flow chemistry will allow controlled synthesis and functionalization of these peptides, and their physico chemical features will be well characterized for their biomedical applications. Functionalities that will be integrated include drugs, ligands, imaging probes, which will lead to a true theranostic agent.

Anna-Mélodie DONNART

Dual magnetic and redox molecular switches for molecular electronics

PhD advisor: Rodrigue Lescouëzec ; Volodymyr Malytskyi

Laboratory: ERMMES team, IPCM, 33-43 5th floor

anna-melodie.donnart@sorbonne-universite.fr

These last years, the ERMMES team has developed original cubic switches showing multiple accessible redox and magnetic states. The aim of this PhD is to use these molecules to design original devices. On one hand, we will explore the formation of ultra-thin films deposited on conductive surfaces, to target electronic device prototypes (eg. resistive memories). The chosen synthetic pathway involves diazonium salts ($-N_2^+$), which are very reactive. Two approaches will be studied: the synthesis of diazonium-bearing complexes, then grafted on surfaces ; and the functionalization of a surface with diazonium-functionalized ligands, which would then react with the complexes. On the other hand, we will develop supramolecular networks whose integration into devices could lead to electrochemical sensors. Those networks are formed through functionalization of the switches by coordinative groups.

Alvaro LOPEZ SANCHEZ

Development of Pt(IV) conjugates of oxaliplatin and redox modulators as anticancer agents with reduced neurotoxicity

PhD advisor: Hélène Bertrand

Laboratory: Laboratoire des Biomolécules (SU, ENS-PSL, CNRS) 24 rue Lhomond, 75005 PARIS

alvaro.lopez-sanchez@ens.psl.eu

Oxaliplatin-induced peripheral neuropathy (OIPN) is one of the main dose-limiting side effects of oxaliplatin, a first-line Pt(II)-based anticancer agent that is widely used for colorectal cancer and that has shown efficacy towards cisplatin-resistant tumors. Its mechanism of action relies on cell cycle arrest mainly due to its ability to bind DNA's nitrogenous bases. However, a burst in oxidative stress is also generated when oxaliplatin is applied, and it has been thought to be one of the factors implied at the origin of OIPN. Therefore, my PhD

project relies on this hypothesis and it will consist on the synthesis, characterization, in vitro and in vivo evaluation of new Pt(IV) compounds that will combine oxaliplatin and redox modulators (mainly small Mn(II) complexes that mimic superoxide dismutase (SOD), one of the main antioxidant enzymes of our organism). This will include Pt(IV) chemistry, starting from the chemical synthesis in round bottom flasks, but also cell biology in order to evaluate the toxicity, cell penetration and antioxidant activity of the synthesized compounds, as well as in vivo experiments on a mice model to test their efficacy. Finally, an analytical approach is also considered in order to understand the intracellular faith and biomineralization processes of Pt and Mn in cells.

Pablo MSELLEM

Molecular tweezers for multifunctional switchable organogels

PhD advisor: Guillaume VIVES (IPCM), Clément GUIBERT (LRS)

Laboratory: IPCM, GOBS team

pablo.msellem@sorbonne-universite.fr

Gels are soft materials composed of a liquid trapped in the three-dimensional network of a solid. Recently, organogels have attracted great interest due to their applications as new soft materials. This class of gels results from the self-assembly of low molecular weight gelators (LMWG) into fibrous gel networks. The main objective of this doctoral project is to exploit the mechanical motion of switchable molecular tweezers carrying gelling groups to obtain multifunctional switchable organogels. The large structural reorganization driven by the opening and closing motion of the tweezers should modulate their gelation properties by promoting inter- or intramolecular interactions between tweezers depending on their conformation. By using emissive functional units bearing transition metals, reversible luminescent gels that can be activated by external stimuli are aimed to be obtained.

Yaping CHENG

Luminescent NHC-Coinage Metal Complexes Containing Organic Chromophores:Towards Panchromatic Emitters For OLED Devices

PhD advisor: Hani AMOURI

Laboratory:IPCM CC 229 Bâtiment 32-42 – 4ème étage, 4 place Jussieu, 75252 Paris

e-mail address: yaping.cheng@sorbonne-universite.fr

In my PhD project, we designed novel family of panchromatic emitters of de type [L'-M–≡–Ar]. In these compounds the organic chromphore is based on pyrene or pyrelene, which are highly luminescent organic chromophores. Moreover the presence of strong s-donor ligands of the type "acetylide-Ar" enhances the stability of the molecule and amplifies the luminescence properties of the coinage metals as well. Moreover, we expect to induce Au---Au aurophilic interactionswhich should also provide low energy emission properties ithe red region of the visible spectrum.

Marie HUYNH

Synthesis and Characterization of Radioactive Auger-Emitter Ruthenium Bioconjugates in view of Delivery to the Nucleus of Cancer Cells for Cancer Treatment

PhD advisor: Pr. Gilles Gasser, Dr. Benjamin Gibert

Laboratory: Chemical Inorganic Biology team, I-CLeHs, Chimie Paris Tech – 11 rue Pierre et Marie Curie 75005 Paris

marie.huynh@chimieparistech.psl.eu

Recently, new antitumoral therapies using radioactive isotopes are emerging and taking advantage of decay modes such as alpha-particle emission or electronic capture, which gives way to Auger-electron emission, to target cancer cells. In this project, we will synthesize novel bifunctional chelators to develop Ruthenium-radiolabeled bioconjugates. These bioconjugates will target the nucleus of cancer cells, where the Auger-electron emitter property of radioactive Ruthenium would act to kill them efficiently.

Marcel ANNEREAU

Silica Nanoparticle – photoinduced CO releasing molecule – sugar conjugates: towards a new approach for the treatment of liver cancer

PhD advisor: Dr Michèle Salmain and Dr Vincent Corcé

IPCM ChemBio, Sorbonne Université

4 place Jussieu, 75252 Paris Cedex 05

marcel.annereau@sorbonne-universite.fr

Carbon monoxide (CO) is known in the popular culture as an odourless lethal gas, earning his name of "silent killer". Since the past decade, CO has emerged as a promising therapeutic agent for anticancer treatment when administrated in optimal concentrations. However, due to its gaseous form, CO remains difficult to handle. To overcome this issue, Carbon Monoxide Releasing Molecules (CORMs) have emerged as a suitable mode of administration of CO. Even more efficient are CORMs delivering CO upon a given external stimulus, such as visible light, i.e. PhotoCORMs. On this basis, the objective of this PhD thesis is to encage PhotoCORMs within silica nanoparticle-based (SiNPs) nanocarriers for the selective delivery of a toxic dose of CO to hepatocellular carcinoma (HCC) cells. These SiNPs find increasing utility as drug delivery systems due to their ease of synthesis, size control and porosity, biocompatibility and versatile surface chemistry. Spatial control of CO delivery will be ensured by decorating the SiNPs with galactose or *N*-acetylgalactosamine ligands to take advantage of their affinity for ASGP-R, overexpressed in HCC cells. This will allow multivalent presentation of the sugar entities to the surface of HCC cells thus increasing the efficiency of their cell uptake.

Clara TESTARD

Synthesis and characterization of tren-bridged cyclodextrin regioisomers for enantioselective applications

PhD advisor: Pr. Matthieu Sollogoub, Dr. Yongmin Zhang

Laboratory: IPCM, GOBS team, 4 place Jussieu, 75005 Paris

clara.testard@sorbonne-universite.fr

Our group developed NHC-bridged cyclodextrins (CDs) that complex transition metals inside their cavity. The resulting complexes are active in catalysis and display interesting chemo-, regio-, and stereo-selectivities. It was proved that the 2-point bridging of CD induces an helicoidal distortion of its cavity, and that this distortion accounts for the observed stereoselectivity. However, no control of the stereoselectivity was possible through 2-point bridging as it can only lead to a distortion into a M-helix.

The goal of my PhD project is to bridge the cavity of the CD asymmetrically in three points using a tripodal moiety such as a tren group, in order to obtain mirror image cavities with opposite enantioselectivities.

Using a synthesis previously developed in the lab, we propose to synthesize two pseudo-enantiomeric tren-bridged CD-metal complexes and study their enantioselectivity in catalysis or molecular recognition.

Xinyu Zhang

Tandem Catalysis for Advanced Materials Synthesis: New Modular Approaches

PhD advisor: Regis GAUVIN

Laboratory: Thomas Group. COCP, Institut de Recherche de Chimie Paris (IRCP),11 rue Pierre et Marie Curie

e-mail address: xinyu.zhang@chimieparistech.psl.eu

Due to the serious situation of worldwide plastic pollution, biodegradable polymers and derived hybrid materials are in great requirement for the next decades. By using metal based tandem catalysts and supported molecular systems, we will synthesize new polymeric materials with original properties. As a first application, from these new biodegradable polymers, we will design self-assembled nanostructures from weak interactions. Following molecular engineering of initiating sites within supported systems, we will also produce hybrid materials and probe their affinity towards biomolecules.

Florian LHOSTIS

High-pressure electrochemical reduction of CO_2 to formic acid and *in situ* conversion of formic acid

PhD advisors: Prof. Marc Fontecave, Dr. Ngoc Huan Tran

Laboratoire de Chimie des Processus Biologiques, Collège de France, 11 pl. Marcelin Berthelot

florian.lhostis@college-de-france.fr

This Veolia-funded PhD project aims at developing efficient and robust metallic electrocatalysts for the selective reduction of CO_2 to formic acid in industry-compatible conditions (i.e current densities > 100 mA.cm^{-}

^{2}). For this project, a prototype of high-pressure electrochemical cell is being developed. By performing electrolysis under elevated CO_2 pressure, high current densities can be reached, and these specific conditions also open the path for the *in situ* conversion of formic acid into other products, particularly methanol which is difficult to produce by direct CO_2 electroreduction. The molecular catalyst necessary for formic acid to methanol conversion is being developed by collaborators in CEA Saclay, and our common goal is to find the right conditions for both catalysts (the electrocatalyst and the molecular catalyst) to work simultaneously in order to have a proof of concept that methanol can be produced via this innovative path.

María BALLARIN MARION

Gold catalysis under visible light

PhD advisors: Louis Fensterbank, Virginie Mouriès-Mansuy and Cyril Ollivier

Laboratory: Institut Parisien de Chimie Moléculaire, 4 Place Jussieu, 75005 Paris

maria.ballarin_marion@sorbonne-universite.fr

Gold(I) catalysis is an efficient method of activating π-bonds and generally leads to products resulting from the protodeauration of the organogold intermediate. In situ post-functionalization of the organogold intermediate is desirable, for instance via cross-coupling reactions. This implies a Au(I)/Au(III) cycle which is difficult to establish as Au(I) complexes are remarkably reluctant to oxidative additions due to the high redox potential of the Au(III)/Au(I) couple (E^0 = 1.41 V). Recently, our team has developed a new type of dual catalysis (gold/photocatalysis) in which the photoactivation step involves an energy transfer (photosensitization) instead of a redox process. My PhD project aims to extend this new dual catalysis to different heteroaromatic nucleophiles, such as 1,3-diketones and carboxylic acids, as well as to evaluate other unsaturated compounds, such as allenes. Among possible fields of application, carbohydrate and nucleoside derivatives would constitute valuable targets.

Yupeng FU

Photosensitive & Steric-selective Bimetallic Ruthenium Catalyst based on Cyclodextrin

PhD advisor: Matthieu Sollogoub, Yongmin Zhang, Sylvain Roland

Laboratory: Glycochimie Organique Biologique et Supramoléculaire (GOBS)

4 Place Jussieu, 75005 Paris, couloir 42-43 5ème étage

e-mail: matthieu.sollogoub@sorbonne-universite.fr

The bimetallic ruthenium complexes have been developed as photosensitive catalysts along with other transition metals. These types of compounds could be applied in many realms including chemistry, energy and biology, exhibiting great prospects. Previously our group reported series of bimetallic complexes based on NHC-modified cyclodextrins (CD) and their steric selective catalytic effects which derive from the size of CD. We also proved that the electron communications in these conjugated bimetallic complex systems could influence the catalyzation. In this project, we manage to combine the photosensitivity of ruthenium complex and the steric selectivity of CD, synthesizing a bimetallic complex to catalyze reactions under light control. Thus, we could manipulate the catalytic process by controlling the irradiation and obtain specific isomer due to the CD steric selectivity.

Rebecca CHURAMANI

Supramolecular assemblies of functionalized cyclodextrins for transfection.

PhD advisors: Pr. Matthieu Sollogoub, Dr. Pierre-Alexandre Driguez

Laboratory: IPCM, Team GOBS, 4 place Jussieu, 75005 Paris

e-mail address: rebecca.churamani@sorbonne-universite.fr

A well-known barrier to genetic material treatments is the low efficacy of the transfection agents used, whether viral or not. Non-viral synthetic vectors are always cationic polymers. It allows to neutralize the negative charges of the nucleic acids and to ease the penetration of the cells. However, in these systems, cytotoxicity has been encountered. Therefore, an ideal transfection agent should be both polycationic and non-polymeric. To reconcile this apparent antinomy, this work focuses on the use of supramolecular polymers of cationic units based on multifunctionalized cyclodextrins. These molecules have been shown to compact DNA (150 kbp), interact with siRNA, transfect siRNA and form stable and well-defined assemblies with RNA/DNA (6-72mers). The goal of this PhD project is to develop novel transfection agents by improving the existing systems. To do so, different directions are considered. The optimisation of the molecular block, the nucleic acids interaction, the cellular uptake, the endosomal escape and the targeting. To achieve this, the combination of synthetic chemistry and supramolecular assemblies with biological testing is essential.

Emile ESCOUDÉ

Exploring the Unique Reactivity of Geometrically Constrained Phosphorus Compounds

PhD advisor: Dr Laurence Grimaud and Dr Maxime Vitale

Laboratory: Laboratoire des biomolécules (École Normale Supérieure de Paris 24 rue Lhomond 75005 Paris)

emilebabao@gmail.com

In this work, geometrically constrained phosphorus and boron compounds will be synthesized and studied by the means of NMR and electrochemistry. These T-shaped phosphorus compounds are known for their unique amphiphilic properties which confer them the ability of performing formal oxidative addition in protic compounds such as amines and alcohols. We intend to use this unique property to activate the N-H or O-H bond and open the chemistry of alcohols and amine to radical based reactions through hydrogen abstraction transfer. The use electrochemistry or photochemistry could be of great interest to achieve such goal. We intend to develop a methodology in which these phosphorous compounds are used in a catalytic fashion. In a similar way we would like to develop a methodology in which a photogeneration of radicals by a constrained boron specie is used to perform a radical reaction.

Xueying LIU

High Performance Biobased Poly(meth)acrylates synthesized by One-Pot Approach

PhD advisor: Christophe M. Thomas

Laboratory: PSL University, Chimie ParisTech, CNRS, Institut de Recherche de Chimie Paris, 75005 Paris (France)

e-mail address: xueying.liu@chimieparistech.psl.eu

Shifting from petrochemical feedstocks to renewable resources can address some of the environmental issues associated with petrochemical extraction and make plastics production sustainable. Therefore, there is a growing interest in selective methods for transforming abundant renewable feedstocks into monomers suitable for polymer production. In this work, several kinds of biobased alcohols were empolyed to synthesis biobased poly(meth)acrylates. Though adjusting the molar ratio of as-prepared bio-monomers, biopolymers with different glass-transition temperature (Tg) and thermal decomposition temperature ($T_{5\%}$) will be obtained.

Sofia Frida RUSSI

Electronically active thin-films based on cubic switches

PhD advisor: Rodrigue LESCOUEZEC, Volodymyr MALYTSKYI

Laboratory: 4 Place Jussieu, Équipe ERMMES, 33-43

sofia.russi@sorbonne-universite.fr

Recently, strong efforts have been made for the design of interfaces that could find potential applications in future electronic and spintronic devices through the deposition of magnetic switches onto surfaces. The aim of the PhD project is to develop an original and simple synthetic approach for the deposition of polymetallic magnetic switches to lead electronically-active (semi)-conductive thin-films deposited on conductive substrates. Thus, the focus is on the synthesis and characterization of cubic switchable complexes bearing electropolymerizable units (such as thiophene) in order to make possible electro-polymerization and electro-deposition of the obtained molecules on surfaces. To do this, different ligands will be considered in order to assess their qualities in terms of polymerisation and deposition. Once prepared, molecular complexes are going to be transformed into robust polymerized surface films. Those are going to be optimized and studied by AFM and c-AFM methods in order to probe their memristor properties.

Iulia COCOSILA

Molecular Catalysis for CO2 electroreduction

PhD advisor: Marc Fontecave, Yun Xu-Li

Laboratory: Chimie des Processus Biologiques, Collège de France

iulia.cocosila@college-de-france.fr

The main objective is the development of catalysts for the reduction of CO2. The products of the CO2 reduction could be used as a carbon source in organic chemistry or, as chemical storage of energy.
The project concerns the development of molecular systems based on organometallic complexes, their coupling with imidazolium functions (or analogues) as ionic liquid, and their grafting on electrodes.

This project involves organic synthesis (the ligands and their modification in order to introduce imidazolium groups and functionalities allowing the grafting of the catalyst on the electrode), organometallic synthesis (the development of complexes) and catalysis.
Finally, catalysts will be studied by electrochemical and photochemical techniques.

Thanaphon KHRUEAWATTHANAWET

Mixed (Anti)Aromaticity Unorthodox Interaction and Topologies

PhD advisor: Dr. Mickaël MÉNAND

Laboratory: Glycochimie Organique Biologique et Supramoléculaire (GOBS), Sorbonne Université, 4 Place Jussieu, 75252 Paris cedex 5 Couloir 42-43 5ème étage

e-mail address thanaphon.khrueawatthanawet@sorbonne-universite.fr

Aromaticity is a property of cyclic molecules containing π electrons which π delocalization reaches to lower energy. Conversely, antiaromaticity is a property of that of which π delocalization reaches to higher energy.[1] Due to instability of antiaromatic compounds, it is challenging to generate and handle them. However, porphyrinoid macrocycles made of pyrrole subunits are known to stabilize such property. For example, Shinokubo developed antiaromatic norcorrole skeleton with high stability.[2] Recently, our research team also studied this property with hybrid molecules composed of a cyclodextrin and an hexaphyrin subunits. Previously, we showed that those hybrids were behaving as switchable Hückel (Anti)Aromatic systems,[3] adaptable hosts,[4] dual-responsive devices[5] and were able to induce chiral preference in Möbius topology.[6] Now, we aim to use this family of molecules to study unorthodox antiaromatic π-type interactions. For this purpose, we planned to synthesize a 3D dimeric hybrid embedding an (anti)aromatic confined space able to generate unorthodox interactions (Host-guest interaction, cation-π interaction, etc.).

Alessia MORI

Selective C-H functionalization of furfural and its derivatives

PhD advisor: Oble Julie

*Laboratory: Équipe **ROCS,** Sorbonne Université, 4 Place Jussieu, 75252 Paris cedex 5 Couloir 32-42 4ème étage*

alessia.mori@sorbonne-universite-fr

Furfural and 5-hydroxymethylfurfural (HMF) are renewable products derived from lignocellulosic biomass, which are raw materials for sustainable production of high value-added chemicals. Their selective functionalization is currently an emerging field and subject of many research efforts. A special quest for stabilizing substituents at C3 and/or C4 positions of furanic platforms is essential to improve chemical and thermal stability of the furanic core. Our goal is to develop methods to achieve the selective borylation at C3 position of furfurals by transition metal-catalysed C-H activation exploiting the aldehyde function to install a directing group. This strategy provide access to reagents that can be used as nucleophilic partners in cross-couplings, as well as serve as directing agent for transition-metal-catalysed C4-H functionalizations. The development of this method is crucial for solving the important practical problem of furans instability and pave for the synthesis of new biomass derived building block and consecutively for new industrial applications.

Kanokon Upitak

Tandem Catalysis: a New Approach to Biodegradable Polymers from Renewable Resources and towards bio-related nanostructures

PhD advisor: Prof. Dr. Christophe THOMAS

Laboratory: Institut de Recherche de Chimie Paris (IRCP), ENSCP Chimie Paris Tech-CNRS

11 rue Pierre et Marie Curie, 75231 Paris Cedex 05, France

e-mail address: christophe.thomas@chimieparistech.psl.eu

Tandem catalysis, which involves the sequential or concurrent action of two or more catalytic cycles in a single reactor to yield a product with minimum workup, or change in conditions, has attracted much attention in recent years. The main objective of this research program is to study the conversion of renewable resources into novel biodegradable polymers through the use of chemo- and stereoselective tandem catalytic systems. Moreover, This project aims to synthesize a new achiral iron complex and investigate the influence of the ligand substituent on the catalytic performance for the one-pot polymerization of cyclic ester monomers and methyl methacrylate.

Mikaël LE ROCH

Structure and reactivity of low-valent Zn(I) systems

PhD advisor: Fabrice CHEMLA / Stéphanie HALBERT

Laboratory : Institut Parisien de Chimie Moléculaire (ROCS Team) and Laboratoire de Chimie Théorique

Mikael.le_roch@sorbonne-universite.fr

The proposed combined experimental and theoretical research project is focused on the examination of the reactivity of low-valent Zn(I)- and Mg(I)-based bimetallic compounds, with a particular interest in the potentialfor the functionalization of C–C multiple bonds and the controlled reduction of carbonyl or imine functions toaccess umpoled -hydroxy- or -amino anion equivalents. The idea is to use theoretical chemistry in parallel of experimental chemistry in order to understand the mechanism and the influence factors.

Yiyi ZHANG

Selective Tumor Delivery of Metal-based Photosensitizers for the Combination of Photodynamic Therapy and Immunotherapy

PhD advisors: Prof. Gilles Gasser: Dr. Bich-Thuy Doan

Chimie Paristech, PSL University, CNRS, Institute of Chemistry for Life and Health Sciences, Teams ICB & SEISAD, 75005 Paris

e-mail address: yiyi.zhang@chimieparistech.psl.eu

Nowadays, chemotherapy, photodynamic therapy (PDT), photothermal therapy (PTT) and immunotherapy are the main methods for tumor treatment. However, monotherapy has a limited effectiveness. During a photodynamic therapy treatment, reactive oxygen species (ROS) produced by photosensitizers (PSs) are the keys to kill tumor cells. It was reported that ROS also play an important role in immunotherapy, including polarizing macrophages, activating dendritic cells (DCs), etc. Therefore, the combination of PDT and

immunotherapy is expected to produce an enhanced effect. In this project, a metal-based PDT PS capable of inducing an immune response will be used and linked to a chemotherapeutic agent to elicit an immune effect. Chemistry design, chemical characterisations, in vitro to in vivo evaluation, histology will be implemented to assess these combined therapies.

Laora BOULO

New supra-molecular anti-adhesive agents against SARS-CoV-2

PhD advisor: Pr. Matthieu SOLLOGOUB & Pr. Vincent CALVEZ

Laboratory: IPCM, 4 Place Jussieu 75005 PARIS

laora.boulo@sorbonne-universite.fr

The aim of this project is to design and synthetize new anti-adhesive agents to prevent viral infections, in particular by SARS-CoV-2, the causative virus of COVID-19. This pathogen has a deactivating interaction with sialic acid. The anti-adhesive strategy is based on a multivalent effect with sialic acid conjugated to macro-structures in order to increase its interaction with the virus and thus to decrease its pathogenicity. However current polymeric agents imply solubility and toxicity issues. This thesis project aims to use functionalized self-assembling cyclodextrins to form non-covalent and multivalent supramolecular assemblies in order to overcome the drawbacks of polymeric agents. Preliminary results have been obtained with a first system which will be optimized during the thesis. The possible optimizations imply the use of other sugars or proteins to improve the interaction with the virus.

Amal LAKHAL

Access to new polycyclic structures by radical cascade reactions triggered by trifluoromethylation under photoredox catalysis

PhD advisor: Cyril OLLIVIER, Louis FENSTERBANK

Laboratory: MACO, IPCM 4 Place Jussieu, 75252 Paris cedex 5

amal.lakhal@sorbonne-universite.fr

The synthesis of compounds containing a fluorine atom or a trifluoromethyl group is very attractive, as it allows access to molecules with biological activity. In this project we are particularly interested in trifluoromethylation reactions under photocatalyzed conditions. We are focusing on ynamides, a sub-class of alkynes as the starting material for the radical reaction. Our aim is the development of cascade reactions initiated by radical addition of a trifluoromethyl group on the ynamide, which allows the formation of high structural complexity in a single step under mild conditions.

Yandong MA

Polymer nanoparticles with chemiluminescence resonance energy transfer (CRET) for photodynamic therapy (PDT)

PhD student: Yandong MA

PhD supervisor: Min-Hui LI

Laboratory: Institut de Recherche de Chimie Paris (IRCP)

e-mail address: yandong.ma@chimieparistech.psl.eu

Photosensitizers in the form of molecules or incorporated in nanoparticles (colloids) have been used in photodynamic therapy (PDT). However, the use of light as trigger needs special optical equipment and light presents limited depth of tissue penetration. Moreover, if short wave lengths should be employed, their biocompatibility poor. To address these issues, we propose to develop PDT polymer nanoparticles with chemiluminescence resonance energy transfer (CRET), where the photosensitizer is chemiexcited instead of photoexcited. The polymer nanoparticles can be polymer micelles or vesicles. The polymer nanoparticles contained a photosensitizer (energy acceptor) such as Ru complexes or aggregation-induced emission (AIE) photosensitizer and a donor such as luminol or Bis[3,4,6-trichloro-2-(pentyloxycarbonyl)phenyl] Oxalate (CPPO) through chemical conjugation or encapsulation. Mechanistically, H_2O_2 and myeloperoxidase (MPO) rich in the tumor microenvironment trigger CRET and the production of singlet oxygen ($^1O_2$) that can kill cancer cells. The thesis work includes chemical syntheses, study of self-assembly, physical chemical investigation of PDT polymer nanoparticles AIE feature and ROS-generation, etc.), and their biochemical study (toxicity, PDT effect in vitro and in vivo).

Alexandre SIMON

New developments in electrosynthesis and photosynthesis for multicomponent processes (MCRs)

PhD advisor: Maxime Vitale/ Laurence Grimaud

Laboratory: LBM UMR 7203. 24, rue Lhomond 75005

e-mail address : alexandre.simoncs@gmail.com

Recently, encouraged by the contemporary standardization and affordability of electrochemical apparatus, electrosynthesis is becoming a multipurpose technology applicable to the preparation of both bulk and fine chemicals. On one hand, the development of electrochemically-induced multicomponent reactions (Electro-MCRs) has known sporadic developments so far. It is a considerable shortage when considering that MCRs typically proceed with high atom and step economy, high reaction efficiency and, thereby, nearly faultlessly meet the concept of “ideal synthesis”. Hence, our first objective will be to explore isocyanide-based multicomponent ractions “Electro-IMCRs”. Indeed, isocyanides are particularly appealing considering their prominent use in multicomponent processes and their remarkable high stability in a wide range of positive potentials.

William PARISOT

Development of new iron catalysts for asymmetric reductions and cycloaddition reactions

PhD advisor: Virginie Vidal et Phannarath Phansavath

Laboratory: Institute of Chemistry for Life and Health Sciences, 11 Rue Pierre et Marie Curie, 75005 Paris.

william.parisot@chimieparistech.psl.eu

The first goal of this project is to develop new chiral iron complexes which will be used in highly enantioselective hydrogenation and transfer hydrogenation of organic substrates, leading to a variety of targets of synthetic and pharmaceutical interest. In order to ensure the robustness and the versatility of the system, various classic liquid hydrogen vectors will be used as well (e.g. formic acid, Hantzsch esters, cyclohexa-1,4-diene) as H_2 surrogates. The second part of this project will be devoted to the development of new iron-catalyzed arene rings construction by [2+2+2] alkyne cyclotrimerization. Construction of aromatic molecules by [2+2+2] cycloadditions is an extremely atom-economic method, and several iron(0)-catalyzed systems have already been reported in the past. Our goal is to extend the scope of this methodology, since the use of iron(0) catalysts can hamper the transformation of functionalized substrates bearing easily reduced groups or acidic functions (e.g. aldehydes, ketones, alcohols).

Norbert REIHANIAN HADANY

Use of organometallic chemistry for the synthesis of chiral nanocatalysts applied to imine and ketone reduction.

PhD advisors : Dr. Marc PETIT (IPCM) and Dr. Caroline SALZEMANN (MONARIS)

Laboratories : Team MACO (IPCM UMR 8232, 32-42, 5ème étage), Team NARCOS (MONARIS UMR 8233, 34-44, 3ème étage)

Email adress : norbert.reihanian_hadany@sorbonne-universite.fr

Enantioselective catalysis is one of the most efficient processes to access the chiral molecules needed in pharmaceutical industry. Despite being the incontestable leader in laboratory small scale synthesis, homogeneous catalysis represents only 20% of the most relevant industrial processes contrary to heterogeneous catalysis. This is due to the fact that heterogeneous catalysis permits an easier recycling of the catalyst and a minimization of metal leaching as well as a low cost. This project is based on a mild and tunable nanoparticles (NPs) synthesis by dismutation of $[CoCl(PPh_3)_3]$, recently developed in the laboratory, on 3d metals such as Co, Ni and CoNi alloys. In a first place, the aim is to develop chiral ligand tuned NPs to induce chirality in reduction reactions. In a second place, the aim is the development of new Co(I) complexes including one chiral ligand to induce chirality during the dismutation process to access to new and chiral NPs.

Raphaël LABIDI

Towards CO_2 reductases: combining proteins and synthetic catalysts

PhD advisor: Marc Fontecave

Laboratoire de chimie des processus biologiques

raphael.labidi@gmail.com

The project consists in the isolation, purification and characterization of proteins, to combine them with metallic cofactors and to test their catalytic activity for CO2 reduction and H2 production.

Fan YANG

Smart multi-catalytic systems for the production of biocompatible polymers

PhD advisor: Christophe THOMAS

Laboratory: COCP, Chimie Paris Tech

e-mail address: fan.yang@chimieparistech.psl.eu

Biocompatible materials such as polyesters and polyamides hold a prominent position in the portfolio of specialty and commodity polymers. Controlling their structural features such as chain size and microstructure is key in establishing specific properties. In this context, organometallic catalysis is instrumental, thanks to its outstanding ability to achieve both high degree of stereoselectivity and mass control. Smart approaches such as tandem catalysis can be game changers: Combining several complementary systems is a unique opportunity to perform series of chemical reactions with higher efficiency. In this project, hydrogen borrowing, a clean, atom-economical technology, will be harnessed in a first step to synthesize lactones or lactones monomers from biosourced raw materials. These will then be polymerized via stereoselective ring opening polymerization, affording novel polyesters or polyamides. A strong emphasis will be put on the design of novel organometallic catalysts based on Earth-abundant metals, as well as on establishing catalysts structure and polymers' physicochemical properties relationships.

Francisca FIGUEIREDO

Synthesis of copper complexes for *in cellulo* photocatalysis

PhD advisors: GASSER Gilles, CARIOU Kevin

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

francisca.figueiredo@chimieparistech.psl.eu

My PhD project aims at developing photoactivatable reactions *in cellulo* by using a family of water-soluble copper complexes. More particularly, the photo-oxidation of relevant naturally occurring compounds in water and in biological media will be studied by using specifically designed biocompatible light-activatable copper complexes. A particular focus will be put on molecules whose regulation could be exploited for the therapy of diseases. Therefore, the project also aims at exploring light-induced copper-catalysis to induce cell/bacteria death. In this setting, light is a traceless and benign way for targeting specific cells, bacteria or tissues, opening new avenues in the treatment of different types of diseases such as Alzheimer, Parkinson, autoimmune diseases, diabetes or cancer.

Zhihang ZHANG

Graphene-based quantum dots as new generation of theranostic agents

PhD advisor: Anne Varenne, Laura Trapiella-Alfonso, Bith-Thuy Doan, Fanny d'Orlyé ,Camille Lescot

Laboratory: Team SEISAD, ICLeHS, UMR 8060 , ENSCP -Université PSL

zhihang.zhang@chimieparistech.psl.eu

In recent years, we are living an exhaustive and deeper research on Carbon-based nanomaterials for bioimaging applications due to their high biocompatibility, water solubility, and exciting properties. Particularly, graphene quantum dots (GQDs) have gain attention thanks to their photo-physical properties (e.g., photoluminescence, up-conversion and photo-thermal that makes them good candidates for bioimaging purposes and therapy as well. Regarding the synthesis, although several methods have been proposed to produce GQDs (top-down & bottom-up approaches) several issues remain to be addressed such as the improvement of the photo-luminescent quantum yield, the batch-to-batch reproducibility, the control of the size/shape production and thus the control of the properties, and the expansion of the optical window from the UV-vis to the NIR region, among others. Rationalizing the interrelationship between the synthetic process by the study of the impact of different parameters (e.g., synthetic methodology, precursors, reaction time and temperature, doping heteroatoms, etc.), the final structure (type, edges effect, stacking) and observed properties is highly demanded because this connection remains unclear. This step is crucial in the development of good candidates for bioimaging and therapy.The main objective of this proposal is to conduct a rational study of the impact of synthesis parameters into the GQDs structure and properties relationship to shed new light on the mechanisms involved in their growth and photo-physical properties for the development of multimodal imaging nanoprobes.

Hugo MADEC

Design/synthesis of water-soluble and photoactivatable Cu complexes based on modified cyclodextrins for *in cellulo* applications

PhD advisor: Dr. Sylvain Roland Pr. Matthieu Sollogoub

Laboratory: Glycochimie Organique Biologique et Supramoléculaire

e-mail address : hugo.madec@sorbonne-universite.fr

The project aims at developing photoactivatable reactions *in cellulo* by using a family of water-soluble copper complexes based on modified cyclodextrins (CDs). More particularly, the oxidation of thiols into disulfide compounds in water and in biological media will be studied by using specifically designed biocompatible light-activatable copper complexes. A particularly relevant biological thiol is glutathione (GSH) whose regulation could be exploited for the therapy of diseases. Therefore, the project also aims at exploring light-induced copper-catalysis to induce cell/bacteria death through GSH oxidation, which will disrupt the redox imbalance of the cell. In this setting, light is a traceless and benign way for targeting specific cells, bacteria or tissues, opening new avenues in the treatment of different types of diseases such as Alzeihmer, Parkinson, autoimmune diseases, diabetes or cancer.

Sun JIE

New electrochemical devices for the detection of emerging pollutant

PhD advisor: Cyrine Slim, Sophie Griveau, Yvette Tran

Laboratory: SEISAD, i-CLeHS, 11, rue Pierre et Marie Curie – 75005 PARIS

jie.sun@chimieparistech.psl.eu

Nowadays, the effect of emerging contaminants becomes serious. They are commonly present at trace concentrations and characterized by their long-term health effects, such as nervous system damage, toxicity, or cancer appearance because of their accumulation and persistence, even at very low concentrations. Until now, its detection essentially depends on conventional techniques, such as HPLC and GC-MS. They are expensive, time consuming and require experts. To deal with this problem, electrochemical methods are wildly applied owing to the advantage of easy integration, rapid response, simplicity, portable as well as low cost. The objectives of the thesis are to develop cheap, portable, sensitive, and selective electrochemical biosensors to detect trace level emerging pollutants.

The biosensor will be based on the principle of molecular recognition through the immobilization of synthetic antibodies (aptamers) which are specific to the required target thus improving the selectivity of the device. The immobilization of these aptamers will be achieved thanks to the use of matrices such as biocompatible polymers or metallic nanoparticles which will improve the sensitivity of the biosensor.

Baptiste NEIL

Catalytic Metalation of Unactivated C-H bonds with Silyldiazenes

PhD advisor: Clément Chauvier

Laboratory: Equipe MACO, Institut Parisien de Chimie Moléculaire, Sorbonne Université

4 Place Jussieu, 75005 Paris, France

baptiste.neil@sorbonne-universite.fr

Organosilanes have found applications in fields as diverse as materials chemistry or drug discovery and serve as stable intermediates in organic synthesis. Most organosilanes have traditionally been synthesized from the corresponding arylhalides (bromide or iodide) via stoichiometric reactions. The direct intermolecular silylation of C–H bonds represents an atom-economical alternative as it bypasses the substrate pre-functionalization step, yet poses significant reactivity and selectivity challenges, especially when it comes to devising catalytic protocols. The main objective of my thesis is to use silyldiazenes (R'-N=N-SiR_3) in association with a s-block based metal catalyst to metalate unactivated C-H bonds (pKa > 35). The metalated substrate can then be silylated in an overall catalytic process. The metalated substrate could also potentially react with an electrophile, which would potentially generate new C-C bonds. A significant part of my thesis will also be devoted to the synthesis of new diazenes and to mechanistic investigations.

Jiaxu ZHANG

Synthesis and Biological Study of Ganglioside GM3 Derivatives as Anticancer Vaccine Candidates

PhD advisor: Yongmin ZHANG, Matthieu SOLLOGOUB

Laboratory: Glycochimie Organique Biologique et Supramoléculaire (GOBS)

4 Place Jussieu, 75005 Paris, Couloir 42-43 5ème étage

e-mail address: jiaxu.zhang@sorbonne-universite.fr

Glycosphingolipids (GSLs) are cell-surface antigens, and it was therefore suggested that changes in their composition would result in changes in the antigenicity (ability to bind antibody) and immunogenicity (ability to induce immune response) of the tumor cells expressing them. The idea of GSLs as tumor associated carbohydrate antigens (TACAs) is the basis for attempts to utilize GSLs for anticancer vaccine development. Previously, a series of ganglioside GM3 analogues were synthesized and evaluated for anticancer activity. In this project, we plan to develop a new type of anticancer vaccine by using GM3 analogues as antigens. A series of glycoconjugates are planned to be synthesized which combine the glycosyl of GM3 analogues with highly immunogenic protein carriers.

Lucas BACHELEY

Valorization of vinyl halides in fine chemistry: application to the synthesis of polyfunctional high added value intermediates. Synthesis of oxygen-, nitrogen- and fluorine- containing heterocycles

PhD advisor: Virginie VIDAL, Phannarath PHANSAVATH

Industrial supervisor: Gerard GUILLAMOT

Laboratory: Institute of Chemistry for Life and Health Sciences (i-CLeHS), CSB2D Team

Chimie ParisTech-PSL, 11 rue Pierre et Marie Curie, 75005 Paris

lucas.bacheley@chimieparistech.psl.eu

The objective of this thesis is to valorize a new platform molecule of vinyl halide type to be used for the preparation of a range of polyfunctional intermediates which could be exploited industrially by the fine chemistrycompagny SEQENS, and on the other hand to access original high added value oxygen-, nitrogen- and fluorine- containing molecules.