SEPTEMBER 2022

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Attention: Please check the assigned rooms

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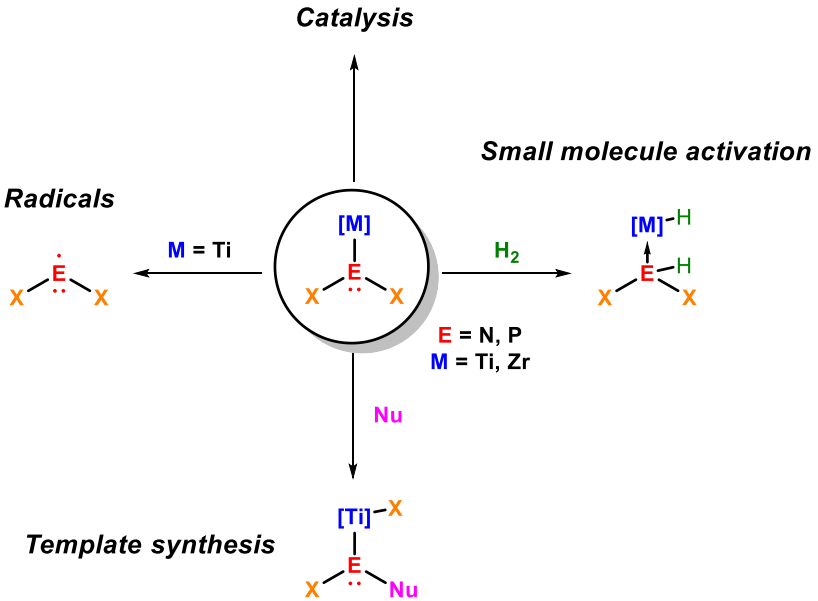
Sept. 12th, 11h
Room 101, 1er étage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Adrien NORMAND (Université de Bourgogne-Franche-Comté)
adrien.normand@u-bourgogne.fr

Ambiphilic group 4 amides and phosphides: synthetically usefullreagents and catalysts

Abstract. Metallic amides and phosphides can usually de described as Lewis basic/nucleophilic reagents. Yet, depending on the substitution pattern at the pnictogen atom, or the metallic fragment bound thereto, they can display ambiphilic properties, *i.e.* also act as Lewis acids/electrophiles.
We have been investigating the properties of Group 4 metals (Ti, Zr) amides and phosphides for a number of years. Their ambiphilic reactivity can be harnessed for the activation of small molecules (*e.g.* H_2, CO_2, alkynes, silanes,…) and eventually leads to exceptional catalytic activities in hydrogenation, dehydrogenative coupling or reduction reactions.
In the case of Titanium complexes, additional aspects of their chemistry includes: *i)* single electron transfer between the ligand and the metal, leading to the release of aminyl and phophinyl radicals; *ii)* the template synthesis of pincer-type ligands resulting from the coupling on an intrinsically ambiphilic phosphide ligand with Ti-activated terminal alkynes.



References: *J. Am. Chem. Soc.*, **2015**, *137*, 10796; *Chem. Eur. J.*, **2019**, *25*, 2803; *Chem. Sci.*, **2021**, *12*, 253; *Chem. Eur. J.*, **2021**, *27*, 18175; *Inorg. Chem.*, **2022**, *61*, 7642.

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Sept. 19th, 11h
Room 101, 1er étage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Paola B. ARIMONDO (EpiCBio – CNRS Institut Pasteur UMR3523 Chem4Life)
paola.arimondo@cnrs.fr

AntiDOTes for diseases: Chemistry and Biology match together to tackle Epigenetics

Abstract. Infectious diseases are a major health treat and there is a need to find innovative targets and new compounds targeting them. A common phenomenon in most microbial infections is the attenuation of the host's immediate immune response, allowing for long-term colonization. Many pathogens achieve this by manipulating the epigenetic regulation of the host. Indeed, pathogens either release factors that directly targets the host chromatin or hijack its epigenetic machinery, both resulting in alterations of the host epigenome. Thus, inhibiting these phenomena will give an advantage to the host and thus facilitate the elimination of the microbe. Importantly, epigenetic modifications, such as DNA and histone modifications, are reversible and modulate gene expression without changing the DNA sequence. This makes them ideal drug targets. In cancer treatment, epigenetic regulators (enzymes and chromatin-binding proteins) are already validated drug targets, with several molecules approved for clinical use. In the context of infection, drugs targeting chromatin have been explored very little. Among the major epigenetic modifications, there is the methylation of DNA and histones that play a key role in gene expression regulation.
We are synthetizing a specific chemical library targeting the methyltransferases of DNA and histone and setting-up biochemical and cellular assays to screen it. We developed a reliable chemical biology high-content imaging strategy to screen compound libraries simultaneously on multiple histone marks inside cells. Interestingly, this assay pointed out a synergistic interaction between two histone methyltransferases (CARM1 and DOT1L), suggesting possible effective synergistic drug combinations.
The inhibitors can be used either as chemical scalpels to probe the epigenetic mechanisms that are aberrant in the diseases or as potential leads for new therapeutic strategies. The design of the chemical library was successful as it allowed us identify two families of epigenetic inhibitors that are active against resistant parasite responsible of malaria and identify novel inhibitors of human DOT1L.

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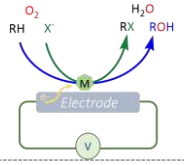
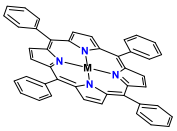
Sept. 26th, 11h
Room 101, 1er étage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Elodie ANXOLABEHERE (Laboratoire d'Electrochimie Moléculaire-Université Paris Cité)
elodie.anxolabehere@u-paris.fr

Electrochemical O_2 reductive activation with bioinspired metallic complexes

Abstract. The current economic and environmental contexts require to replace the energy demanding or harmful technologies often used in oxidation chemistry with economically viable and environmentally sound alternatives. In this context, we aim at reproducing metalloenzymes activities, such as the one of oxygenases. These enzymes are able to unravel the O_2 potent oxidizing power through the partial and controlled reduction of O_2 bound at a Fe site to efficiently and selectively oxidize organic molecules under mild conditions. Our strategy is to develop efficient catalysts for electrochemical O_2 activation using earth abundant transition metal catalysts. Such an objective requires deciphering the parameters that control the factors governing the reactivity of the catalysts and the nature of the intermediates. We address these questions through electrochemical methods coupled to spectroscopies. We illustrate our work with recent examples on O_2 reductive activation using Mn or Fe complexes and present promising results of electrocatalysis experiments substrates oxidation.





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OCTOBER 2022

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Attention: Please check the assigned rooms

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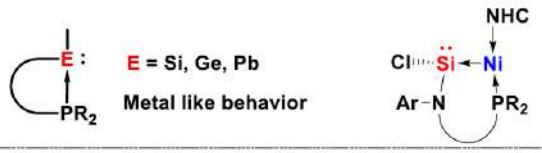
Oct. 3rd, 11h
Room 101, 1er étage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Tsuyoshi KATO (Laboratoire d'Hétrochimie Fondamentale et Appliquée -Université de Toulouse III Paul Sabatier)
tsuyoshi.kato@univ-tlse3.fr

Metal-like behavior of E(II)-complexes (E = group-14 elements) and transition metal-stabilized silylenes

Abstract. The transition metal-like behavior of non-metallic species is a current hot topic in chemistry. We have developed an original system of phosphine-based ligands that induces the particular properties of low valence group 14 species (E(II)-complexes), including their metal-like behavior. I will present their synthesis and reactivity as well as their applications in catalysis. I will also present some very recent results concerning the particular way to use transition metals to stabilize silylenes (divalent silicon species).



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For any information, please contact:
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Oct. 10th, 11h
Room 101, 1st stage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Nathalie GAGEY-EILSTEIN (Université Paris Cité)
nathalie.eilstein@u-paris.fr

Array-based sensors for Optical Fingerprinting: From Identification of Protein to prediction of pathological statues

Abstract. To this day, biosensors based on specific antibody-antigen interaction and enzymatic reactions continue to remain the 'gold standard' for a number of relevant biomolecules. However, these systems often suffer due to limited range of detectable analytes, low stability and high costs. Chemical sensors have thereby emerged as a new class of sensors where functional molecules containing a recognition element for analyte binding and a transduction element for generation of readily quantifiable signals are being used for detection and quantification of analytes. A 'chemical nose' sensor is one such subclass of sensors that provide an alternative array-based strategy using synthetic molecules/materials to mimic the functioning of the mammalian olfactory system. This kind of sensing, unlike specific sensing, works on the principle of selective binding between an analyte and an array of cross-reactive receptors to generate distinct responses – fingerprint - for each analyte. The output responses can then be linked back to the analyte through pattern recognition and machine learning algorithms. Therefore, enabling such systems to detect multiple analytes with relatively few sensor elements.[1,2]

I will present our sensors array based on the pan-selective molecular recognition feature of a cucurbit[7]uril (CB[7]) macrocyclic receptor covalently tethering with a library of fluorescent reporters. We first used this strategy to rapidly discriminate a diverse range of protein analytes. The macrocyclic sensor was then applied to probe conformational changes in the protein structure and identify the formation of oligomeric and fibrillar species from misfolded proteins. Ultimately, this sensor system predicted clinically relevant changes by fingerprinting serum samples from a cohort of pregnant women.[3]

(1) Lavigne, J. J.; Anslyn, E. V. Sensing A Paradigm Shift in the Field of Molecular Recognition: From Selective to Differential Receptors. *Angew. Chem. Int. Ed.* **2001**, *40* (17), 3118–3130.
(2) Wright, A. T.; Anslyn, E. V. Differential Receptor Arrays and Assays for Solution-Based Molecular Recognition. *Chem. Soc. Rev.* **2006**, *35* (1), 14–28.
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For any information, please contact:
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Oct. 17th, 11h
Room 101, 1er floor
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Carole DUBOC (CNRS, Univ. Grenoble Alpes)
carole.duboc@univ-grenoble-alpes.fr

Molecular bio-inspired complexes for the activation of small molecules

Abstract. The presentation will focus on the synthesis and characterization of thiolate-based transition metal complexes (M = Fe, Ni, Mn, Co), as well as the investigation of their reactivity. More precisely, it will highlight how the bio-inspiration approach can provide efficient, selective and robust catalysts for H_2 production, CO_2 reduction or O_2 reduction. An important part of the presentation will also be devoted to explain the importance of the understanding of the catalytic mechanism for rational design of systems with optimal performance, and how it can be determined.

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Oct. 24th, 11h
Room 101, 1er floor
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Luke MACALEESE (Université de Lyon)
luke.mac-aleese@univ-lyon1.fr

Lasers and Mass Spectrometry, some principles of action spectroscopy and applications across various fields of chemistry and biology

Abstract. Coupling light sources with mass spectrometers has long proven its interests in particular in the field of chemical physics where the photo-dissociation yield can be used as a readout for the optical properties of mass selected ions. Schematically, mass spectrometry is used to characterize the raw formula of a given, isolated ion while the energy range of the photons may be chosen to characterize its vibrational or electronic spectrum, reflecting information on its functional groups, its structure, conformation, metal oxidation state, etc.

Over the years and throughout multiple collaborations, our group in Lyon has worked on the development of multiple methods using various light sources and mass spectrometers both for pure analytical purposes (e.g. quantification and identification of biomolecules in complex media in collaboration with M. Girod and J. Lemoine at Institut des Sciences Analytiques in Lyon) and more fundamental applications including structural biology in the gas phase or, lately, chemical reactivity studies in the gas phase.

After a short introduction on action spectroscopy, with a special focus on the mechanisms at play for ion photo-dissociation in the visible range, a selection of examples will illustrate the large variety of fields to which the laser-MS coupling can be applied. First, some details will be given on the development of the action-FRET methods, with applications to the collaborative project MS SPIDOC in the field of native MS and protein structural characterization. Then, a time-resolved implementation of action spectroscopy will be shown that evidences how intramolecular proton transfer and conformational dynamics may be intricated in peptides. Eventually, we will describe the application of such a laser-MS coupling to the characterization of rhodamine 6G ion photo-excited states dynamics and its specific photo-reactivity via the formation of a long-lived triplet state. The latter theme will provide another, more chemical angle, opening towards the field of photo-catalysis.

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NOVEMBER 2022

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November 7th, 11h
Room 101, 1st stage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Frédéric FRISCOURT (Université de Bordeaux, IECB, ISM UMR5255)
f.friscourt@iecb.u-bordeaux.fr / www.friscourtlab.com

Exploiting Bioorthogonal Chemical Reporters for Controlling the Processing of Sialosides by Glyco-enzymes in Living cells

Abstract. Sialic acids are anionic nine-carbon carbohydrates generally found as terminal sugars of mammalian cell-surface glycoproteins and glycolipids. Because of their distinct cellular location, sialo-glycoconjugates (also known as sialosides) are often key mediators of physiological and pathological events, including cell adhesion, host–pathogen interactions, and cancer progression.
Due to the posttranslational nature of sialoconjugates, applications of classical biochemical imaging tools such as the use of fusion fluorescent proteins are not amenable for tracking these complex carbohydrates in living cells. The bioorthogonal chemical reporter strategy, which elegantly combines the use of metabolically labeled azido-sugars and highly reactive cyclooctyne probes, is emerging as a versatile technology for labeling and visualizing sialosides. This strategy relies on the fact that bioorthogonal chemical reporters are highly reactive species while being biologically noninvasive.
During this talk, I will present our recent efforts to show that chemical bioorthogonal reporters may actually impact sialosides processing enzymes activity, providing us with novel, more selective, chemical biology tools for studying and controlling the biological roles of cell- surface sialosides.

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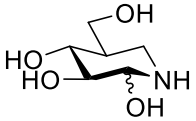
November 14th, 11h
Room 101, 1st stage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Mikael BOLS (Université de Copenhague)
bols@chem.ku.dk

Azasugars and the physical organic chemistry we can learn from them

Abstract. 1-Azasugars, such as Noeuromycin, are some of the most potent inhibitors of glycosidases binding thousands of times better to these enzymes than the substrate carbohydrates. The lecture will discuss the synthesis, the role of the crucial nitrogen atom in these molecules, their properties, and what these properties tell us about the chemical and biochemical behavior of carbohydrates and amine containing molecules.



K_i (almond β-glu): 69 nM
K_i (almond α-glu): 22 nM

Noeuromycin

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For any information, please contact:
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November 21th, 11h
Room 101, 1st stage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Jean-Marc VINCENT (Université de Bordeaux)
jean-marc.vincent@u-bordeaux.fr

Copper(II), benzophenone and sun: a good match for photolatent click chemistry, but not only.

Abstract. In the area of catalyst development a reactivity *vs* stability dilemma exists as extremely reactive catalysts are difficult to store/handle, which limits the scope of their use. This is particularly true for catalysis mediated by low-valent M(0/I) species possessing open coordination sites, whose oxygen sensitivity typically requires handling in a glovebox. To address this key issue, a powerful approach consists in developing photoreducible precatalysts.
In the lecture, our contribution toward this goal will be presented with a focus on copper catalysis. It will be shown that Cu(II) precatalysts which integrate a benzophenone photosensitizer in their structure could find their place in the chemist's toolbox. After presenting the synthesis of such complexes and their photoreduction properties, their scope and limitation for application in key transformations, including CuAAC, trifluoromethylation of alkenes and C(sp^3)–H alkylations will be described.

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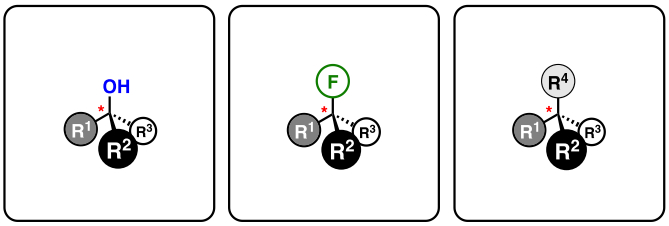
November 28th, 11h
Room 101, 1st stage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Cyril BRESSY (Aix-Marseille Université – Institut des Sciences Moléculaires de Marseille, iSm2, UMR7313)
cyril.bressy@univ-amu.fr

Kinetic Resolution: Amplification Phenomenon and Indirect Strategy

Abstract. To reach a high level of enantiopurity is often a difficult goal in enantioselective catalysis. For several years, we developed methodologies using amplification of enantioselectivity phenomenon in organocatalyzed acylation reactions. To use such amplification, the catalyst has to perform several consecutive transformations on a polyfunctional substrate. A desymmetrization can be combined in synergy with a kinetic resolution in *subtractive* amplification using *meso* substrates[1] or, two kinetic resolutions can be associated through an *additive* amplification starting from racemic substrates.[2]
To tackle synthetic challenges, such as the enantiocontrol of building blocks bearing a tertiary alcohol,[3] a fluorinated tetrasubstituted stereocenter[4,5] or a quaternary stereocenter,[6] indirect strategies were developed. Starting from diastereocontrolled racemic substrates, acylative kinetic resolutions were performed on a secondary alcohol adjacent to the targeted functions or motifs. Highly enantioenriched building blocks were obtained through these indirect strategies.



References: (1a) *Angew. Chem. Int. Ed.* **2014**, *53*, 766-770; (1b) *Org. Lett.* **2015**, *17*, 2118-2121; (2a) *Angew. Chem. Int. Ed.* **2017**, *56*, 16052-16056; (2b) *Angew. Chem. Int. Ed.* **2021**, *60*, 24924-24929; (3) *Org. Lett.* **2021**, *23*, 4332-4336; (4) *Chem. Eur. J.* **2022**, e202103874 (hot paper); (5) *Eur. J. Org. Chem.* **2022**, e202200031; (6) *Eur. J. Org. Chem.* **2022**, e202101475.

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DECEMBER 2022

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December 5th, 11h

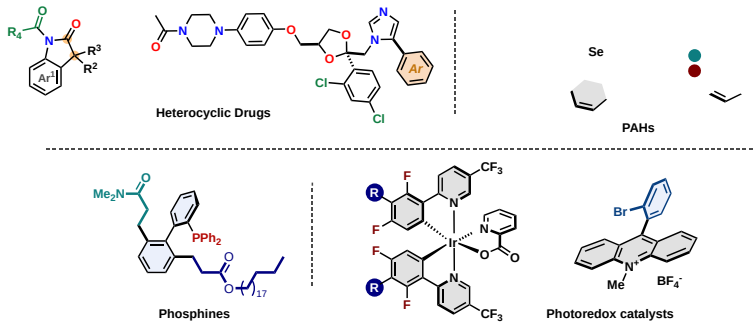
Room 101, 1st stage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

Jean-François SOULÉ (Chimie ParisTech | PSL University)
jean-francois.soule@chimieparistech.psl.eu

Catalytic C–H Bond Functionalizations to Improve Molecular Diversity, Materials and Catalysts

Abstract. Over the last decades, catalytic C–H bond functionalization methodologies have drastically improved the way to prepare intricate molecules.[1] However, one of the main challenges of this chemistry is the regioselectivity of the C–H bond functionalization. In this context, our research focuses on controlling and switching the regioselectivity with a minimum environmental impact by employing simple catalytic systems and reducing/avoiding additives, and use "non-conventional" directing groups. The regiocontrol is mainly accomplished through a catalyst-control *via* a rational design of novel ligands, catalysts, and reaction conditions.

This presentation will focus on our recent contributions to how the development of novel regioselective C–H bond functionalizations can reshape the access to improved molecules such as polycyclic aromatic hydrocarbon (PAH),[2] luminescent cyclometalated iridium complexes,[3] phosphines,[4] and acridinium-based photoredox catalysts.[5]



[1] a) J. Wencel-Delord, F. Glorius *Nature Chem* **2013**, *5*, 369–375; b) C.-S Wang,. P.H. Dixneuf, J.-F. Soulé *Chem. Rev.* **2018**, *118*, 7532-7585.; c) B. Li, A. I. M Ali, H. Ge *Chem* **2020**, *6*, 2591-2657; d) S. K. Sinha, S. Guin, S. Maiti, J.P. Biswas, S. Porey, D. Maiti *Chem. Rev.* **2022**, *122*, 5682-5841.
[2] W. Hagui, H. Doucet, J.-F. Soulé, *Chem* **2019**, *5*, 2006-2078.
[3] M. Peng, J. Lin, W. Lu, T. Roisnel, V. Guerchais, H. Doucet, J. F. Soulé, *Chem. Eur. J.* **2021**, *27*, 12552-12557.
[4] Z. Zhang, T. Roisnel, P. H. Dixneuf, J.-F. Soulé, *Angew. Chem. Int. Ed.* **2019**, *58*, 14110-14114.
[5] Y.-X. Cao, G. Zhu, Y. Li, N. Le Breton, C. Gourlaouen, S. Choua, J. Boixel, H.-P. Jacquot de Rouville, J.-F. Soulé, *J. Am. Chem. Soc.* **2022**, *144*, 5902-5909.

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SPECIAL SEMINAR

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December 8th, 11h

Room 101, 1st stage
Corridor 32-42
Campus P et M Curie
Sorbonne Université

Olivier BASLÉ (Laboratoire de Chimie de Coordination, LCC-Toulouse)
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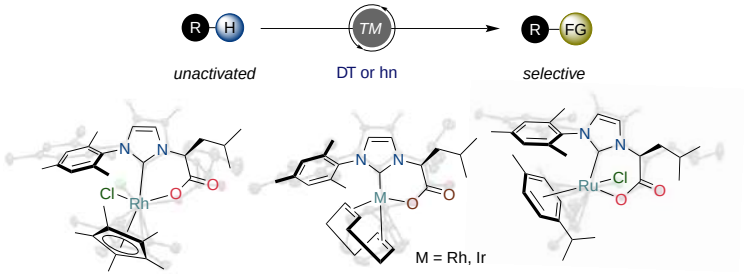
Bidentate NHC ligands for highly selective homogeneous transition metal-(photo)catalysis

Abstract. Over the past few decades, direct functionalization of carbon-hydrogen bonds has emerged as a preferred alternative to conventional cross-coupling reactions requiring pre-functionalized substrates. Moreover, photocatalysis offers the possibility to use visible light as a safe, abundant and renewable energy source.
Based on our expertise in the design of transition metal (TM) catalysts, we have recently developed a new class of *N*-heterocyclic carbene (NHC) ligands that have demonstrated utility in the preparation of particularly robust Ir(III) photocatalysts,[1] as well as in the development of efficient Rh(III) catalysts for the borylation of C-H bonds.[2] More recently, we discovered a visible light-induced regioselective C-H functionalization catalyzed at room temperature by a Rh(I) complex.[3] Following on from this study,[4] Ru(II) and Ir(I) complexes have demonstrated interesting catalytic activities in the regioselective borylation of arylphosphines[5] and in dehydrogenative directed C-H silylation of arenes,[6] respectively.



1. R. Manguin, D. Pichon, R. Tarrieu, T. Vives, T. Roisnel, V. Dorcet, C, Crévisy, K. Miqueu, L. Favereau, J. Crassous, M. Mauduit, O. Baslé, *Chem. Commun*. **2019**, *55*, 6058.
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5. J. Thongpaen,R. Manguin, T. Kittikool, A. Camy, T. Roisnel, V. Dorcet, S. Yotphan, Y. Canac, M. Mauduit, O. Baslé, **2022**, 58, 12082.
6. R. Manguin, M. Galiana-Cameo, T. Kittikool, J. Thongpaen, E. Bancal, S. Mallet-Ladeira, S. Yotphan, R. Castarlenas, M. Mauduit, J.-B. Sortais, O. Baslé, under review, **2022**.

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December 12th, 11h

Room 101, 1st stage
Corridor 23-24
Campus P et M Curie
Sorbonne Université

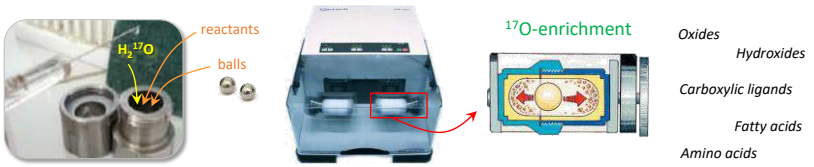
Danielle LAURENCIN (ICGM Montpellier)
danielle.laurencin@umontpellier.fr

Fatty acids, amino acids, nanoparticles, MOFs and more... from ^{17}O isotopic labeling using mechanochemistry to high resolution NMR analyses

Abstract. Oxygen is everywhere. It is present in the vast majority of natural and synthetic molecules and materials, forming covalent, ionic, coordination or hydrogen bonds with neighboring atoms. Thus, in order to be able to rationalize and optimize the structure and properties of different systems, it is important to finely identify oxygen bonding environments.

Oxygen-17 NMR spectroscopy appears as ideally suited for this purpose. However, it intrinsically suffers from a very poor sensitivity, the natural abundance of ^{17}O being only 0.04%. This implies that ^{17}O-labeling is most-often necessary to perform high resolution analyses. Unfortunately, up until recently, the most-widely used labeling protocols suffered from various drawbacks, including (very) high costs, long reaction times, and/or constraining chemical reactions or experimental set-ups.

In recent years, we have focused our research on implementing cost-effective and user-friendly ^{17}O-labeling protocols based on mechanochemistry.[1] We have shown that ball milling procedures are highly attractive for the ^{17}O-labeling of a variety of organic and inorganic compounds, using microliter quantities of ^{17}O-enriched water, and working under ambient temperature and pressure. Here, some of our most recent examples will be presented, from the isotopic labeling of key biomolecules (fatty acids and amino acids), to the ^{17}O NMR study of grafted nanoparticles and of coordination networks like MOFs.[2-5]



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[5] "From *operando* Raman mechanochemistry to "NMR crystallography": understanding the structures and interconversion of Zn-terephthalate networks using selective ^{17}O-labelling", C. Leroy, T.-X. Métro, I. Hung, Z. Gan, C. Gervais, D. Laurencin, *Chem. Mater.* **2022**, *34*, 2292-2312.

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For any information, please contact:
Dr Cyril Ollivier, Sorbonne Université, Campus Pierre et Marie Curie, Tour 32-42, 5ème étage, case 229, 4 place Jussieu, 75005 Paris. ☎ 01 44 27 38 50. Courriel : cyril.ollivier@sorbonne-universite.fr

JANUARY 2023

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Attention: Please check the assigned rooms

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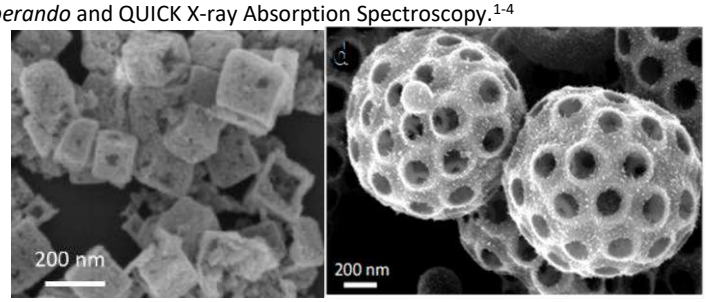
January 9th, 11h
Room 101, 1st stage
Corridor 32-42
Campus P et M Curie
Sorbonne Université

Marion GIRAUD (ITODYS, Université Paris Cité)
marion.giraud@u-paris.fr

Porous Ir-based electrocatalysts for the production of hydrogen: synthesis and study by X-ray absorption spectroscopy

Abstract. Proton Exchange Membrane Water Electrolysis (PEMWE) technology is the ideal technology to produce H_2 in a "zero-carbon" and renewable manner. Indeed it can be coupled with intermittent electricity production modes and allows for the production of ultra-pure H_2 at a high rate. However, the operating conditions of PEMWE systems are very demanding, especially at the anode of the device where H_2O is oxidized into O_2 at very high pH and potential. IrO_2 is the only catalyst material that offers high efficiency and high stability in these drastic anodic conditions; but it suffers from scarcity and high cost.

In the recent years, we have developed different synthetic ways to achieve the formation of porous Ir-based materials with two purposes: (i) a very high surface area to maximize the atomic utilization of Ir and (ii) a suitable architecture to be implemented in the catalytic layers of real PEMWE devices. A special attention has been paid to unraveling the mechanism of formation of these porous materials as well as their structure-properties relationships by the use of several advanced techniques and in particular *in situ*, *operando* and QUICK X-ray Absorption Spectroscopy.[1-4]



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2. "Aerosol synthesis of thermally stable porous noble metals and alloys by using bi-functional templates", Odziomek, M., *et al.*, *Mater. Horizons*, **2020**, 7, 541-550. doi: 10.1039/C9MH01408J.
3. "The origin of the high electrochemical activity of pseudo-amorphous iridium oxides", Elmaalouf, M., *et al.*, *Nature Commun.*, **2021**, 12, 3935. doi: 10.1038/s41467-021-24181-x.
4. "Green synthesis of water splitting electrocatalysts: IrO2 nanocages via Pearson's chemistry", Elmaalouf, M., *et al.*, *Chemical Science*, **2022**, 13, 11807-11816. doi: 10.1039/D2SC03640A.

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For any information, please contact:
Dr Cyril Ollivier, Sorbonne Université, Campus Pierre et Marie Curie, Tour 32-42, 5ème étage, case 229, 4 place Jussieu, 75005 Paris. ☎ 01 44 27 38 50. Courriel : cyril.ollivier@sorbonne-universite.fr

SPECIAL SEMINAR

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January 12th, 16h
Room 101, 1st stage
Corridor 32-42
Campus P et M Curie
Sorbonne Université

Martin ALBRECHT (University of Bern)
martin.albrecht@unibe.ch

Design and Application of NHC based Ligands for Organometallic Reduction and Oxidation Catalysis

Abstract. While catalytic reductions (hydrogenation, hydroelement functionalizations) are very well understood mechanistically and many high activity catalysts are available nowadays, oxidation catalysis is much less developed. This is due in parts to the mechanistic complexity of oxidation reactions (substrate recognition, multistep multi-electron transformations), and in other parts due to the harsh conditions for oxidation reactions, requiring catalysts with a specific set of properties that impart high activity and high robustness. In the search of suitable ligands that meet these criteria, we have become particularly intrigued by ligands that can formally adopt either a neutral or a zwitterionic form. Through their different bonding modes, these ligands provide opportunities to (transiently) store protons and electrons, which is an excellent prerequisite for mediating oxidation reactions. The presentation will demonstrate the potential of these donor-flexible ligands to induce challenging bond activation catalysis for synthetic and energy-related applications such as water oxidation, CO2 reduction, and recently also CH bond amination.

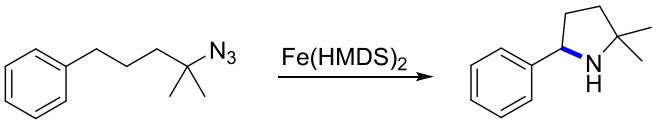

Figure 1: Catalyst optimization for the intramolecular C–H amination by Fe(HMDS)2

References:

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S. Bertini, M. Rahaman, A. Dutta, P. Schollhammer, A. V. Rudnev, F. Gloaguen, P. Broekmann, M. Albrecht *Green Chem.*, **2021**,*23*, 3365-3373.

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For any information, please contact:
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January 16th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

JOURNEES DE CHIMIE MOLECULAIRE 2022 … SUITE

1. **Jean BOUVET**, Laboratoire des Biomolécules – ENS
Sorbonne Université/PSL Université Paris
Jean.bouvet@ens.psl.eu
Cu peptides as SOD mimics

2. **Elodie DAVID**, Institut Parisien de Chimie Moléculaire et
Institut de Biologie Paris Seine
Sorbonne Université
elodie.david@sorbonne-universite.fr
Design and pharmacological evaluation of neuropsin inhibitors (Kallikrein-related peptidase 8) as therapeutics and potential diagnosis tools for Alzheimer's Disease and associated dementias

3. **Thomas DEIS**, Institut Parisien de Chimie Moléculaire
Sorbonne Université
thomas.deis@sorbonne-universite.fr
Martin's Spirosilane-based Pentacoordinated Organosilicons: Synthesis, Optical Resolution & Configurational Stability

4. **Sonia KHEMAISSA**, Laboratoire des Biomolécules
Sorbonne Université/PSL Université Paris
sonia.khemaissa@sorbonne-universite.fr
Arg/Trp cell-penetrating peptides incorporating Trp analogues: internalisation properties and interactions with cell membrane components

5. **Diana MELIS,** Institute of Chemistry for Life and Health Sciences (i-CLeHS), Chimie ParisTech
PSL Université Paris
diana.melis@chimieparistech.psl.eu
Development of an in-house $^{188}W/^{188}Re$ generator for ^{188}Re production and its use in the production of ^{188}Re-radiopharmaceuticals

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For any information, please contact:
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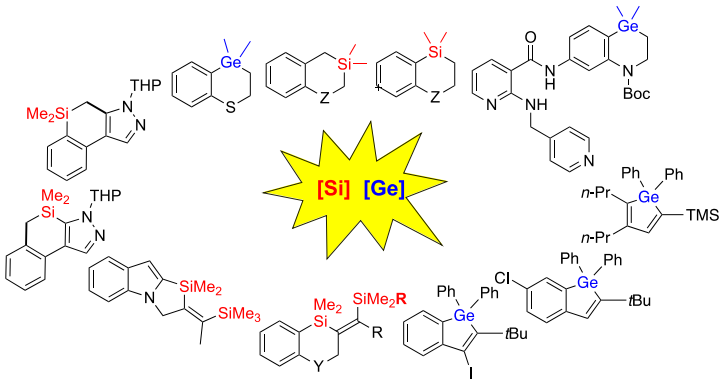
January 23rd, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Muriel DURANDETTI (Université de Rouen)
muriel.durandetti@univ-rouen.fr

Efficient access to Silylated or Germylated heterocycles

Abstract. Carbon, silicon and germanium atoms have structural similarities (valence, geometry), which are at the origin of an isostery between them. Recently, our group has engaged in a research program devoted to the access to silylated or germylated heterocycles through cyclization reactions, the presence of silicon/germanium atom being known to increase the lipophilicity of silylated/germylated molecules compared to their carbon analogues. We first developed a convenient access to silylated and germylated heterocycles based on an anionic rearrangement.[1] Then, we developed a cyclization process, involving a C–H activation step on a sp^3 carbon under palladium catalysis. In this reaction, the C–H bonds of a trimethylsilyl group were involved.[2] Later on, we developed intramolecular regio- and stereoselective silapalladation reactions of alkynes, starting from disilanes.[3] The oxidative addition of Pd(0) into the Si–Si bond provides, after cyclization and reductive elimination, heterocyclic derivatives in good yields, as single (*Z*) isomers, through a *syn* addition process. Currently, our interest is focused on a simple access to germoles by treatment of *o*-alkynyl aryldiphenylgermanes in the presence of diethylzinc and AIBN as radical initiator.[4] Interestingly, the application of this process to more challenging alkynes, led to a polar germylzincation process, without the need for a radical initiator. This presentation will focus on our recent contributions to the development of silylated and germylated heterocycles.



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4) S. Kassamba, A. Perez-Luna, F. Ferreira and M. Durandetti, *Chem. Commun.* 2022, **58**, 3901–3904.

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Dr Cyril Ollivier, Sorbonne Université, Campus Pierre et Marie Curie, Tour 32-42, 5ème étage, case 229, 4 place Jussieu, 75005 Paris. ☎ 01 44 27 38 50. Courriel : cyril.ollivier@sorbonne-universite.fr

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January 30th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Carlos AFONSO (Université de Rouen)
carlos.afonso@univ-rouen.fr

Ion Mobility and Mass Spectrometry: How to reach the 3rd dimension?

Abstract: https://www.lab-cobra.fr/annuaire/afonso-carlos/
https://www.lab-cobra.fr/equipes/analyse-et-modelisation/

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For any information, please contact:
Dr Cyril Ollivier, Sorbonne Université, Campus Pierre et Marie Curie, Tour 32-42, 5ème étage, case 229, 4 place Jussieu, 75005 Paris. ☎ 01 44 27 38 50. Courriel : **cyril.ollivier@sorbonne-universite.fr**

FEBRUARY 2023

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Attention: Please check the assigned rooms

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February 6th, 11h
Amphi Chaudron
Chimie ParisTech – PSL
11, Rue P et M Curie

Bouchemal KAWTHAR (IRCP, Chimie ParisTech)
kawthar.bouchemal@chimieparistech.psl.eu

Morphology controlled nanomaterials to navigate mucosal barriers

Abstract. Drug delivery to mucosal barriers is preferred in comparison with invasive parenteral routes. However, designing drug carriers to avoid dilution with physiological fluids and mucus clearance still represents an unmet challenge. Nanomaterials (NMs) coated with mucoadhesive polymers have shown their ability to partially address these problems due to their small size and mucoadhesive surface. However, while NM size and surface properties have been extensively studied, there is a lack of investigations on the morphology-dependent behaviors of NMs toward mucosal barriers. The strategy we envisioned is to consider the morphology of NMs as a relevant parameter to reach mucus avoiding dilution with biological fluids, accumulating at high concentrations close to the mucosal epithelium and internalized by epithelial cells. Understanding whether NM morphology impacts their transport into the mucus and mucoadhesive behaviors requires robust technological tools to manufacture NMs with controlled properties. In this context, our research group has recently developed complementary processes to design morphology-controlled NMs with simultaneous control of aspect ratio, size, and versatile surface modification. Nonspherical particles, denoted as nanoplatelets, were formed by supramolecular and hierarchical self-assembly in water of polysaccharides hydrophobically modified with palmitic acid and α-cyclodextrin. Nanoplatelets have flat surfaces, sharp edges, and a high aspect ratio (~20), as characterized by AFM. We revealed that NMs with a nonspherical morphology exhibited different physical and biological behaviors than spherical particles. Indeed, the nanoplatelets had faster mobility in biological fluids and higher cell internalization. They exhibited faster bioadhesion than spherical particles. Using real-time in vivo imaging on a rat model, we revealed that nanoplatelets had a longer residence time in the intestine and in the bladder compared to spherical particles. Finally, we showed that the nanoplatelets did not exhibit the same biological behaviors as spherical particles to treat mucosal infections and inflammation.

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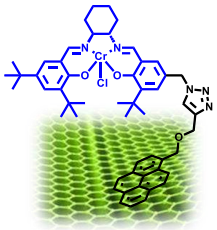
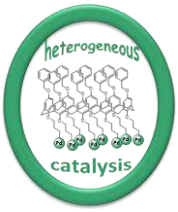
February 13th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Emmanuelle SCHULZ (Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay)
emmanuelle.schulz@universite-paris-saclay.fr

Homogeneous supported (asymmetric) catalysis

Abstract. The role of organometallic catalysis allowing the targeted production of high value-added products no longer needs to be demonstrated, but the fine chemicals sector dedicated to health applications remains very demanding for innovative and sustainable synthesis routes. On the one hand, the search for an efficient synthesis of enantioenriched functionalized molecules is still topical. Making precious chiral catalysts insoluble and therefore easily recoverable and reusable is an elegant way to answer the principles of green chemistry and sustainable development. On the other hand, obtaining minimal residual traces of metal in the target products is another important objective. Most transition metals are indeed toxic species, and their presence in valuable chemicals is accurately regulated, depending on their mode of administration. Additionally, residual amounts of metals can interfere with subsequent synthetic steps of the process. It is in this context that we work on the one hand on different modes of immobilization of chiral salen complexes and study their efficiency in the heterogeneous catalysis of enantioselective formation of C-C, C-O and C-N bonds. Since cross-coupling reactions are prevalent tools in the fine chemical industry, we also propose the synthesis and the evaluation of the catalytic activity of Pd–NHC complexes covalently grafted on calix[8]arene supports in Suzuki-Miyaura and Buchwald-Hartwig reactions.





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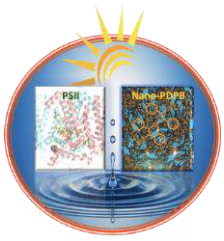
February 20th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

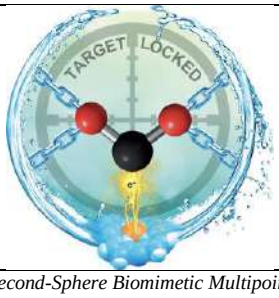
Ally AUKAULOO (Université Paris-Saclay)
Ally.aukauloo@universite-paris-saclay.fr

New Directions to Development of Photocatalytic CO_2 Reduction

Abstract. Photosynthesis is the process that uses sunlight as sole energy input to flush carbon dioxide (CO_2) from our atmosphere and convert it into a chemical energy vector. In my talk I will focus on examples how we are learning lessons from natural systems ie. enzymes involved in the transduction of energy and designing new molecular catalysts and nonstructured systems to replicate these functions.



Biohybrid approaches for energy conversion and 2020 Chemical Science HOT Article Collection



Second-Sphere Biomimetic Multipoint Hydrogen-Bonding Patterns to Boost CO2 Reduction of Iron Porphyrins (ANIE 2020)

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February 27th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Cyrille COSTENTIN (Université Grenoble Alpes)
cyrille.costentin@univ-grenoble-alpes.fr

Molecular catalysis of electrochemical reactions: principles and applications to small molecules activation.

Abstract. The basic principles of molecular catalysis of electrochemical reactions based on the use of cyclic voltammetry as an analytical tool for fast processes and constant potential spectro-electrolysis for slower processes will be first presented. Several examples will then be discussed: (i) catalysis of CO_2 reduction with iron porphyrins (FeTPP) including recent developments involving reactivity of Fe(I)TPP; (ii) catalysis of N_2O-to-N_2 conversion illustration the role of ligand exchange in the self-moderation of catalysis.

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CULTURCHEM

MARCH 2023

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Attention: Please check the assigned rooms

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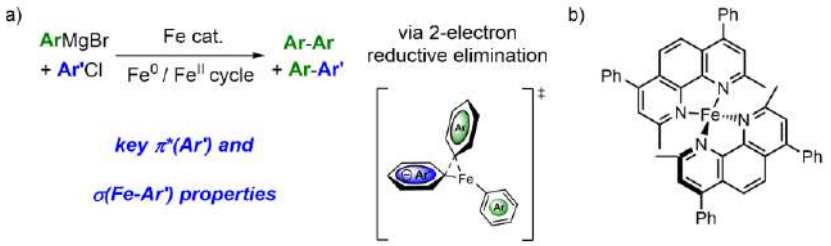
March 6th, 14h
Amphi Chaudron
Chimie ParisTech – PSL
11, Rue P et M Curie

Guillaume LEFEVRE (Chimie ParisTech, CNRS)
guillaume.lefevre@chimieparistech.psl.eu

Juggling with iron (not so) well-defined oxidation states : the curse and the blessing of Fe-catalyzed C-C bond formations

Abstract. Iron catalysis is of high interest in a context of green and sustainable chemistry, owing to the low cost and toxicity of this metal. However, in numerous catalytic processes, the reactive iron species are usually air- and moisture-sensitive, thermally unstable, making their characterization and monitoring rather difficult. Moreover, such complexes can also accommodate several spin multiplicities, leading to a large panel of paramagnetic structures. Those considerations lead to a mechanistic understanding of Fe-mediated processes which is still in its infancy, important milestones being still to be met in this field. We will discuss in details how physical-inorganic methods such as ^{57}Fe-Mössbauer, EPR and multinuclear paramagnetic NMR spectroscopies, associated with theoretical modellings, allowed us to map and govern the reactivity of new sensitive iron species with low oxidation states (from Fe^0 to Fe^{II}). A focus will be put on some recent systems that were recently investigated in our group, which led to the full characterization of the first iron-mediated cross-coupling sequences relying on genuine two-electron processes (Scheme 1a), and to the development of a new thermally stable non-innocent neutral $(N,N)_2Fe$ species, able to promote cycloaddition transformations (Scheme 1b). In both cases, significant improvements in the mechanistic understanding and the rational design of the iron coordination sphere were drawn from physical-inorganic experiments, which helped us to unlock new catalytic patterns.



Scheme 1

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For any informations, please contact:
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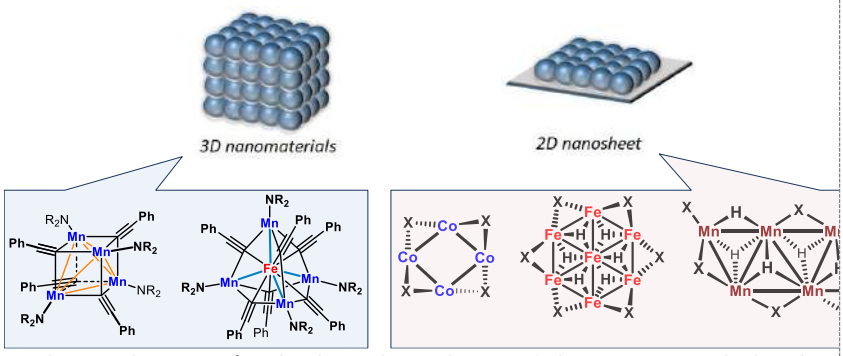
March 9th, 14h30
Room 101
T 56-66
Campus P et M Curie
Sorbonne Université

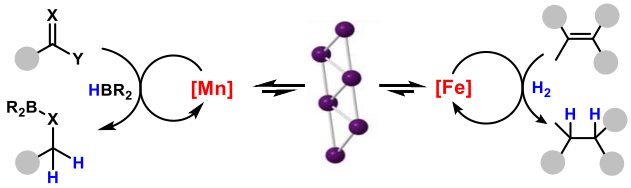
Axel JACOBI VON WANGELIN
(Dept. of Chemistry, University of Hamburg, Germany)
axel.jacobi@uni-hamburg.de

3d Metal Amides becoming Nanoclusters & Catalysts

Abstract. Metal nanoclusters have recently gained a strong foothold in the field of nanoscience due to their unique structural, magnetic, and catalytic properties. Discrete metal clusters constitute nanoscale snapshots of cluster growth but are especially rare owing to rapid aggregation or decomposition pathways. We have developed a synthetic strategy that enables the rapid and high-yielding access to 3d metal nanoclusters (M = Mn, Fe, Co; n = 4-8).[1]



Catalytic applications of such 3d metal complexes and clusters were studied in the context of hydrogenations, oligomerizations, and hydroborations.[1]



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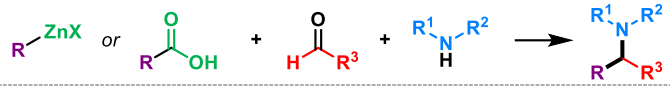
March 13th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Marc PRESSET (Institut de Chimie et des Matériaux Paris-Est - Université Paris-Est Créteil)
marc.presset@u-pec.fr

New approaches in multicomponent Mannich reactions and related transformations

Abstract. Multicomponent reactions represent an important trend in organic synthesis, because they tend to fit with the concepts of atom- and step-economy, hence constituting a relevant response to growing environmental concerns. They also constitute powerful tools for the preparation of complex scaffolds in one step. Amon them, the Mannich reaction plays a significant role as it affords a straightforward access to densely substituted amines by the formation of both C–C and C–N bonds in only one step. Since the mid-2000s, our group focuses on organometallic Mannich reactions involving organozinc reagents as nucleophiles. This approach leads to the development of new transformations using simple reaction protocols, which allow to greatly expand the scope of this classical reaction. More recently, the use of other pro-nucleophiles, such as substituted malonic acid half oxyesters, has been explored. Recent results will illustrate our efforts in the elaboration of eco-compatible and practical methodologies.



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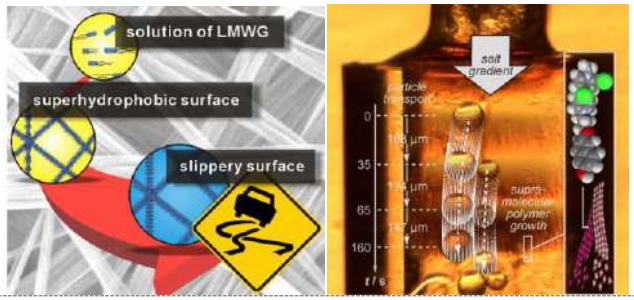
March 20th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Christoph A. SCHALLEY (Freie Universität Berlin)
schalley@zedat.fu-berlin.de

Supramolecular Gels & Polymers: From Superhydrophobic and Slippery Surfaces to Directional Transport along Gradients

Abstract. In the first part, a very simple production procedure for superhydrophobic and slippery surfaces is demonstrated. The deposition of a gel leads to the surface roughness needed for superhydrophobicity and in a way mimics the Lotus leaf effect. While the superhydrophobic surfaces repel water, but not solutions of detergents such as SDS, infusion of a lubricant into the cavities of a gel provides a slippery surface, which also repels SDS solutions and more complex liquids such as serum or blood. Both surfaces are stable to extended exposure to running water. In addition, the slippery surfaces are self-healing.The second part discusses how to use a supramolecular polymer self-assembling from easy-to-synthesize monomers as a supramolecular machine for the directional transport of particles as their cargo over millimeter distances. The direction is defined by a salt gradient and the energy dissipated in the process comes from the crystallization of flexible, bent and partially amorphous ribbons into rigid rods. Overall, this supramolecular machine generates external work from chemical energy. The structural details have been unraveled by electron microscopy, small and wide angle X-ray scattering and electron diffraction experiments.



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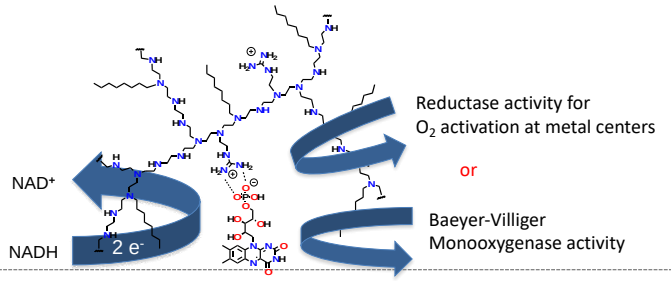
March 27th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Frédéric AVENIER
(Institut de Chimie Moléculaire et des Matériaux d'Orsay)
frederic.avenier@universite-paris-saclay.fr

Bio-inspired dioxygen activation for selective oxidation catalysis

Abstract. Selective oxidation reactions are of upmost importance for organic synthesis. However, current industrial oxidation processes mostly rely on harsh conditions associated with strong oxidants and potentially harmful catalysts. Interestingly, nature has figured out an elegant manner to catalyze such reactions thanks to the reductive activation of dioxygen at the active site of iron monooxygenases or flavine monooxygenases. We are thus working on the development of bioinspired catalysts mimicking the activity of these enzymes, with the aim to perform selective oxidation in water, using molecular oxygen as a cheap and readily available oxidant. Thanks to flavin cofactors incorporated into a polymeric matrix, these catalysts can collect electrons from NADH and either transfer them to a metal center for O_2 activation, or directly activate O_2 as an organic peroxo species to mimic the activity of Baeyer-Villiger monooxygenases.



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CULTURCHEM

APRIL 2023

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April 3rd, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Francesco PINEIDER (University of Pisa)
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Some interesting applications of magnetoplasmonics

Abstract. Magnetoplasmonics studies the interaction between plasmon resonances and magnetic field. In its simplest form, the interaction between charge carriers of a plasmonic unit with a static magnetic field can be rationalized as a Lorentz force component that alters carriers' trajectories in the conductor. [1,2,3] In recent years, several approaches have been proposed to capitalize on this interaction and boost it up to a usable magnitude. [4,5] From plasmon-enhanced magneto-optical spectroscopy to active modulation of resonances through magnetic fields, several exciting applications of magnetoplasmonics have been proposed. In this talk, I will introduce the basic concepts of the discipline, review the current progress toward viable applications and highlight some novel concepts involving magnetic fields interacting with plasmon resonances.
I will focus especially on the potential of magnetoplasmonics with three different case studies:
- high-performance plasmonic refractometric sensing of (bio)molecules through magnetic modulation of the plasmon resonance; [6-8]
- field-enhanced magneto-optical spectroscopy of ultrathin films of magnetic molecules on surfaces; [9]
- quantitative sensing of magnetic fields at the nanoscale with magnetoplasmonic nanostructures.

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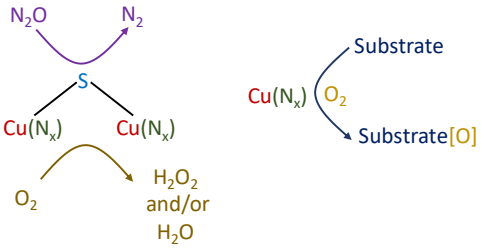
April 17th, 11h
Room 209, 2nd stage
Corridor 14-24
Campus P et M Curie
Sorbonne Université

Stéphane TORELLI (UMR 5249 – CEA Grenoble / CNRS/ Université Grenoble Alpes - Laboratoire de Chimie et Biologie des Métaux)
stephane.torelli@cea.fr

Bio-Inspired Copper-based complexes for small molecules (N_2O, O_2, H_2O) activation and reactivity

Abstract. Small molecules such as O_2, N_2O and H_2O are abundant on earth and of particular interest for environmental and sustainable considerations. Their chemical inert nature/stability remain an issue and preclude any direct utilization without activation. However, they are co-substrates for crucial processes performed by Nature, and more precisely by sophisticated edifices known as metalloenzymes. The latter combine a protein skeleton in which abundant and non-toxic d-metal ions are present with precise and dedicated coordination spheres. The particularity of these enzymes is to be capable of using and activating these chemically inert molecules to perform efficient catalytic activities. Copper-containing enzymes part of this superfamily and are involved in chemical bio-transformations and electron transfer.[1] For instance, nitrous oxide (N_2O) reduction into dinitrogen by nitrous oxide reductase is a key step in the denitrification pathway in bacteria[2] whereas dioxygen (O_2) activation by Cu monooxygenases mainly leads to oxidation reactions.[3]
Exploring the multiple facets of these processes is an amazing playground for chemists, not only to ascertain mechanistic aspects but also to imagine new reactions. *To do so, the use of bio-inspired copper models of these metalloenzymes active sites is an appealing strategy.*
In this line we develop different axis based of the preparation, characterization and reactivity study of Cu-containing systems with N or N/S environments suitable for N_2O and O_2 reduction but also for organic transformation.[4] The reactivity strongly depends on the metal coordination spheres when exogenous positions are present. These aspects will be discussed and illustrated with examples.



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3. *Chem. Rev.* **2017,** *117* (3), 2059-2107.
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CULTURCHEM

MAY 2023

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May 15th, 11h
Amphitheater Friedel
Chimie ParisTech – PSL
11 rue P et M Curie

Eva HEVIA (University of Bern)
eva.hevia@unibe.ch

Tailoring Organosodium Reagents for Arene Functionalisation

Abstract. Organosodium compounds have attracted the attention of the scientific community in recent years as an alternative to widely used organolithium reagents.[1] Lithium alkyls and amides reside at the front of organometallic synthesis as key players in countless transformations, owing to their availability, substantial stability and solubility in hydrocarbon solvents.[2] However, these desirable traits are often pitfalls of heavier alkali-metal organometallics, meaning that their applications have remained underexplored. While recent reports have hinted at the untapped potential of these reagents,[3] the constitution of the organometallic intermediates that operate in these reactions has been overlooked, missing an opportunity to tackle their high reactivity and improve their poor solubility. Filling this gap in the knowledge, the preparation of organosodium compounds soluble in hydrocarbon solvents and the isolation and characterization of reactive sodium organometallic intermediates in the solid state and in solution by X-Ray crystallography and ^{1}H DOSY (Diffusion Ordered SpectroscopY) have allowed the development of new protocols for the functionalisation of organic molecules. Our efforts have been focused on selective deprotonative metalation reactions of synthetically attractive arenes, providing access to the selective functionalization of these scaffolds, including the borylation[5] and the perdeuteration of aromatic scaffolds,[6] and the aroylation of toluene derivatives via selective benzylic metalation.[7] The reactivity and/or selectivity obtained with organosodium compounds was different to the one with its lithium analogues, opening new vistas in the use of polar organometallic reagents for the functionalization of organic molecules.

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[1] P. B. De, S. Asako, L. Ilies, *Synthesis* **2021**, *53*, 3180–3192.
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[7] D.E. Anderson, A. Tortajada, E. Hevia *Angew. Chem. Int. Ed.* **2023**, *62*, e202218498.

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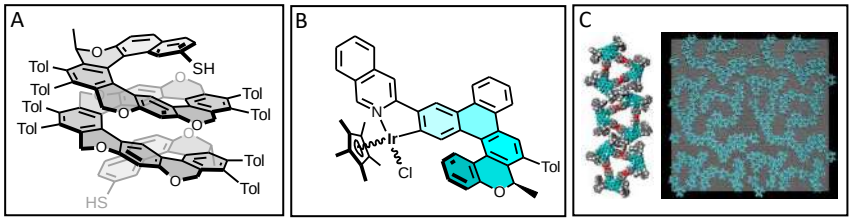
May 22nd, 11h
Amphitheater Herpin
Esclangon Building
Campus P et M Curie
Sorbonne Université

Irena G. STARÁ (Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences - IOCB Prague, Czech Republic)
stara@uochb.cas.cz

Unveiling the Fascinating World of Helicenes: From Synthesis to Their Intriguing Properties

Abstract. Recent advances in the synthesis of (hetero)helicenes and their long homologues have given new stimuli to use these inherently chiral 3D aromatic systems as functional molecules in enantioselective catalysis, molecular recognition, self-assembly, surface science, chiral materials and other fields of science. To illustrate that, three studies will be presented: (a) Synthesis of enantiopure extremely long (hetero)helicenes by multiple intramolecular diastereoselective [2+2+2] cycloisomerisation of centrally chiral aromatic oligoalkynes,[1] (Fig. 1A) and measurement of their single molecule electrical conductance by the STM break-junction method,[2] (b) asymmetric synthesis of optically pure and conformationally locked oxabenzo[5]helicenes with heteroaromatic substituents converted to the corresponding cycloiridated helicenes and the first example of the use of these cyclometalated helicenes in enantioselective catalysis[3] (Fig. 1B) and, finally, (c) helically chiral π-electron macrocycles and their self-assembly into well-ordered 2D molecular crystals observed by ambient AFM on HOPG (Fig. 1C) corroborated by MD simulations.[4]

Figure 1



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3. *ACS Catal*. **2022**, *12*, 10793.
4. *Nanoscale* **2023**, *15*, 1542.

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CULTURCHEM - JUNE 2023

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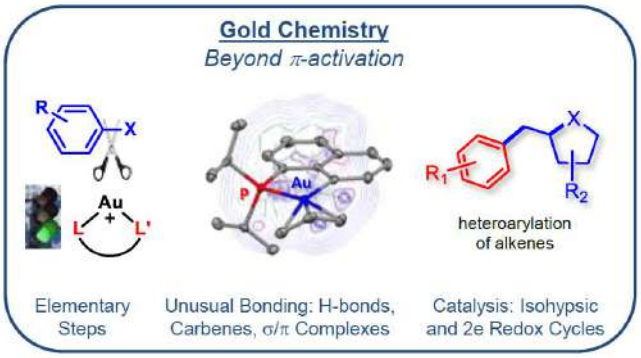
June 5th, 11h
Amphitheater Astier
Esclangon Building
Campus P et M Curie
Sorbonne Université

Didier BOURISSOU (LHFA -Université de Toulouse -CNRS)
didier.bourissou@univ-tlse3.fr

Gold Chemistry under Ligand Control

Abstract. With the aim to open new avenues in gold chemistry, we are designing and exploring new ligand designs. Three complementary facets will be discussed in this lecture: - the ability of chelating (P,P) and hemilabile (P,N) ligands to trigger oxidative addition to gold and achieve 2-electron redox catalysis, - the rich and unique reactivity of P^C and N^C cyclometallated Au(III) complexes, - π-allyl gold(III) complexes, from their first authentication and versatile behavior, to catalytic allylation.



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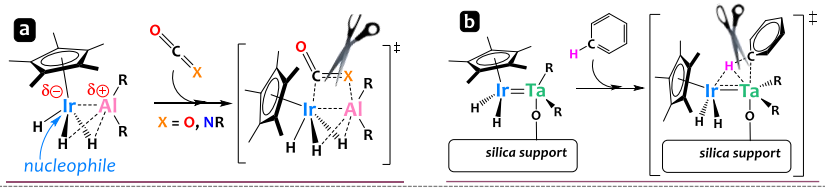
June 12th, 11h
Amphitheater Astier
Esclangon Building
Campus P et M Curie
Sorbonne Université

Clément CAMP (CNRS – Laboratory of Catalysis, Polymerization Processes and Materials UMR 5128)
clement.camp@univ-lyon1.fr

Cooperative heterobimetallic reactivity: from molecules to catalytic materials

Abstract. One of the current frontiers in organometallic catalysis is to study the combined action of two metal centers to promote novel modes of reactivity, where the two metal centers act in synergy, in order to access a chemistry not possible with monometallic species. Our approach is to use Surface OrganoMetallic Chemistry (SOMC) to isolate highly unsaturated heterobimetallic species at the surface of solid supports. The latter are able to activate challenging substrates in a concerted way on both metal centers, which explains why these bimetallic systems have a catalytic activity largely superior to monometallic analogues.



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June 19th, 11h
Amphitheater Astier
Esclangon Building
Campus P et M Curie
Sorbonne Université

Pascal MARCHAND (Nantes Université, Cibles et médicaments des infections et de l'immunité, IICiMed, UR 1155)
pascal.marchand@univ-nantes.fr

Targeting casein kinase 1 as a novel strategy for the design of antileishmanial agents

Abstract. According to a recent WHO report[1], leishmaniasis affects nearly 12 million people, with 350 million others at risk, and is responsible for nearly 40,000 deaths per year. In 2012, mainly due to global warming, visceral leishmaniasis (VL) was declared as a new emerging disease in Europe. Today, there is no effective vaccine, and the limited treatments are unfortunately too toxic and costly. In this context, there is a real emergency to develop new paradigms for antileishmanial therapy, which also limit the devastating impact of parasite resistance. While most of the current drugs as well as those in development target the parasite biology, we propose to target the exoproteome of *Leishmania*, and particularly excreted signaling kinases, to inhibit host-parasite interactions, which will restore the host cell ability to fight the parasite and limit the risk of resistance. To this end, we selected and validated *Leishmania* casein Kinase I paralog 2 (L-CK1.2) as a drug target[2,3]. L-CK1.2 is essential for intracellular parasite survival and released in macrophages via extracellular vesicles[2]. Moreover, several evidence suggest that L-CK1.2 has been evolutionary selected to interact with and phosphorylate host proteins subverting the biological and immune functions of the macrophage[2]. Because of its dual role in the parasite and the host cell, targeting L-CK1.2 would kill the parasite while limiting the emergence of parasite resistance. We previously reported the discovery of **CTN1122**[4,5], an imidazo[1,2-*a*]pyrazine derivative with promising antileishmanial properties that targets L-CK1.2 (Figure 1).

CTN1122

IC_{50} (amastigotes *L. major*) = 0.80 µM (CL)
IC_{50} (amastigotes *L. donovani*) = 2.74 µM (VL)
SI (RAW cells/amastigotes *L. major*) = 52.5
SI (RAW cells/amastigotes *L. donovani*) = 15.3
IC_{50} (*Lm*CK1) = 0.72 µM
SI_{CK1} = 1.3

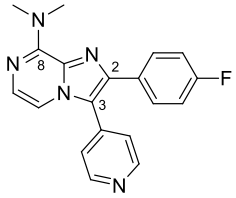

Figure 1. The lead compound **CTN1122**.

When tested *in vivo*, it reduces the parasite load in the liver and spleen of mice infected with *L. donovani*, as well as in the lesion of mice infected with *L. major* with a significant decrease in the size of the lesion. Here, we present the TEXLEISH consortium, which, through a research program dedicated to this chemical series and its target, focuses on three main objectives (1) the optimization of this lead compound by generating new pharmacomodulations of **CTN1122,** (2) the identification of potential off-target effects to limit toxicity and side-effects by using state-of-the-art deconvolution methods and (3) the better understanding of the role of L-CK1.2 in host-pathogen interactions by using system-levels analyses. The TEXLEISH consortium will provide the first evidence that targeting the exoproteome of parasite for drug treatment is an innovative way to discover potent new drugs against leishmaniasis limiting the risk of selecting for drug resistant parasites.

References: [1]World Health Organization, Leishmaniasis, Information site, https://www.who.int/en/news-room/fact-sheets/detail/leishmaniasis, January 2023. [2]N. Rachidi, U. Knippschild, G.F. Späth, *Front. Cell. Infect. Microbiol.* **2021**, *11*, 655700; doi: 10.3389/fcimb.2021.655700. [3]E. Durieu *et al.*, *Antimicrob. Agents Chemother.* **2016**, *60*, 2822–2833. [4]P. Marchand *et al.*, *Eur. J. Med. Chem.* **2015**, *103*, 381-395. [5]M.-A. Bazin *et al.*, *Eur. J. Med. Chem.* **2021**, *210*, 112956.

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June 26th, 11h
Amphitheater Astier
Esclangon Building
Campus P et M Curie
Sorbonne Université

Guillaume PRESTAT (Université Paris Cité, LCBPT UMR 8601)
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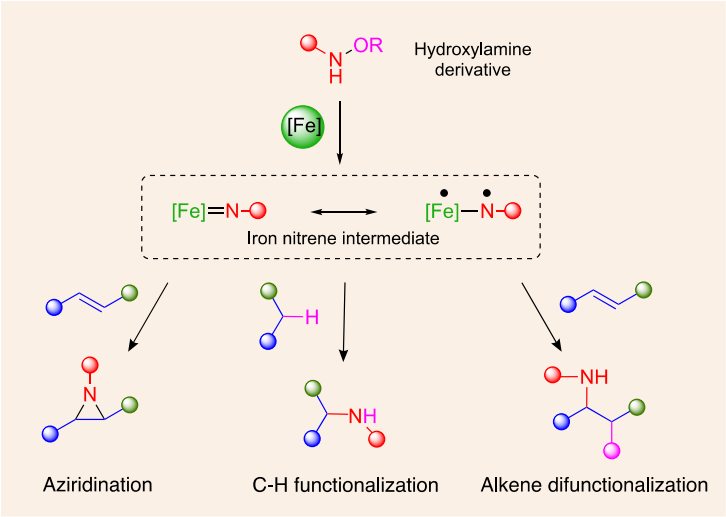
Hydroxylamine derivatives as clean iron nitrenes precursors

Abstract. Transition metal-catalyzed nitrene transfer reactions represent a powerful strategy for the formation of nitrogen-containing molecules.[1] Among the years various catalytic systems have been developed, mostly based on rhodium, ruthenium, iridium or copper complexes and relying mainly on iminoiodinanes and azide reagents as nitrene precursors.[2] Despite their good reaction efficiency, the use of those rare and/or toxic transition-metal is problematic. Furthermore, iminoiodinanes liberate stoichiometric amounts of toxic iodobenzene and azides have significant risks of explosion. Conversely, iron associated with hydroxylamine derivatives represent an interesting solution for the development of such new sustainable protocols. The low toxicity of this metal makes it a catalyst of choice, particularly for the pharmaceutical industry. Moreover, the high concentration of iron in the earth's crust guarantees a sustainable access to a large variety of inexpensive salts. Hydroxylamine derivatives are interesting nitrene precursors. In the one hand they can be efficiently synthesized via straightforward and cost-effective preparations from hydroxylamine. In the other hand they are able to generate the metal-nitrene species without addition of external oxidants.
Our research group focuses his efforts on the development of original iron-catalyzed sustainable methods based on the use of valuable hydroxylamine derivatives.[3] We will present our results on aziridination, intra and inter alkene di-functionalization as well as C-H direct functionalization.



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CULTURCHEM – JULY 2023

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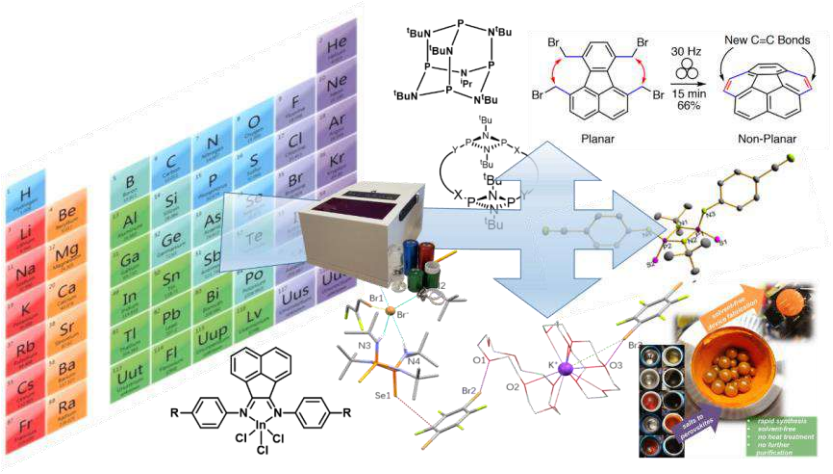
July 03rd, 11h
Amphitheater Astier
Esclangon Building
Campus P et M Curie
Sorbonne Université

Felipe GARCIA (Universidad de Oviedo, Espagne)
garciafelipe@uniovi.es

Mechanochemistry in Main Group Synthesis

Abstract. **Traditionally, solution-based processes have dominated laboratory set-ups and industrial manufacturing protocols. However, the past decade has seen the renaissance of solid-state synthetic routes, driven by the need for more sustainable chemical processes. Within this context, mechanochemistry (*i.e.*, chemical transformations initiated or sustained by mechanical force) has rapidly evolved from being a laboratory curiosity to a widely applicable synthetic technique that not only enables greener chemical transformations but offers exciting opportunities for the synthesis and screening of molecules and materials.**

This seminar will focus on the recent developments in reactive mechanochemistry of main group compounds and materials. The novel application of mechanochemistry to the synthesis of phosphorus-nitrogen frameworks – from orthogonal synthesis to "unattainable" molecules – will be discussed, followed by their implementation in the rational design of high-order organic-inorganic hybrid multicomponent cocrystals. This will be followed by a discussion on the challenges facing the broader adoption of mechanochemistry in industry, with focus on the upscaled synthesis of metal complexes and perovskite materials.



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July 10th, 11h
Amphitheater Astier
Esclangon Building
Campus P et M Curie
Sorbonne Université

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In the search for sustainable efficient lighting

Abstract. The design of more efficient sustainable SSL (solid state lighting) LEDs (light emitting diods), OLEDs (organic light emitting diods) and LECs (light emitting electrochemical cells) is an important focus of interest in materials science. These systems are key technologies for modern screens in TVs and mobile phones and are also implemented in prototypes of organic solar cells, flexible panels and next-gen devices.

During the last years, we have developed different approaches to improve the benchmarking devices accessible.

For example, the use of FP (fluorescent proteins) is a promising alternative to the use of inorganic transition metal complexes in down converting LEDs technologies. Other materials employed in SSL can be successfully substituted by other biogenic materials. Precisely, we have employed Cellulose as sustainable electrolyte.

From the other side, optical devices such as OLEDs and LECs require active materials capable of generate efficient electroluminescence. In electroluminescence, the light is generated by the exciton, but according to spin orientation statistics the excitons are formed in a 1:3 ratio singlet:triplet. TADF (thermally activated delayed fluorescence) process is characterized by the risc (reverse intersystem crossing) mechanism, capable of re-populate the singlet state with the triplet excitons. This means that the theoretical limit in efficiency for the conversion of electrons in photons is 100%. In particular, we have explored TADF in earth abundant ions Cu(I), and Ag(I) and we have successfully manufactured efficient TADF SSL devices.

Last but not less, the problem of achieving long stabilities for conventional emitters can be overcome by the use of encapsulation strategies. We have recently used MOFs (Metal Organic Frameworks) in a double strategy of encapsulating and emitting material.

All the different topics will be covered, presenting the theory behind, the approach that has been employed in the Chair of Biogenic and Functional Materials and also the perspective for the future of these technologies.

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