

CulturChem 406

2018-2019

September

Monday Sept 10th
T 54-55 Room 205, 11h

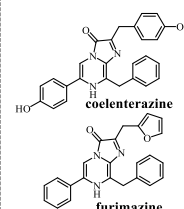


Yves L. Janin (CNRS-Institut Pasteur)

yves.janin@pasteur.fr

Heterocycles from the sea, a light from the abyss

Abstract. A growing proportion of bioluminescent reporting systems are using imidazo[1,2-*a*]pyrazine luciferins such as the natural product coelenterazine or the analog furimazine along with photoproteins or luciferases from sea creatures. Our contribution has led to an original (gram-scale) synthesis of this heterocyclic system, the preparation of close to 150 analogues and thus to extensive insights in the structure-bioluminescence relationship when using NanoLuc/nanoKaz as the luciferase.



1

Monday Sept 17th
T 54-55 Room 205, 11h



Aude Demessence (IRCELYON)

aude.demessence@ircelyon.univ-lyon1.fr

Emerging 1D and 2D d¹⁰ Coinage Metal Organic Chalcogenolate Coordination Polymers for Optical Technologies

Abstract. Hybrid materials with chalcogenolate ligands (ER = SR, SeR, TeR) and d¹⁰ coinage metals (M(I) = Cu, Ag and Au) are known for a long time mainly in the domains of biology and pharmaceuticals. Indeed, copper-thiolates are present in most of the living organisms as metalloproteins, silver-thiolates are recognized for their anti-bacterial activity and some gold-thiolates, as the Myochrysin, have been used as antiarthritic drugs. Today, the d¹⁰ coinage Metal Organic Chalcogenates (MOCs) are gaining a growing relevance in materials science for their semiconductivity and photoluminescence properties.¹ Indeed, the photoemission of these compounds is attributed to the presence of d¹⁰ coinage metals and their ability to display metallophilic interactions. Neutral MOCs, defined with the formula [M(ER)]_n, can form cyclic oligomers and extended coordination polymers with anisotropic 1D or 2D structures. In this presentation, we will show the variety of the chain-like and lamellar structures of these MOCs, associated to a rich palette of photophysical properties (Fig. 1).² Thus, some compounds exhibit high quantum yield (~70 %) in the solid state and some have an intrinsic triple emission associated with luminescence thermochromism allowing optical temperature sensing. This study will show the great potential of the MOCs as phosphorescent hybrid materials and their great potential in electronic devices, sensors or photocatalysis.

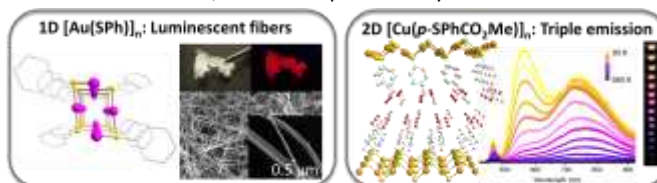


Figure 1 Examples of two MOCs.

[1]. O. Veselska; A. Demessence, *Coord. Chem. Rev.*, **2018**, 355, 240.

[2]. (a) C. Lavenn; L. Okhrimenko; N. Guillou; M. Monge; G. Ledoux; C. Dujardin; R. Chiriac; A. Fateeva; A. Demessence, *J. Mater Chem. C*, **2015**, 3, 4115; (b) C. Lavenn; N. Guillou; M. Monge; D. Podbevšek; G. Ledoux; A. Fateeva; A. Demessence, *Chem. Commun.*, **2016**, 52, 9063; (c) O. Veselska; L. Okhrimenko; N. Guillou; D. Podbevšek; G. Ledoux; C. Dujardin; M. Monge; D. M. Chevrier; R. Yang; P. Zhang; A. Fateeva; A. Demessence, *J. Mater Chem. C*, **2017**, 5, 9843; (d) O. Veselska; D. Podbevšek; G. Ledoux; A. Fateeva; A. Demessence, *Chem. Commun.*, **2017**, 53, 12225; (e) O. Veselska; L. Cai; D. Podbevšek; G. Ledoux; N. Guillou; G. Pilet; A. Fateeva; A. Demessence, *Inorg. Chem.*, **2018**, 57, 2736.

2

Monday Sept 24th
T 54-55 Room 205, 11h



Olga Iranzo (Institut des Sciences Moléculaires de Marseille- UMR
CNRS 7313, Aix-Marseille Université)

olga.iranzo@univ-amu.fr

*Engineering catalytic sites and molecular recognition in designed
peptide scaffolds*

Abstract. Peptide-based frameworks constitute very attractive and versatile platforms for the development of novel systems with tailor-made properties and functionalities. They are chiral and have structural and chemical diversity (proteinogenic and non-proteinogenic amino acids), accessible chemical synthesis by well-established solid-phase methodologies and water solubility. In this seminar, different sets of peptidic scaffolds will be presented and their potential applications as catalysts for oxidation reactions and as affinity reagents for bioseparations will be discussed.

3

Pour tous renseignements, veuillez contacter :

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

October

Monday October 1st
T 54-55 Room 205, 11h



Heeyoon Lee (Korean Advanced Institute of Science & Technology)
leehy@kaist.ac.kr

Development of radical based synthetic strategies for the total synthesis of natural products and Posttranslational modification of proteins

Abstract. Tandem cycloaddition reaction of allenylidiazao precursor via trimethylenemethane(TMM)-diyl was developed to construct complex polycyclic structures in a single operation. This TMM-diyl cycloaddition reaction was successfully applied to the total synthesis of natural products with very challenging structural features. Radical based C-C bond forming reaction was developed for the study of posttranslational modification (PTM) and demonstrated to mimic Lys modification in PTM.

4

Monday October 8th
T 54-55 Room 205, 11h



Ali Tavassoli (University of Southampton)
a.tavassoli@soton.ac.uk

Platforms for the generation and high-throughput screening of SICLOPPS cyclic peptide libraries

Abstract. Cyclic peptide libraries have demonstrated significant potential when employed against challenging targets such as protein– protein interactions. SICLOPPS is a method for the intracellular generation of cyclic peptide libraries of over a hundred million members. We have interfaced SICLOPPS libraries with a variety of cell-based assays for the identification of inhibitors of a variety of targets. The discovery and development of our cyclic peptide HIF-1 inhibitors will be discussed, along with details of a newly developed ultra-high throughput screening platform that allows the generation of SICLOPPS cyclic peptide libraries in femtomolitized microfluidic droplets.

5

Pour tous renseignements, veuillez contacter :

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

Monday October 15th
T 54-55 Room 205, 11h



Aude Demessence (IRCELYON)

aude.demessence@ircelyon.univ-lyon1.fr

Emerging 1D and 2D d¹⁰ Coinage Metal Organic Chalcogenolate Coordination Polymers for Optical Technologies

Abstract. Hybrid materials with chalcogenate ligands (ER = SR, SeR, TeR) and d¹⁰ coinage metals (M(I) = Cu, Ag and Au) are known for a long time mainly in the domains of biology and pharmaceuticals. Indeed, copper-thiolates are present in most of the living organisms as metalloproteins, silver-thiolates are recognized for their anti-bacterial activity and some gold-thiolates, as the Myochrysin, have been used as antiarthritic drugs. Today, the d¹⁰ coinage Metal Organic Chalcogenates (MOCs) are gaining a growing relevance in materials science for their semiconductivity and photoluminescence properties.¹ Indeed, the photoemission of these compounds is attributed to the presence of d¹⁰ coinage metals and their ability to display metallophilic interactions. Neutral MOCs, defined with the formula [M(ER)]_n, can form cyclic oligomers and extended coordination polymers with anisotropic 1D or 2D structures. In this presentation, we will show the variety of the chain-like and lamellar structures of these MOCs, associated to a rich palette of photophysical properties (Fig. 1).² Thus, some compounds exhibit high quantum yield (~70 %) in the solid state and some have an intrinsic triple emission associated with luminescence thermochromism allowing optical temperature sensing. This study will show the great potential of the MOCs as phosphorescent hybrid materials and their great potential in electronic devices, sensors or photocatalysis.

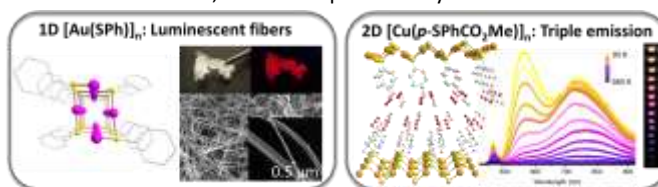


Figure 1 Examples of two MOCs.

[1]. O. Veselska; A. Demessence, *Coord. Chem. Rev.*, **2018**, 355, 240.

[2]. (a) C. Lavenn; L. Okhrimenko; N. Guillou; M. Monge; G. Ledoux; C. Dujardin; R. Chiriac; A. Fateeva; A. Demessence, *J. Mater Chem. C*, **2015**, 3, 4115; (b) C. Lavenn; N. Guillou; M. Monge; D. Podbevšek; G. Ledoux; A. Fateeva; A. Demessence, *Chem. Commun.*, **2016**, 52, 9063; (c) O. Veselska; L. Okhrimenko; N. Guillou; D. Podbevšek; G. Ledoux; C. Dujardin; M. Monge; D. M. Chevrier; R. Yang; P. Zhang; A. Fateeva; A. Demessence, *J. Mater Chem. C*, **2017**, 5, 9843; (d) O. Veselska; D. Podbevšek; G. Ledoux; A. Fateeva; A. Demessence, *Chem. Commun.*, **2017**, 53, 12225; (e) O. Veselska; L. Cai; D. Podbevšek; G. Ledoux; N. Guillou; G. Pilet; A. Fateeva; A. Demessence, *Inorg. Chem.*, **2018**, 57, 2736.

Pour tous renseignements, veuillez contacter :

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

Monday October 22nd
T 54-55 Room 205, 11h



Damien LAAGE

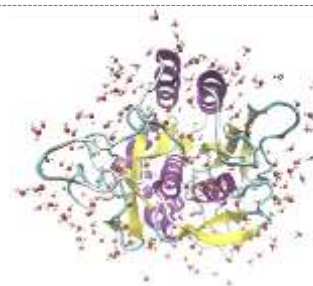
(Department of Chemistry, Ecole Normale Supérieure, PSL-SU-CNRS)
damien.laage@ens.fr

Biomolecular Hydration Shells: Dynamics and Biochemical Role

Abstract. The structure and function of biomolecules are strongly influenced by their hydration shells. Two key challenges are thus first to determine the extent to which the structural and dynamical properties of these shells differ from those of bulk water, and second to elucidate the role played by water in the functioning of biomolecules.

We will first review the recent advances in theory, simulations and experiment that have led to new and detailed insight in the dynamical properties of water molecules in the hydration shells of proteins and DNA. Three central questions will be addressed: what is the size of the hydration shell? To what degree are the shell water dynamics different from bulk water? And what is the molecular origin of the effect induced by the biomolecule on the water dynamics, is it rather due to the shape of the molecule or to the chemical nature of the exposed groups?

We will then consider the influence of water on the function of proteins, and focus on the role of the hydration shell in the catalytic activity of enzymes. Water is usually depicted as a lubricant which facilitates the protein conformational transitions occurring during enzyme catalysis. Through the study of a paradigm enzyme in a water-cosolvent mixture, we will show that this picture is not justified. We will identify the molecular origin of the catalytic activity enhancement by water, and use it to suggest new routes to optimize enzymatic activities in non-aqueous solvents.



7

Monday October 29th
T 54-55 Room 205, 11h



Raphaël Tripier (Université de Brest)

raphael.tripier@univ-brest.fr

Organic-, coordination-chemistry and theranostic: influence of the full control of the macrocycle design on the biological properties

Abstract. If the importance of azamacrocyclic chelates in imaging (MRI, PET, optical probes) and therapy (radiotherapy) is now well established, the challenge to find good chelators able to be used in both diagnostic and therapeutic applications persists. Indeed, there is still no "ideal" ligand able to coordinate different metallic cations of interest and to allow, only by changing the cationic core, imaging and therapeutic purpose. We will then present our investigation in this area, which are now close to propose such new chelators associated with copper(II) or lanthanides(III).

8

Pour tous renseignements, veuillez contacter :

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

November

Monday November 5th
T 54-55 Room 205, 11h



Philip A. Gale (The University of Sydney, Australia)

philip.gale@sydney.edu.au

Selective anion transport

Abstract. My group is interested in designing new transporters to facilitate the transport of anions across lipid bilayer membranes and the design of new assays to measure transmembrane transport processes. Our aim is to develop selective transporters that may find application in a number of areas including the treatment of disease.

Supramolecular transmembrane anion transport: new assays and insights. *X. Wu, E.N.W. Howe and P.A. Gale, Acc. Chem. Res. 2018, 51, 1870-1879; DOI: 10.1021/acs/accounts.8b00264*

Monday November 5th
T 22-23 Room 317, 14h



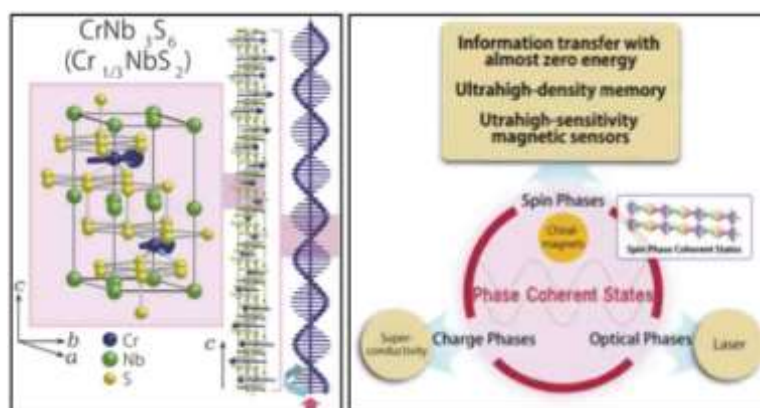
Katsuya Inoue (Hiroshima University, Japan)

kxi@hiroshima-u.ac.jp

Chirality in Nature

Abstract. Chirality can be found at all time and space scale in nature. In this seminar I shall explore what is important from basic particle physics to large scale natural world. I shall start from chiral spin system and show how to connect static chirality and spin chirality. Next, I shall introduce the common properties to biomolecules and chiral (magnetic) liquid crystals. Next, I shall make efforts to find out the commonality between the chiral spin and the QCD systems. Based on these facts, I discuss the nature of nonlinear defects of chiral solitons, skyrmions, Hopfions. In conclusion, I shall present prospects in chiral science.

<https://home.hiroshima-u.ac.jp/kotai/>



10

Pour tous renseignements, veuillez contacter :

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

Monday November 12th
T 54-55 Room 205, 11h

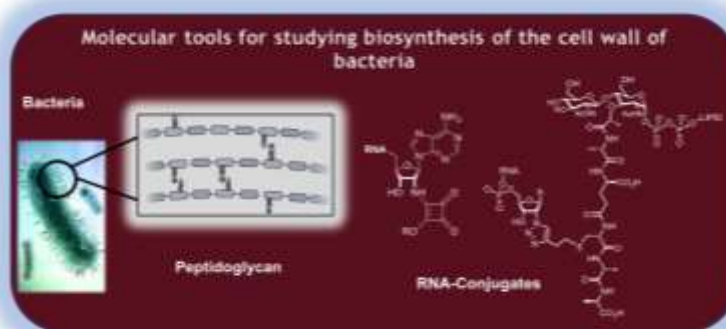


Mélanie Etheve-Quelquejeu (Université Paris Descartes)

melanie.etheve-quelquejeu@parisdescartes.fr

Synthetic RNA as molecular tools for the structural and functional study of enzymes

Abstract. The role of RNAs in cellular processes is one of the most dynamic areas in Biology. In addition to their key functions in protein synthesis, new RNA activities are constantly discovered. To study these different biological processes, in particular, the enzymes that interact with these RNAs, we have developed synthetic methodologies to obtain stable RNAs, reactive RNAs or peptidyl-conjugates. The use of nucleoside and nucleotides chemistry, solid support synthesis, enzymatic reactions or post-functionalization methods allowed us to obtain a large variety of modified RNAs, which will be presented here. These RNA analogs were used for the study of Fem aminoacyl transferases, a tRNA-dependent enzyme that catalyze an essential step in peptidoglycan synthesis of the bacterial wall and for the study of m⁶A-RNA methyltransferases.



11

Monday November 19th
T 54-55 Room 205, 11h



Xavier Moreau (Université de Versailles Saint-Quentin-en-Yvelines)

xavier.moreau@uvsq.fr

Dienals as versatile substrates for the stereoselective synthesis of polycyclic architectures

Abstract. Polycyclic architectures encompass a broad range of natural and biologically relevant products. The vast array of structural diversity and complexity reached by these molecules has fascinated synthetic organic chemists over the years. Within the context of total synthesis or synthetic chemistry methodology, considerable endeavors have been devoted to the design of efficient domino transformations that generate elaborated polycyclic tridimensional scaffolds bearing multiple stereogenic centers. Beyond that, diversity-oriented synthesis (DOS) based around readily available and versatile starting materials is one of the most attractive strategy to achieve skeletal diversity. Thus, merging domino polycyclizations with DOS approach could lead to intricate small-molecule libraries. In this context, our current interest in designing new methodologies to afford functionalized polycyclic scaffolds from simple unsaturated aldehydes will be presented.

12

Pour tous renseignements, veuillez contacter :

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

Monday November 26th
T 54-55 Room 205, 11h



Carlos C. Romão (Universidade Nova de Lisboa- ITQB NOVA, Portugal)

ccr@itqb.unl.pt

Therapy with CO: where do we stand?

Abstract. The promise to use CO (carbon monoxide) as a therapeutic principle appeared with the turn of the century following the discovery of CO's signalling and cytoprotective effects. The ensuing research effort confirmed the therapeutic action of CO. Inhaled CO gas has been tested in many human clinical trials. Different kinds of organometallic and organic prodrugs and a large variety of materials and devices have been successfully tested. However, CO has not yet entered the clinic and the question to ask is: why? The meanders and highlights of this journey will be discussed in an attempt to identify the reasons for this impasse and outline reasonable pathways to overcome it.

13

Pour tous renseignements, veuillez contacter :

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

December

Monday December 3rd
T 54-55 Room 205, 11h



Benjamin Abecassis (Laboratoire de Chimie de l'ENS Lyon)

Benjamin.Abecassis@ens-lyon.fr

Auto-assemblage de Nano-plaquettes Semi-Conductrices

Abstract. Les nanoplaquettes semi-conductrices (NPL) de CdSe sont des nanoparticules colloïdales 2D composées d'un cœur cristallin dont l'épaisseur peut être contrôlée à la couche atomique près et recouvertes d'une couche de ligands organiques. Elles possèdent des propriétés de luminescence exceptionnelles. J'exposerai nos résultats sur l'assemblage de ces NPL sous diverses formes comme de longues aiguilles ou des chapelets flexibles. Je montrerai qu'il est possible, en jouant sur la chimie de surface, d'obtenir des plaquettes plates, enroulées ou twistées et montrerai comment ces contraintes de surface peuvent être exploitées pour former des assemblages frustrés.

14

Monday December 10th
T 54-55 Room 205, 11h

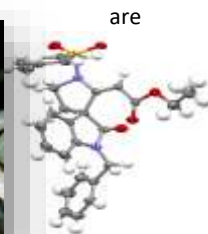
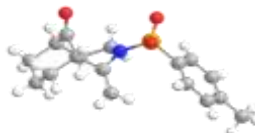


Laurence Miesch (Strasbourg University)

lmiesch@unistra.fr

Ynamides and enamides providing access to valuable building blocks

Abstract. Ynamides and enamides are versatile synthons to create nitrogen-containing scaffolds highly prevalent in natural products that exhibit pharmacological profiles. Silver-catalyzed cyclization of ene-yne-sulfonamides provide rapid access to bridged bicyclic ketoenamides, whereas keto-sulfonamides lead to spiro-enamides in a one pot fashion via keto-ynamides. Substructures of man-made psychoactive molecules of the benzodiazepine family accessible through *N*-imides equipped with enamides.



15

Pour tous renseignements, veuillez contacter :

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

Monday December 17th
 T 54-55 Room 205, 11h



16

Christophe Hardouin (Oril Industrie)

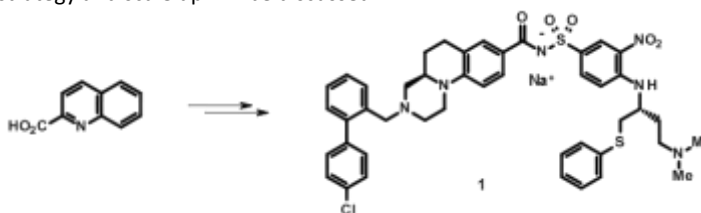
christophe.hardouin@servier.com

**Multi kilogram-scale synthesis of an anticancer drug candidate:
 a journey towards development of some key reactions**

Abstract. In order to evaluate a new drug in preclinical or clinical testing, the pharmaceutical industry needs bulk quantities of final product (from kg to hundreds of kg). Converting reactions from laboratory into industrial-scale manufacturing processes remains a challenge for process chemists while taking into account safety, legislation, environmental and cost of goods requirements.

As part of a drug discovery program at Servier Group, compound **1** was selected. To enable further clinical studies, we explored an efficient route to synthesize **1** implementing some key reactions.

Both strategy and scale up will be discussed.



For any informations, please contact :

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

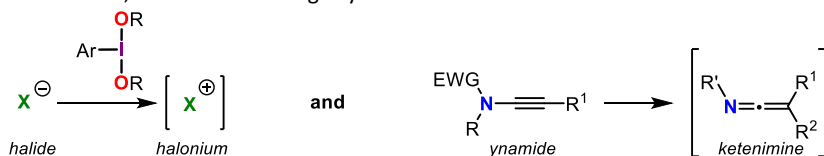
January

Monday January 14th
T 54-55 room 125, 11h



Kevin CARIOU (CNRS- Institut de Chimie de Substances Naturelles)
kevin.cariou@cnrs.fr
Iodine(III)-Mediated Halogenation Reactions & Ynamides as Ketenimines Precursors

Abstract. In our group we develop synthetic methodologies that enable the construction of original molecular scaffolds possessing interesting biological properties. In particular, we try to bypass the use of unstable yet reactive intermediates by generating these species *in situ*. We pursue two lines of research in this direction, one deals with hypervalent iodine reagents and the second with the chemistry of ynamides. We use the former as mediators to trigger chemoselective halogenation reactions through the mild oxidation of halides. The latter are employed as readily available and stable precursors for the generation of ketenimines, which then undergo cycloaddition reactions.



17

Monday January 21st
T 54-55 room 125, 11h



Carsten STREB (Ulm University, Germany)
carsten.streb@uni-ulm.de
Polyoxometalate Composites - from water purification to energy storage

Abstract. The combination of polyoxometalates – molecular metal oxide anions – with functional substrates such as nanostructured carbon or porous silica will be described as a means to access (multi)functional composite materials. Tuning of each component will be reported as a facile means of controlling reactivity and developing materials with unusual properties for chemical and biological applications. Particular focus will be (a) on the design of conductive composites with use in energy conversion and storage, e.g. in battery electrodes or water electrolysis. (b) the use of POM-ionic liquids as reactive surface coatings will be discussed and control of rheology and materials chemistry will be demonstrated to enable applications in corrosion protection and water purification

18

For any informations, please contact :

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

Monday January 28th
T 54-55 room 125, 11h

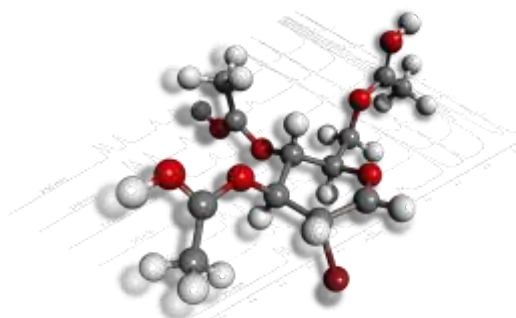


Sébastien THIBAudeau (IC2MP Poitiers University)

sebastien.thibaudeau@univ-poitiers.fr

Creating New (Bioactive) Molecules with Superacids

Abstract. In superacid, such as HF/SbF₅, functionalized organic molecules can be (poly)protonated to furnish electrophilic species which can react with very poor nucleophiles. This superelectrophilic activation can be applied to the development of unprecedented organic reactions. This work opens new possibilities for the direct and effective preparation of elaborated compounds of high synthetic and biological values



19

For any informations, please contact :

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

February

Monday February 4th
Astier (Esclangon), 11h



20

Stéphanie Norsikian (CNRS -ICSN)

Stephanie.norsikian@cnr.fr

Stereoselective synthesis of polyfunctional molecules- Use of the borono-Mannich reaction and glycosylations

Abstract. The Borono-Mannich reaction, also known as Petasis reaction, is a multi-component reaction between a carbonyl derivative, an amine and a boronic acid. We apply this methodology to the stereoselective preparation of chiral elaborate molecules and examine new variants of this reaction. We are also working on the total synthesis of ticamycin B, a natural antibiotic. Our efforts are focused on the development of the rhamnoside and novioside fragments as well as the key 1,2-cis glycosylations needed to bind them to the macrolide.

Monday February 11th
Astier (Escanglon), 11h



21

Victor Maurizot (University of Bordeaux)

victor.maurizot@u-bordeaux.fr

How to control Aromatic Oligoamide Foldamers

Abstract. Functions and properties of molecules are intimately related to their shape. This is particularly true in Nature where biomolecules functions only arise from the folding of linear oligomeric peptides or nucleotides into 3-D architectures. With the objective of mimicking functional natural biomolecules, chemists have developed synthetic oligomeric molecules named as "foldamers" that are designed to fold into compact architectures. Over the last decades our group has focused its attention toward the construction of Aromatic Oligoamide Foldamers and has tried to control not only their shapes by producing helices and sheets but also their self-assembly.



For any informations, please contact :

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

Monday February 18th
Astier (Esclançon), 11h



Laurence Miesch (Strasbourg University)

lmiesch@unistra.fr

Ynamides and enamides providing access to valuable building blocks

Abstract. Ynamides and enamides are versatile synthons to create nitrogen-containing scaffolds highly prevalent in natural products that exhibit pharmacological profiles. Silver-catalyzed cyclization of ene-yne-sulfonamides provide rapid access to bridged bicyclic ketoenamides, whereas keto-sulfonamides lead to spiro-enamides in a one pot fashion via keto-ynamides. Substructures of man-made psychoactive molecules of the benzodiazepine family are accessible though *N*-imides equipped with enamides.



22

Monday February 25th
Astier (Esclançon), 11h



Fahmi Himo (Stockholm University)

fahmi.himo@su.se

Quantum Chemical Modeling of Enzymatic and Homogeneous Catalysis

Abstract. Using modern density functional theory methods, it is today possible to routinely and accurately treat relatively large systems. The calculated energies can be used to rule out or substantiate reaction mechanisms and have also been shown to be sufficiently accurate to satisfactorily reproduce various kinds of selectivities. These developments have made it possible to tackle increasingly difficult problems in homogeneous catalysis and also to model enzyme active sites in a more realistic way. This talk will give a brief account of the methods used in these two fields, and it will be argued that very similar approaches can be employed. The status of this methodology will be assessed and a number of recent examples from our work will be discussed.

23

For any informations, please contact :

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

March

Monday March 4th
Astier (Escanglon), 11h



Eva JAKAB TOTH (Centre de Biophysique Moléculaire, Orléans)
eva.jakabtoth@cnrs-orleans.fr
Lanthanide-Based Probes in Molecular Imaging

Abstract. One important field in molecular imaging is the detection of physico-chemical parameters of tissues, concentration of ions, metabolites, etc. by smart, activatable probes. MRI is well adapted to the design of responsive probes, involving Gd³⁺-based or PARACEST (Paramagnetic Chemical Exchange Saturation Transfer) agents. The MRI efficacy (relaxivity or CEST properties) of the probe has to be selectively influenced, based on coordination chemistry concepts, by the particular biomarker that we wish to detect. We develop potential smart contrast agents to detect cation or neurotransmitter concentration changes in the extracellular space or to monitor enzyme activity.

24

Monday March 11th
Astier (Escanglon), 11h



Bruno FABRE (Institut des Sciences Chimiques de Rennes)
bruno.fabre@univ-rennes1.fr
Fonctionnalisation de surfaces de silicium pour la (photo)électronique moléculaire et la catalyse photoélectrochimique

Abstract. La fonctionnalisation de surfaces de silicium à terminaison hydrogène (Si-H) par des assemblages électroactifs constitue une voie privilégiée pour la mise au point de nouvelles interfaces parfaitement définies pour de nombreuses applications, telles que l'électronique moléculaire et la catalyse photoélectrochimique. A travers quelques exemples représentatifs, nous montrerons que de telles surfaces fonctionnelles peuvent se comporter comme des portes logiques photo-adressables ou bien permettre l'activation de petites molécules (H₂, O₂ et CO₂) sous énergie solaire.

25

For any informations, please contact :

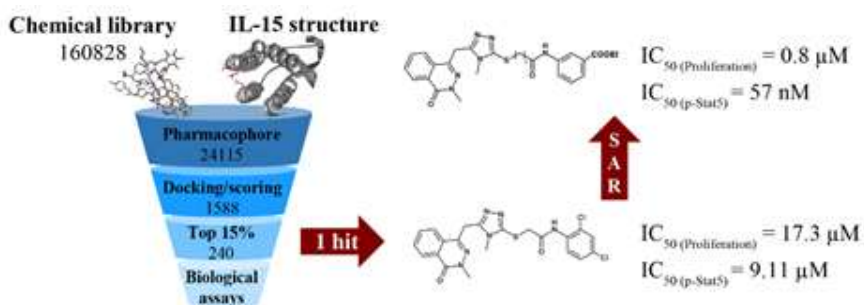
Dr Cyril Ollivier, Sorbonne Université, Campus Pierre et Marie Curie, Tour 32-42, 5^{ème} étage, case 229,
4 place Jussieu, 75005 Paris. ☎ 01 44 27 38 50. Courriel : cyril.ollivier@sorbonne-universite.fr

Monday March 18th
Astier (Escanglon), 11h



Jacques LEBRETON (CEISAM UMR CNRS 6230-Université de Nantes)
jacques.lebreton@univ-nantes.fr
Identification, synthèse et évaluation biologique de la première famille d'inhibiteurs de système interleukine 15

Résumé. L'IL-15 est une cytokine majeure impliquée dans l'activation des effecteurs de l'immunité. Sa surexpression est associée au développement de pathologies auto-immunes ou inflammatoires. A travers une approche rationnelle s'appuyant sur les structures 3D de complexes de l'IL-15 avec son récepteur en utilisant des méthodes in silico par criblage de banques de molécules nous avons identifié une molécule hit, qui via une étude SAR a conduit au 1^{er} inhibiteur de l'IL15 au nanomolaire.



26

Monday March 25th
Astier (Escanglon), 11h



Osamu ISHITANI (Tokyo Institute of Technology)
ishitani@chem.titech.ac.jp
New Directions to Development of Photocatalytic CO₂ Reduction

Abstract. Both the problems of the global warming and shortage of the fossil resources have brought us great interests in photochemical utilization of CO₂ with solar energy. Efficient photocatalysts for CO₂ reduction must be necessary for development of such an important technology. We have developed novel types of photocatalysts using metal complexes as key players in not only homogeneous solutions but also in heterogeneous systems including semiconductor photocatalysts. In this presentation, I will mainly discuss about two recent topics; (1) photocatalytic CO₂ reduction using water as a reductant (Scheme) and (2) CO₂ reduction photocatalytic systems consisting of only earth-abundant elements.



27

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

April

Monday April 1st
Auditorium Astier 11h



28

Jérôme LONG (Institut Charles Gerhardt, Montpellier)

jerome.long@umontpellier.fr

Multifunctional molecule-based magnets : slow relaxation, luminescence and ferroelectricity

Abstract. Coordination chemistry of lanthanide ions allows the tailored design of multifunctional molecule-based materials. We investigate here by using luminescent and magnetically anisotropic lanthanide ions assembled with enantiopure ligands the synthesis of high-temperature molecular ferroelectrics exhibiting Single-Molecule Magnet behavior and lanthanide luminescence. These systems exhibit an electrical bistability above 180 K of the Curie temperature of BaTiO₃ while investigation of the magnetoelctrical coupling at room temperature confirms their great potentiality.

Monday April 8th
Auditorium Astier 11h



29

Eduardo PERIS (Universitat Jaume I, Castellón (Spain))

eperis@uji.es

Polyaromatic-adorned N-Heterocyclic Carbenes. From Homogeneous Catalysis to Host-guest Chemistry Studies

Abstract. In the course of our most recent research, we demonstrated how homogeneous catalysts with polyaromatic functionalities possess properties that clearly differ from those shown by analogues lacking these polyaromatic systems. The differences arise from the ability of the polyaromatic groups to afford non-covalent interactions with aromatic molecules, which can either be substrates in a homogeneous catalysed reaction, or the same catalysts to afford self-assembled systems. We also prepared a large variety of metallo-supramolecular complexes, including metallocrowns, metallo-rectangles, metallo-folders and bowl-shaped metallo-structures. Depending on their structural features, these species were used for the recognition of a variety of organic substrates, such as electron-deficient aromatic substrates, polycyclic aromatic hydrocarbons and heavy metal cations. The most relevant results in this research will be presented.

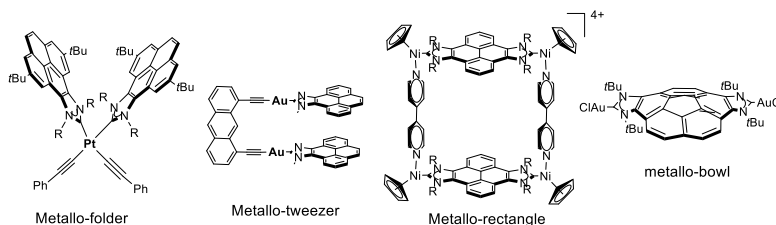


Figure. Some representative metallo-supramolecules

For any informations, please contact :

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

Monday April 15th
Auditorium Astier 11h



Bert MEIJER (Eindhoven University of Technology)

e.w.meijer@tue.nl

Supramolecular polymerizations - chirality as a muse

Abstract. Although the word polymer was already coined by Jöns Jakob Berzelius in 1833, it was through the pioneering work of Hermann Staudinger in 1920, that it was recognized that the macroscopic properties of polymers both in solution and solid state are the result of the macromolecular nature of the molecules. The impressive progress in supramolecular chemistry, however, paved the way to design polymers and polymeric materials that lack the macromolecular structure. Instead, highly directional secondary interactions are used to assemble the many repeating units into a polymer array. By adequate design, these systems should still have all of those material properties that make polymers so valuable and on top of that we may expect some unprecedented behavior – like self-healing - as a result of the reversibility of the supramolecular design. Multiple hydrogen bonding units will be shown to be highly attractive to produce supramolecular polymers with unique properties. Like covalent polymers, or macromolecules, the supramolecular counterparts are prepared by different mechanisms. Especially ordered arrays of monomers are highly interesting due to the cooperative nature of their supramolecular polymerization processes. These supramolecular polymers will be used to create artificial extracellular matrices, hydrogels and super-selectivity in molecular recognition. In the lecture, the concept of supramolecular polymers will be illustrated with a detailed analysis of the pathways in these non-covalent polymerizations and how these supramolecular polymers are used.

30

For any informations, please contact :

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

May

Monday May 6th
T 54-55 Room 125, 11h



Christophe BIOT (Lille University)

christophe.biot@univ-lille.fr

Illuminer le vivant par des approches de chemobiologie

Abstract. Dans notre équipe, nous développons de nouvelles approches d'imagerie des glycanes en utilisant la stratégie du rapporteur chimique bioorthogonal couplée à une sonde détectable en microscopie pour localiser et quantifier des changements dynamiques de glycosylation. Récemment, nous avons décrit une nouvelle méthodologie qui, grâce à l'utilisation de deux analogues métaboliques marqués, nous a permis de distinguer les deux grandes voies métaboliques de l'acide sialique. L'utilisation distincte d'un analogue de la N-acétyl-mannosamine (ManNAc) et de l'acide N-acétyl Neuraminique (Neu5Ac) permet en effet de visualiser respectivement la voie de biosynthèse endogène de l'acide sialique mais également la voie d'importation et de recyclage de l'acide sialique exogène. Notre stratégie de marquage nous a ainsi permis de mettre en évidence les mécanismes d'entrée cellulaire de nos deux rapporteurs.

De plus, nous avons appliqué cette méthodologie du rapporteur chimique pour révéler la complexité du végétal. Trois rapporteurs bioorthogonaux, analogues de monomères naturels des lignines, ont été conçus et synthétisés pour porter des étiquettes chimiques. Une fois incorporés dans le processus de formation des lignines de plantes, ces rapporteurs ont montré que trois réactions de bioconjugaison peuvent être utilisées simultanément au sein d'un même échantillon vivant.



Chem. Sci., 2018, 9, 7585-7595

Angew Chem Int Ed Engl. 2018, 57, 16665-16671

31

Monday May 13th
T 54-55 Room 125, 11h



Emmanuel MAISONHAUTE (LISE, SU)

emmanuel.maisonhaute@sorbonne-universite.fr

Extracting mechanistic information in molecular electrochemistry

Abstract. This presentation will aim at giving specific clues when one wishes to lead an electrochemical mechanistic investigation for systems either reacting in solution or adsorbed onto the electrode. Starting from simple electron transfer reactions, we will next consider coupled chemical reactions. The frequently encountered square scheme mechanism will be particularly detailed. Finally, for macromolecules bearing several redox centers (dendrimers, rotaxanes), we will explain how the intramolecular electron hopping can be measured thanks to ultrafast cyclic voltammetry, and what can be deduced about molecular movements.

32

For any informations, please contact :

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

Monday May 20th
T 54-55 Room 125, 11h



Manfred Bochmann (University of East Anglia / UK)

m.bochmann@uea.ac.uk

Recent advances in Gold Chemistry

Abstract. The chemistry of gold has seen a meteoric rise in recent years, due to novel applications in synthesis, catalysis, and luminescent compounds. This lecture will discuss recent advances in gold chemistry in terms of ligand architecture, structure and bonding, with emphasis on gold(III) chemistry. It will be shown how ligand design can be exploited in the synthesis of hitherto unknown compound classes, notably alkene, alkyne and hydride complexes, and for the control of photophysical and anti-cancer properties.

33

Monday May 28th
T 54-55 Room 125, 11h

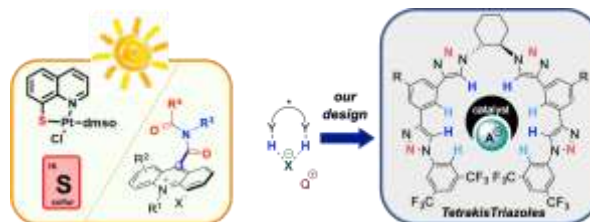


Olga GARCÍA MANCHEÑO (Münster University)

olga.garcia@uni.-muenster.de

Design of Novel (Organo)Catalytic Systems for Photoredox & Anion-Binding Catalysis

Abstract. In the past years, the areas of photoredox and asymmetric anion-binding catalysis have attracted a great interest since their unusual activation modes allow the discovery of unprecedented transformations. However, there is a continuous demand of new, efficient catalytic systems to overcome unsolved synthetic challenges. In this regard, we have recently design new visible light photoredox catalysts based on acridinium salts and Pt-complexes, as well as a new class of chiral triazole anion-binding catalysts with enhanced activity and broad synthetic applications.



34

For any informations, please contact :

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

June

Lundi 3 Juin
Amphi Astier

Pr. **Francesc Lloret**. Icmol Universitat de València
francisco.lloret@uv.es

Conception de polymères de coordination magnétique poreux.



Abstract. Dans la présente communication, nous discutons sur la conception et la synthèse de polymères de coordination poreuse magnétique (PCPM) à partir de précurseurs tétraoxamate de Cu(II) lesquels agissent en tant que ligands tétrakis-didentés vers d'autres ions métalliques [Mn(II), Co(II) et Ni(II)]. L'implication de tous les groupes oxamates du précurseur dinucléaire dans la coordination des ions métalliques conduit à la formation de plans hexagonaux ou octogonaux. Tous ces plans sont reliés les uns aux autres de manière rigide, ce qui conduit à la formation de larges canaux hexagonaux ou octogonaux.

Monday June 24th
Auditorium Astier 11h

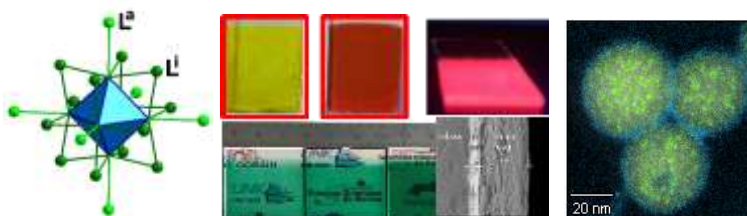
Fabien GRASSET (CNRS UMI3629 LINK)

fabien.grasset@univ-rennes1.fr

Synthesis and Characterizations of New Nanocomposites Materials based on Metal Atoms Clusters for Biomedical, Optical, Energy and Environmental Applications



Abstract. Composite nanoarchitectures represent a class of nanostructured entities that integrate various dissimilar nanoscale building blocks including clusters, particles, wires and films. The heterogeneous composite nanostructured materials are composed by definition of multi-(nano)components, each tailored to address different requirements. As one of the nanocomponents, nanometer sized transition metal clusters (<2 nm), which consist of less than a few dozens of metal atoms, could be defined as a link between atom and nanoparticle. Multifunctional properties could be achieved by a combination of several materials in a best-defined architecture. During the last decade, we developed a simple, versatile, highly reproducible and efficient methods based on solution based chemistry and sol-gel processes to prepare large amount of multifunctional nanocomposites (particles, colloids and films). In this presentation, we will focus on our latest results on nanocomposites, nanoparticles and thin films, involving mostly Mo₆, Nb₆ or Ta₆ atom cluster units, γ -Fe₂O₃, SiO₂ or ZnO for biomedical, optical, energy and environmental applications.



Pour tous renseignements veuillez contacter : **Prof Giovanni Poli**, Bâtiment F, 2^{ème} étage, case 229, 4 place Jussieu, 75005 Paris. ☎ 01 44 27 41 14 📠 01 44 27 73 60 e-mail : giovanni.poli@upmc.fr