September

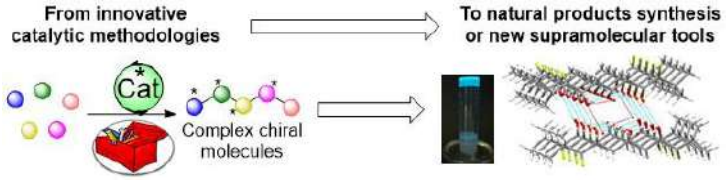
****

Monday September 27th
Auditorium Astier, 11h

Adrien QUINTARD (Aix-Marseille University - CNRS)
adrien.quintard@univ-amu.fr

(Multi)-catalytic strategies, synthetic economies... and some supramolecular applications

Abstract. The presentation will highlight our recent success in the development of multi-catalytic transformations. Based on the combinations between inexpensive iron or copper complexes with organocatalysts, they enable the rapid preparation of a broad range of molecules of interest. This was demonstrated in the context of natural products synthesis but also recently in the elaboration of new type of supramolecular tools.



1

****

For any informations, 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**

NOVEMBER 2021

****

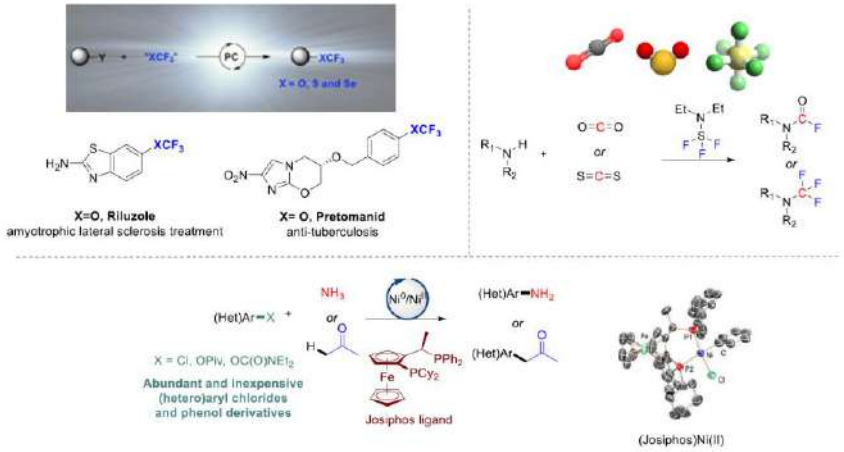
****

Monday Nov 8th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Anis TLILI (Université Lyon 1)
anis.tlili@univ-lyon1.fr

Use and Functionalization of Small Chemical Entities

The valorization of small building blocks to access highly complex and valuable molecules is of great interest. Our group is therefore focusing on the developments of new reagents or catalysts to enable such transformations. Firstly, the design of a new reagent for trifluoromethylselenolation will be discussed as well as its application under organophotoredox process. [1] Afterwards, a new concept to access fluorinated compounds using CO2 as a C1 source will be detailed. [2] Finally, a family of new air and moisture stable Ni(II) complexes designed with Solvias AG will be presented in the context of the challenging α-arylation of acetone.[3]



[1] C. Ghiazza, L. Khrouz, C. Monnereau, M. Médebielle, T. Billard, A. Tlili, *Angew. Chem. Int. Ed.* **2018**, *57*, 11781; [2] K. Onida, A. Tlili, *Angew. Chem. Int. Ed.* **2019**, *58*, 12545; [3] S. A. Derhamine, T. Krachko, N. Monteiro, G. Pillet, J. Schranck, A.Tlili, A. Amgoune *Angew. Chem. Int. Ed.* **2020**, *59*, 18948.

****

For any informations, 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

****

CulturChem Remote

Monday Nov 15th, 15h30
ZOOM
Login see below

Federica PISANESCHI (UT MD Anderson Cancer Center, Houston)
fpisaneschi@mdanderson.org

^{18}F-Fluoropivalic acid and ^{18}F-4-Fluoronaphthol: Story of Two Radiopharmaceuticals from Bench to Bedside

Abstract. Positron Emission Tomography (PET) is a molecular imaging technique able to visualize biomolecular processes *in vivo*, in real time, via a radiolabeled drug called "tracer". PET is used in many fields of medicine, oncology, neurology, and inflammation to name a few.
In the present talk, two tracers, [^{18}F]fluoropivalic acid ([^{18}F]FPIA) and [^{18}F]fluoronaphthol ([^{18}F]4FN), will be shown.
[^{18}F]FPIA has oncological applications and visualizes lipid metabolism. Initially conceived to map the *de novo* fatty acid synthesis pathway, [^{18}F]FPIA was shown later to be linked to the recruitment of short-chained fatty acids from the extracellular space, via carnitine-shuttle. [^{18}F]FPIA has completed phase 0-I, showing a suitable safety profile and it is currently in phase II, for the visualization and staging of glioblastoma.
[^{18}F]4FN visualizes the production of high-energy reactive oxygen species (ROS), which occurs during acute inflammatory processes when the innate immune system is recruited. 4FN has been validated in several inflammation models, such as arthritis and dermatitis, and is ready to be submitted to FDA as an Investigational New Drug.

Click this link:
https://zoom.us/j/98996517364?pwd=QUEvUlBaOXVqOEI4cHFoMkZvV3JJUT09

****

****

Monday Nov 22nd, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Rodolphe CLERAC (CNRS - Université de Bordeaux)
clerac@crpp-bordeaux.cnrs.fr

A scientific adventure from the control of the magnetic interactions toward metal-organic magnets at room temperature

Abstract. The magnetic properties of a complex or a material usually result from cooperative effects between the magnetic spins. The choice of the linker between the spins is therefore a crucial element to control, as it mediates the communication between them. The use of a redox-active bridging ligand as a linker is a particularly attractive strategy. By oxidation or reduction, it can act as a switch of the magnetic interactions. While in its diamagnetic state, it mediates usually weak magnetic interactions, in its radical form, it can promote a better spin delocalization inducing large magnetic interactions and in the same time, a good electronic conductivity which could lead to new high T_C conductive magnets.

****

For any informations, 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

****

CulturChem Special

Friday Nov 26th, 11h
Room 101
32/42, 1st floor
Campus P et M Curie
Sorbonne Université

Pedro M. P. GOIS (Pharmacy Faculty, Uni. Lisboa.)
pedrogois@ff.ulisboa.pt

New Chemistries for Stimuli-Responsive Targeting Drug Conjugates

Abstract. Targeting drug conjugates emerged as a powerful class of chemotherapeutic agents that are capable of sparing healthy tissues by liberating the cytotoxic payload upon specific antigen recognition. A considerable body of work in this field highlighted that targeting drug conjugates therapeutic efficacy, correlates well with the conjugate homogeneity and activation of the drug at the diseased site. Therefore, the linker technology used to connect both functions contributes decisively to the therapeutic usefulness of these constructs. In this communication will be presented our most recent finding on the design of functional likers for targeting drug conjugates, based on boron complexes (B-complexes) that can be modulated to exhibit fluorescence and to respond to glutathione, pH or reactive oxygen species stimulus.
https://sites.ff.ulisboa.pt/goislab/

****

****

Monday Nov 29th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Grégory NOCTON (Ecole Polytechnique)
gregory.nocton@polytechnique.edu

Organometallic chemistry of low-valent lanthanides: unusual oxidation states and magnetic sandwiches

Abstract. Organolanthanide complexes are an interesting class of organometallic compounds that have been developed in the 1950's and that now concern most of the rare earths in their trivalent and divalent states. The applications for such compounds are numerous for single electron transfer reactivity and also because of their optical and magnetic properties: their Single-Molecule-Magnet behavior have impressed with record blocking temperatures. We will present a short overview of our methodology for the synthesis of organometallic complexes with very original geometry and in which the oxidation state is not trivial to assess because of the development of multiconfigurational electronic states.

****

For any informations, 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**

DECEMBER 2021

****

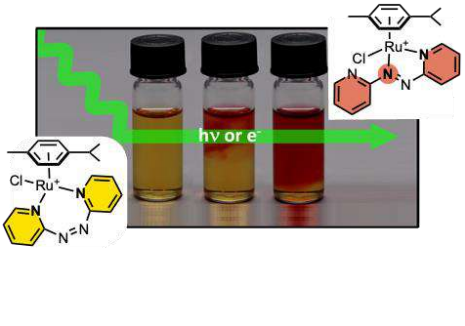
****

Monday Dec 6th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Nicolas BOGLIOTTI (ENS Paris-Saclay)
nicolas.bogliotti@ens-paris-saclay.fr

Stimuli-responsive metal complexes and materials derived from azobenzene

Abstract. The external manipulation of molecular systems with stimuli (light, electrons, molecules) is being increasingly exploited for the control of events at various scales, eventually giving rise to "smart" systems. In the aim of developing new tools for the control of chemical events with implication ranging from catalysis to material sciences, we have investigated various molecular species, notably arene-ruthenium complexes and polyazobenzenes, whose synthesis, structure and properties will be presented.



****

For any informations, 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

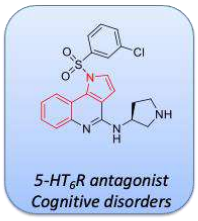
****

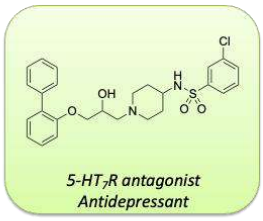
Monday Nov 13th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

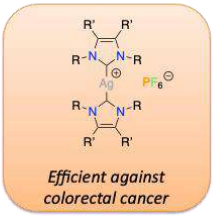
Xavier BANTREIL (Université de Montpellier)
xavier.bantreil@umontpellier.fr

Enabling Technologies for the Sustainable Synthesis of Biologically Active Molecules

Abstract. Medicinal chemistry is often limited to standard bench techniques involving well-known classical reactions. In the past years, in the frame of a collaboration with the group of Prof. Pawel Zajdel (Jagellonian University Medical College, Krakow, Poland), we have studied the synthesis of biologically active molecules, targeting specific serotoninergic receptors, and that could be used for the treatment of the cognitive deficits that are associated with dementia and Alzheimer's disease.[1] A major improvement was found in the use of novel technologies such as flow chemistry[2] and mechanochemistry.[3] Ball-milling was also used as a unique approach for the synthesis of biologically active silver(I) complexes featuring *N*-heterocyclic carbene ligands.[4]







References

1) Zajdel, P.; Grychowska, K.; Mogilski, S.; Kurczab, R.; Satała, G.; Bugno, R.; Kos, T.; Gołębiowska, J.; Malikowska-Racia, N.; Nikiforuk, A.; Chaumont-Dubel, S.; Bantreil, X.; Pawłowski, M.; Martinez, J.; Subra, G.; Lamaty, F.; Marin, P.; Bojarski, A. J.; Popik, P., *J. Med. Chem.* **2021,** *64*, 13279.

2) Drop, M.; Bantreil, X.; Grychowska, K.; Umuhire Mahoro, G.; Colacino, E.; Pawlowski, M.; Martinez, J.; Subra, G.; Zajdel, P.; Lamaty, F. *Green Chem.* **2017**, *19*, 1647.

3) a) Canale, V.; Frisi, V.; Bantreil, X.; Lamaty, F.; Zajdel, P., *J. Org. Chem.* **2020,** *85*, 10958. b) Canale, V.; Kotańska, M.; Dziubina, A.; Stefaniak, M.; Siwek, A.; Starowicz, G.; Marciniec, K.; Kasza, P.; Satała, G.; Duszyńska, B.; Bantreil, X.; Lamaty, F.; Bednarski, M.; Sapa, J.; Zajdel, P., *Molecules* **2021,** *26*, 3828.

4) Beillard, A.; Quintin, F.; Gatignol, J.; Retailleau, P.; Renaud, J.-L.; Gaillard, S.; Métro, T.-X.; Lamaty, F.; Bantreil, X., *Dalton Trans.* **2020,** *49*, 12592.

****

For any informations, 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 2022

****

****

February 7th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Belén ALBELA (Ecole Normale Supérieure de Lyon)
belen.albela@ens-lyon.fr

Mesoporous Solids: Innovative Materials with Multiple Applications

Abstract. Inorganic mesostructured porous solids, discovered by Mobil Company in 1992, offer multiple applications in domains such as depollution, catalysis and medicine. Indeed, the combination of well-defined porosity (pore diameter ~ 2-10 nm), high specific surface (1000 m^2/g) and high thermal and mechanical stability makes them ideal supports for the design of heterogeneous catalysts, depollution systems and drug nano-carriers. Our strategy consists in designing metal active sites supported on mesostructured silica using metalloenzymes as models. The functionalization of the support is a key parameter to tune its activity. The challenge is to obtain single active sites homogeneously distributed in the solid in order to correlate structure and activity. In addition, the pore affords confinement as in the hydrophobic matrix of the enzyme. This approach has been applied to prepare manganese hybrid materials with potential applications in antioxidant therapies.

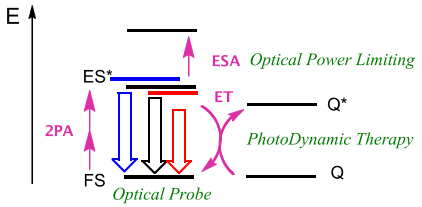
****

February 14th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Gilles LEMERCIER (Université Reims Champagne-Ardenne)
gilles.lemercier@univ-reims.fr

Excited-states of 1,10-phenanthroline derivatives and related Ru(II) (nano)edifices for potential applications

Abstract. The presentation will concern studies in the field of the linear and nonlinear optical properties of ligands and related Ru(II) complexes [1]. One- and two-photon induced (2PI) access to triplet ^{3}MLCT excited states will be discussed both in a fundamental interest and in the perspective of applications in physic and biology such as photodynamic therapy (PDT) [2]. The access to functionalized surfaces and nanoparticles [3] will also be presented and discussed for potential applications in theranostic [4].



[1] E. Rousset, O. Mongin, J. Moreau, L. M. Lawson Daku, M. Beley, P. C. Gros, S. Chevreux, M. Blanchard-Desce, G. Lemercier, *Dalton Trans.*, **2021**, ***50***, 10119. [2] G. Lemercier, M. Four, S. Chevreux, *Coord. Chem. Rev.*, **2018**, *368*, 1; C. Boca, M. Four, A. Bonne, B. van Der Sanden, S. Astilean P. L. Baldeck, G. Lemercier, *Chem. Commun.* **2009**, 4590. [3] Q. Nguyen, E. Rousset, V. Nguyen, V. Colliere, P. Lecante, W. Klysubun, K. Philippot, J. Esvan, M. Respaud, G. Lemercier, P. Tran, C. Amiens, *ACS Applied Materials & Interfaces*, **2021**, ***13***, 45, 53829. [4] C. Truillet, F. Lux, J. Moreau, M. Four, L. Sancey, S. Chevreux, G. Boeuf, P. Perriat, C. Frochot, R. Antoine, P. Dugourd, C. Portefaix, C. Hoeffel, M. Barberi-Heyob, C. Terryn, L. van Gulick, G. Lemercier, O. Tillement, *Dalton Trans.*, **2013**, *42*, 12410; S. Lechevallier, R. Mauricot, H. Gros-Dagnac, S. Chevreux, G. Lemercier, E. Phonesouk, M. Golzio, M. Verelst, *ChemPlusChem.*, **2017**, *82*, 770.

****

****

February 21st, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

José RUIZ (Universidad de Murcia, Spain)
jruiz@um.es

Novel Ir(III) complexes: applications for photodynamic therapy of cancer

Abstract. Photodynamic therapy (PDT) is a non-invasive antitumor approach that uses visible light to activate a prodrug, over a flexible time in a precise space, destroying local tumor cells due to the generation of toxic singlet oxygen and/or reactive oxygen species (ROS).[1] One of the setbacks of this technique is the low concentration of oxygen present in tumors.[2] Interestingly, PDT can exhibit immunomodulatory functions in addition its direct tumor-destroying capability and provides an important opportunity to target CSCs selectively.[3] Over the last years, our research group focused its attention on the development of precious metal complexes as (photo)therapeutic agents against cancer.[4-5] During this talk, we will present our latest results on these topics.

[1] A. Zamora, G. Vigueras, V.Rodríguez, M. D. Santana and J. Ruiz *Coord. Chem. Rev.*, 2018, 360, 34-76. [2] F. J. Ballester, E. Ortega, D. Bautista, M. D. Santana and J. Ruiz *Chem. Commun.*, 2020, 56, 10301-10304. [3] G. Vigueras, L. Markova, V. Novohradsky, A. Marco, N. Cutillas, H. Kostrhunova, J. Kasparkova, J. Ruiz and V. Brabec *Inorg. Chem. Front.*, 2021, 8, 4696–4711. [4] E. Ortega, C. Pérez-Arnaiz, V. Rodríguez, C. Janiak, N. Busto, B. García and J. Ruiz. *Eur. J. Med. Chem.*, 2021, 222, 113600. [5] J. Pracharova, G. Vigueras, V. Novohradsky, N. Cutillas, C. Janiak, H. Kostrhunova, J. Kasparkova, J. Ruiz and V. Brabec *Chem. Eur. J.*, 2018. 24, 4607-4619

****

February 28th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Wadih GHATTAS (Université Paris-Sud Orsay)
wadih.ghattas@u-psud.fr

Artificial enzymes beyond powerful catalytic tools

Abstract. In the context of environmentally friendly green chemistry, enzymes can be used instead of chemical catalysts but their high substrate specificity limits their utility. Additionally, their scope of catalysis is limited to the panel of biochemical reactions while chemists have developed a larger variety of reactions.
To overcome these hurdles artificial enzymes have been developed by incorporating chemical catalysts inside proteins. On the one hand, chemical catalysts bestow artificial enzymes with a wide scope of catalysis, on the other protein residues provide a chiral environment and eco-compatibility. Artificial enzymes are now considered a major development addressing the increasing societal and governmental pressure that demand greener chemistry. The talk will feature a prominent example of the development of artificial Diels-Alderases as well as the potential applications of such biorthogonal artificial enzymes. Indeed, we demonstrated that such artificial enzymes function in living cells thus opening new horizons of applications in therapy and diagnostics.
The chemical and the biological components of artificial metalloenzymes can be separately fine-tuned to optimize the catalysis. Such chemo-genetic optimizations are a unique feature of artificial enzymes and have led to highly efficient examples. Recently while designing the active site of an artificial enzyme, we witnessed how the protein fold can adapt to different metals and how single mutations distant from the active site can affect metal coordination. Studying artificial enzymes is proving to be useful to further improving our understanding of metal coordination in metalloproteins in general.

****

For any informations, 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

MARCH 2022

****

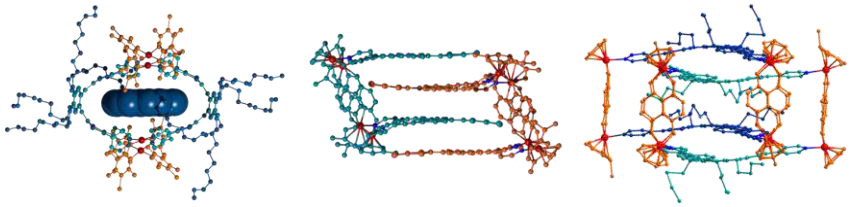
****

March 7th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Sébastien GOEB (Université d'Angers)
sebastien.goeb@univ-angers.fr

Supramolecular Transformations from Self-Assembled Cages

Abstract. Coordination driven self-assembly has allowed the preparation of many molecular polygons and polyhedrons with remarkable properties. They are obtained by association of polytopic ligands and complexes showing a pre-organized geometry. The corresponding host cavities offer promising opportunities for applications in molecular recognition or even in guest transport. We focused our attention for several years in the design of electro-active self-assembled 2D and 3D discrete structures based on the tetrathiafulvalene unit (TTF) and derivatives (exTTF and DTF for example) with the aim of controlling the guest release thanks to a electrochemical stimulus. We are also interested in understanding the key parameters governing the formation of an emergent class of coordination assemblies, i.e. interlocked cages. We believe that such compact objects could offer promising opportunities in controlling the structural organization of donor and acceptor units. For example, we demonstrated recently that truxene based ligands, associated with dinuclear Ruthenium or Rhodium complexes can produce this type of compact interlocked systems.



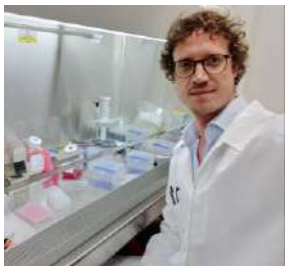
Self-assembled structures constructed from **exTTF** (left), **DTF** (center) and **Truxene** (right)

****

For any informations, 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

****

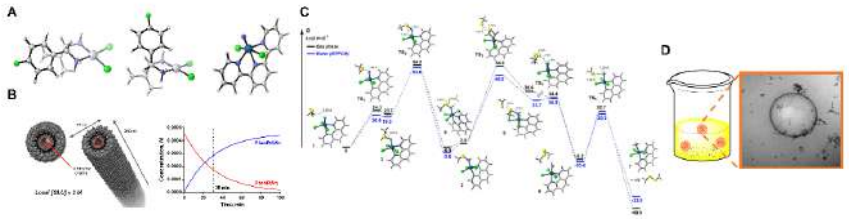
March 14th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université



Gilles BERGER (Université de Bruxelles)
gilles.berger@ulb.be

Metal-Based Anticancer Therapeutics: Short Stories

Abstract. Metal drugs such as gold, mercury and arsenic compounds belong to some of the most ancient remedies knows to humans and can be traced back to ancient Egyptians, Greek and Chinese civilizations, but are also in extensive use in modern societies. Metal complexes and bioinorganic chemistry (re)gained widespread interest with the discovery of cisplatin, one of the first successful anticancer drugs to hit the clinics. Although extremely useful in today's arsenal against cancer, current platinum drugs are associated with severe drawbacks, such as resistance to treatment and toxic effects that limit their use and efficacy. The discovery and development of metal-based chemotherapeutic agents with new mechanisms of action or innovative delivery systems are thus still important goals in cancer research. I will highlight my young journey in the field, focusing on the development of new metal complexes that may be active against cisplatin-resistant cancers and/or have fewer dose-limiting side effects. These will comprise diastereoselective platinum(II) cytotoxic complexes, high valent osmium(VI) nitrido compounds, self-assembling osmium and ruthenium nanosystems, and the viral encapsulation of a monovalent platinum(II) complex.



A: Chiral platinum(II) diastereomers and a high-valent osmium(VI) nitrido complex. B: Loading of a monovalent platinum complex in the tobacco mosaic virus. C: The multistep reduction of Os^{VI} to Os^{III} by thiols. D: Mitochondria-targeting, self-assembling ruthenium and osmium nanoparticles.

****

March 21st, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Peter HESEMANN (Institut Charles Gerhardt, Montpellier)
peter.hesemann@umontpellier.fr

From Ionic Liquids to nanostructured Ionic Solids: Ionosilicas as 'Designer Materials'

Abstract. Silica based materials containing covalently anchored ionic groups are called ionosilicas. Our special concern are purely ionic-inorganic silica hybrids (Figure 1), obtained via hydrolysis-polycondensation reactions exclusively from silylated ionic precursors. These phases can be considered as 'heterogenized Ionic Liquids; they combine the characteristics of mesoporous silicas (porosity, regular architecture on the mesoscopic scale) and the unmatched chemical versatility of ionic liquids.

This talk will focus on the extraordinary polyvalence of ionosilicas. On the one side, the texture and morphology of ionosilicas can be controlled, and various shapes such as ionosilica nanoparticles, monoliths or fibers can be synthesized. On the other side, ionosilicas are functional materials with promising properties for various applications. We will illustrate the polyvalence of ionosilicas by two case studies in drug delivery and organocatalysis.

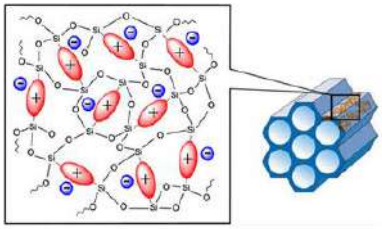


Figure 1. Schematic representation of ionosilica

****

For any informations, 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

****

March 28th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Cédric PLESSE (CY Cergy Paris Université)
cedric.plesse@cyu.fr

Electronic conducting polymers and ionic conducting polymers for electroactive materials

Abstract. Electroactive Polymers (EAPs) belong to the group of smart materials which respond to an electrical stimulus by undergoing large deformations and can therefore be used in biomimetic systems. Electronic conducting polymers (ECP) based actuators have several advantages compared to conventional actuators, including, light weight, biocompatibility and low-operating voltage. Their actuation principle relies of ECP volume variation induced by ion exclusion/expulsion when submitted to a redox process. It is then possible to convert electrochemical energy into volume variation of CP electrodes and then to convert electrical energy into mechanical work. Moreover ECP based ionic devices can operate in a reverse mode and generate electrical signal in response to mechanical stimulation. In the growing field of soft electronics, they could then fulfill tasks non possible with stiff classical technology and arise as promising candidates for the development of artificials muscles and soft Micro-Electro-Mechanical Systems (MEMS)
In this presentation, the synthesis and optimization of the basic components of such devices, i.e. conducting polymer electrodes and ionic conducting materials will be described as well as how macromolecular chemistry can be a powerful tool to develop on demand new applications, from microrobotics to biomedical devices.

****

For any informations, 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**

APRIL 2022

****

****

April 4th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Gustavo GARCIA-MACIAS (SOLEIL Synchrotron)
gustavo.garcia@synchrotron-soleil.fr

Applications of photoelectron spectroscopy for product detection in gas phase chemistry

Abstract. Full detection of all products and intermediates involved at any given time on a chemical reaction is considered as the ultimate goal, leading to a complete description of the reaction mechanism and therefore to its control. Optical methods, although very sensitive, lack the required universality needed for complex determinations. Because every species can be ionised, mass spectrometry also appears as a method of choice, however extensive fragmentation due to the high energy ionisation sources in commercial spectrometers, and the inability to differentiate structural isomers limit its usability. In the past decade, several groups have combined mass spectrometry with VUV tuneable sources to minimise fragmentation by ionising close to the first threshold (soft ionization), and to record the photoion efficiency (PIE) curves as a function of photon energy, which provide structural information, as demonstrated in complex systems such as low-pressure flames.

Because the structural information contained in the PIEs is limited, a more recent development that increases sensitivity and isomer differentiation will be discussed here based on coupling photoelectron spectroscopy to photoion mass spectrometry. Although photoelectron-photoion coincidence (PEPICO) techniques have been applied extensively to acquire detailed knowledge on photoionisation processes since the early seventies, it is only recently that are being applied for advanced product detection in complex gas phase media.

I will present examples of application of modern double imaging PEPICO (i2PEPICO) techniques in combination with tuneable VUV synchrotron radiation for the study of complex systems of environmental interest such as combustion, secondary organic aerosol formation5 or atmospheric oxidation. I will also present a novel method to measure circular dischroism in the gas phase that can also be coupled to mass spectrometry for online enantioselective analysis on products or reactive intermediates, as I will show in the case of pepper oil analysis.

****

****

April 11th, 11h
Auditorium Astier
Building Esclangon
Campus P et M Curie
Sorbonne Université

Silvia PUGLIESE (Collège de France and University of Namur)
silvia.pugliese@college-de-france.fr

Towards artificial photosynthesis: heterogenized molecular complexes for CO_2 electroreduction and optimization of perovskite solar cells

Abstract. Despite its challenges, solar-powered CO_2 electroreduction represents a promising way to tackle both global warming and energy demand. This seminar will focus on the main outcomes of my PhD work, which had the double goal to develop heterogenized molecular complexes for CO_2 electroreduction and to increase the power conversion efficiency (PCE) of fully printable carbon-based perovskite solar cells (PSCs).

Homogeneous catalysts can be immobilized on heterogeneous conductive supports to generate cathode materials for CO_2 electrolyzers: such heterogenized molecular systems thus combine the advantages of a solid material with those of molecular complexes.[1] In this context, $[Ni(cyclam)]^{2+}$ is known to be a good, stable and selective molecular catalyst,[2] however, previous electrode surface modifications with $[Ni(cyclam)]^{2+}$ proved quite inefficient and poorly selective.[3] In the present research, novel N- and C-substituted cyclam derivatives carrying a pyrene moiety were synthesized in order to immobilize $[Ni(cyclam)]^{2+}$ at the surface of carbon-based electrodes. The pyrene-modified complexes were immobilized on carbon nanotube-coated gas diffusion electrodes using a non-covalent approach and the novel electrodes were characterized electrochemically for CO_2 electroreduction.

The manufacturing process of monolithic, fully printable carbon-based PSCs makes this type of devices among the most competitive on the market, with high potential for scalability and applications in future low-cost technologies. Despite this, PCEs of these devices (15.6% at its best[4]) are still lower than conventional PSCs, for which the best certified PCE has been recently increased up to 23.7%.[5] Efforts to increase the PCE of monolithic printable PSCs are therefore necessary to maintain their competitiveness. For this purpose, in the present work, the optimization of the TiO_2-based electron transport layer was addressed. We initially synthesized and fully characterized a range of mesoporous TiO_2 nanomaterials with different morphological features and we introduced them into the solar cells. Successively, we have adopted an even more viable strategy by introducing different degrees of porosity into state-of-the-art nanoparticle based TiO_2 scaffolds by using polymer beads as sacrificial templates.

[1] C. Sun, R. Gobetto, C. Nervi, *New J. Chem.*, **2016**, *40*, 5656–5661.
[2]M. Beley, J. P. Collin, R. Ruppert, J. P. Sauvage, *J. Chem. Soc. - Ser. Chem. Commun.*, **1984**, *2*, 1315–1316.
[3] A. Zhanaidarova, C. E. Moore, M. Gembicky, C. P. Kubiak, *Chem. Commun.*, **2018**, *54*, 4116–4119.
[4] M. Duan, Y. Hu, A. Mei, Y. Rong, H. Han, *Mater. Today Energy*, **2018**, *7*, 221–231.
[5] P. Roy, N. Kumar Sinha, S. Tiwari, A. Khare, *Sol. Energy*, **2020**, *198*, 665–688.

****

****

April 25th, 11h
Room 101
32-42, 1st level
Campus P et M Curie
Sorbonne Université

Debasis BANERJEE (Indian Institute of Technology Roorkee)
debasis.banerjee@cy.iitr.ac.in/ debasis.iitk@gmail.com

Nickel-Catalyzed Oxidant Free (De)-hydrogenation of Alcohols for Sustainable Organic Transformations

Abstract. Amines, amides and N-heterocycles are most valuable compounds ubiquitous in bioactive molecules, alkaloids, and extensively used in pharmaceuticals, agrochemicals and as ligands.[1] Therefore, catalytic selective C–N and C-C bond formation for their synthesis is an ultimate goal in chemical research. Conventional methodologies for their synthesis involves multi-step pathways and suffer from low atom economy, limited selectivity and produced stoichiometric amounts of waste.[1] Direct application of renewable alcohols as electrophilic coupling partner represents a sustainable alternative, as they can be readily available in industrial scale production from lignocellulose biomass.[1]

Recently, there is a potential drive to replace the precious noble-metal catalysts using earth abundant and inexpensive non-noble metals for sustainable organic transformations. Since last couple of years we have developed the applications of Ni-based catalysts for such transformations. We have studied general and practical applications of various primary alcohols, including diols and amino alcohols for selective construction of numerous primary and secondary amines, amides, five or six-membered N-heterocycles, activation of weak sp^3 C-H bond of alkyl substituted N-heteroarenes to E-selective alkenes as well as functionalization of ketone enolates. Our recent studies on the per-fluoroalkylation will also be discussed. A detailed mechanistic and kinetics studies were also established for such transformations.[2-6]

References and Notes:

1. Watson, A. J. A.; Williams, J. M. J. Science **2010**, 329, 635.
2. (a) Vellakkaran, M.; Singh, K.; Banerjee, D. ACS Catal., **2017**, 7, 8152–8158. (b) Singh, K.; Vellakkaran, M.; Banerjee, D. Green Chemistry, **2018**, 20, 2250-2256. (c) Das, J.; Singh, K.; Vellakkaran, M.; Banerjee, D. Org. Lett., **2018**, 20, 5587-5591.
3. (a) Vellakkaran, M.; Das, J.; Banerjee, D. Chem. Commun. **2018**, 54, 12369-12372. (b) Kabadwal, L. M.; Das, J; Banerjee, D. Chem. Commun. **2018**, 54, 14069-14072.
4. (a) Das, J.; Vellakkaran, M.; Banerjee, D. Chem. Commun. **2019**, 55, 7530-7533. (b) Bera, A.; Sk. M.; Singh, K.; Banerjee, D. Chem. Commun. **2019**, 55, 5958-5961.
5. (a) Das, J.; Vellakkaran, M.; Sk. M.; Banerjee, D. Org. Lett., **2019** 21, 7514-7518. (b) Bera, S.; Bera, A.; Banerjee, D.. Org. Lett. **2020**, 22, 6458–6463. (c) Bera, S.; Bera, A.; Banerjee, D. Chem. Commun. **2020**, 56, 6850–6853. (d) Kabadwal, L. M.; Bera, S.; Banerjee, D. Chem. Commun. **2020**, 56, 4777–4780.
6. (a) Bera, A.; Bera, S.; Banerjee, D. Chem. Commun. **2021**, 57, 13042–13058. (b) Kabadwal, L. M.; Bera, S.; Banerjee, D. Org. Chem. Front. **2021**, 8, 7077–7096. (c) Bera, A.; Kabadwal, L. M.; Bera, S.; Banerjee, D. Chem. Commun. **2022**, 58, 10–28.

****

MAY 2022

****

Attention: Please check the assigned rooms

****

May 9th, 11h
INSCP Room 317
T 22-23
Campus P et M Curie
Sorbonne Université

Grégory CHAUME (BioCIS, CY Cergy Paris Université)
gregory.chaume@cyu.fr

Fluorinated proline analogues as original tools for conformational control of peptide chains

Abstract. Nowadays, a whole arsenal of drugs based on peptides and peptidomimetics is available.[1] Their efficacy depends on several factors such as their conformation, hydrophobicity, or resistance to degradation by peptidases. These physicochemical and biological factors can be tuned by the introduction of fluoroalkylated groups within the peptides.[2]
Due to its nature, the peptide bond undergoes a spontaneous *cis–trans* isomerism, and the *cis* isomers are much more difficult to stabilize than the *trans* forms. The Xaa-Pro peptide bond is subject to *cis-trans* isomerization characterized by an increased *cis* population and an activation energy that is low when compared to the other amino acids. Besides, the five-membered ring of the Pro residue can adopt two main distinct conformations (C^{γ} *endo*- or C^{γ} *exo*-puckered). Therefore, a variety of proline analogs have been designed in order to control the conformation of the peptide backbone and consequently to modulate the biological activity of peptides.
Our group is interested in the synthesis of enantiopure fluorinated amino acids and their incorporation into peptides. Because of the crucial role of the proline, we have developed efficient synthetic routes for the synthesis of various fluorinated analogues of proline.[3] Here, I will present the main results obtained from NMR and theoretical studies based on model peptides which established the stereoelectronic effects imparted by the CF_3 and CF_2H groups along the pyrrolidine ring. I will also detail the methodological study developed to optimize their incorporation into peptides. Finally, I will present some applications to peptides of interest.

References:
[1] a) M. Muttenthaler et al. *Nat. Rev. Drug Discov.* ***2021****, 20, 309;* b) L. Wang et al. *Signal Transduct. Target. Ther.* **2022**, *7*, 48.
[2] H. Mei, H. et al. Eur. J. Med. Chem. ***2020****, 186, 111826.*
[3] a) G. Chaume et al. *Org. Lett.* **2006**, *8*, 6123; b) G. Chaume et al. *J. Fluorine Chem.* **2008**, *129*, 1104; c) C. Caupène et al. *Org. Lett.* **2009**, *11*, 209; d) G. Chaume et al. *J. Org. Chem.* **2010**, *75*, 4135; e) H. Lubin et al. *J. Org. Chem.* **2015**, *80*, 2700; f) J. Simon et al. *J. Org. Chem.* **2016**, *81*, 5381; g) C. Gadais et al. *ChemBioChem* **2019**, *20*, 2513 ; h) N. Malequin et al. *Chem. Commun.* **2019**, *55*, 12487; i) S. A. Sanchez et al. *Org. Lett.* **2021**, *23*, 382.

****

For any informations, 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

****

May 16th, 11h
INSCP Room 317
T 22-23
Campus P et M Curie
Sorbonne Université

Gerhard ERKER (Université Münster)
erker@uni-muenster.de

Boranes and Frustrated Lewis Pairs: Searching for New Reactions

Abstract. Acids and bases undergo the neutralization reaction when brought together in solution. In frustrated Lewis pairs (FLPs) this is effectively hindered to make pairs of active Lewis acids and bases coexistent in solution. This leads to some remarkable reactivities. Examples are shown where the FLPs activate dihydrogen and serve as metal free hydrogenation catalysts. The presented reactive intramolecular phosphane/borane FLPs add to olefins, they add examples of carbon, nitrogen and sulfur oxides and they were used to initiate selective reduction reactions of carbon monoxide. A variety of strongly electrophilic boranes were used in FLP chemistry and they were employed in the preparation of reactive BH containing borenium cations. Examples of their specific reactions with small molecules are presented and discussed and they were used for the generation of rare examples of reactive boraalkenes, among them borabutadiene derivatives. Eventually, we made use of the isolobal connection between the cationic C-H^+ and the neutral B-H moieties. This was used to prepare unique borapyramidane examples by isomerization of a corresponding borole precursor. The borole precursor itself was obtained starting form a suitably substituted bis-alkynyl borane by a sequence involving consecutive 1,1-hydroboration and 1,1-carboboration reactions.

Selected references:

"Frustrated Lewis Pair Chemistry: Development and Perspectives", D. W. Stephan, G. Erker, *Angew. Chem. Int. Ed.* **2015**, *54*, 6400-6441 (doi: 10.1002/anie.201409800)
"The $[(NHC)B(H)C_6F_5]^+$ Cations and Their [B](H)-CO Borane Carbonyls", C. Chen, J. Li, C. G. Daniliuc, C. Mück-Lichtenfeld, G. Kehr, G. Erker, *Angew. Chem. Int. Ed.* **2020**, *59*, 21460-21464 (doi: 10.1002/anie.202009353).
"N-Heterocyclic Carbene Stabilized 1-Bora-1,3-butadienes", C. Chen, C. G. Daniliuc, G. Kehr, G. Erker, *J. Am. Chem. Soc.* **2021**, *143*, 21312-21320 (doi: 10.1021/jacs.1c09774

****

For any informations, 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

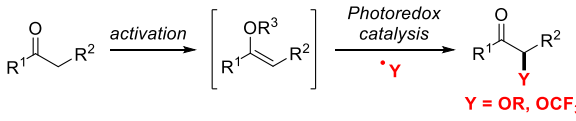
****

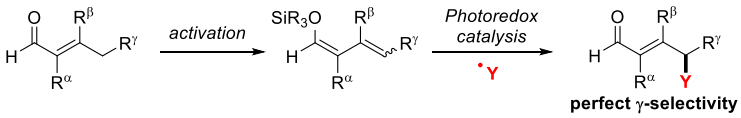
May 23rd, 11h
Auditorium Herpin
Building Esclangon
Campus P et M Curie
Sorbonne Université

Guillaume DAGOUSSET (Institut Lavoisier de Versailles)
guillaume.dagousset@uvsq.fr

New radical strategies for the synthesis of α-functionalized carbonyls and γ-functionalized enals.

Abstract. The C–H functionalization in α position to carbonyl compounds is a powerful approach to access a wide variety of synthetic building blocks of high interest. This key transformation in organic synthesis classically involves the activation of the carbonyl substrate into a nucleophilic intermediate (enolate, silyl enol ether, enamine…) and subsequent reaction with a suitable electrophile. In an analogous manner, the C–H functionalization in γ position to enals generally involves a similar activation of the enal substrate into a dienolate, a silyl dienol ether, or a dienamine, which subsequently reacts with the electrophile. However, these well-known methods have to face two main issues: i) Fist, they are unadapted for some specific reactions such as alkoxylation reactions, because no RO^+ electrophile is readily available; ii) Second, in the case of γ-funtionalization, the selectivity between the two nucleophilic α and γ carbons of the dienolate or dienamine is hard to control and generally leads to a mixture of regioisomers.
This presentation will show how a new radical approach can overcome these limitations. Alkoxyl and trifluoromethoxy radicals, generated under mild photoredox-catalyzed conditions, will enable the α-alkoxylation and α-trifluoromethoxylation of carbonyl compounds, respectively. In addition, a unified photoredox strategy will be described for the highly selective synthesis of γ-alkoxy, γ-amino and γ-alkyl enals.





****

****

May 30th, 11h
Auditorium Herpin
Building Esclangon
Campus P et M Curie
Sorbonne Université

Audrey DENICOURT-NOWICKI (ENS Chimie de Rennes, ISCR, "Organometallics: Materials and Catalysis)
audrey.denicourt@ensc-rennes.fr

Metal nanoparticles: Pertinent catalysts to upgrade terpenic renewables in water. From lab to multigram scale

Abstract. Aqueous suspensions of surfactant-stabilized metal nanoparticles are considered as unavoidable catalysts owing to their unique surface properties, thus affording efficient catalytic performances combined with their recycling through a biphasic approach. During this seminar, I will present some applications of these catalytic systems to upgrade terpenic renewables through oxidation and hydrogenation reactions, as well as the scale-up of these processes for the synthesis of value-added products for fragrances industries.

****

For any informations, 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

JUNE 2022

****

Attention: Please check the assigned rooms

****

June 13th, 11h
Auditorium Durand
Building Esclangon
Campus P et M Curie
Sorbonne Université

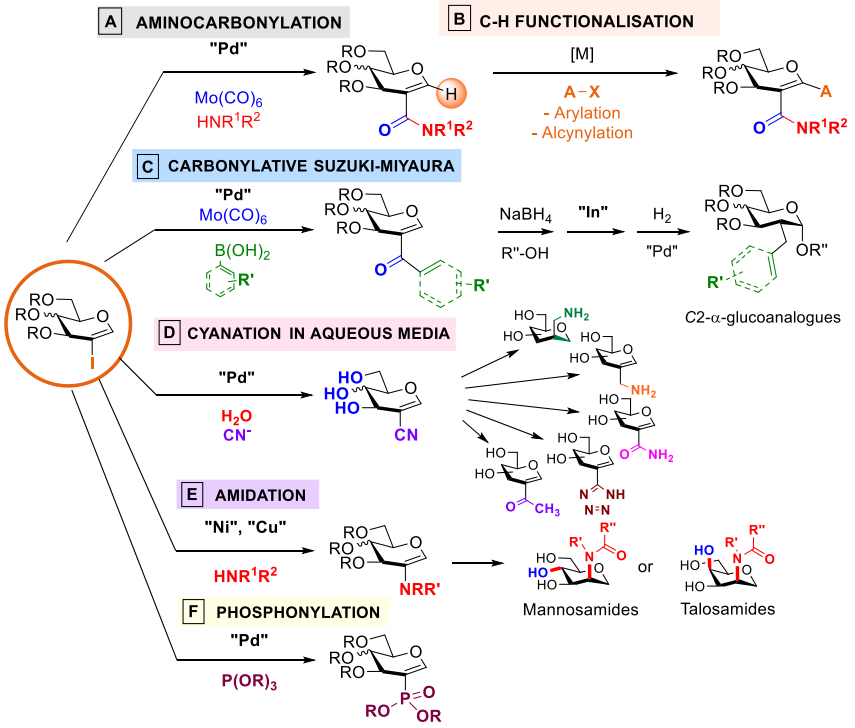
Angélique FERRY (CY Cergy-Paris Université)
angelique.ferry@cyu.fr

Access to unnatural glycosides by metal-catalyzed functionalisation of glycal substrates

Abstract. Development of new access to glycoconjugates has become of great interest in synthetic chemistry. In particular, glycoconjugates possessing an unnatural bond are largely studied due to their enzymatic and chemical stabilities towards C-O and C-N natural links.

Our expertise deals with the metal-catalyzed functionalisation of glycal substrates using two different reactivities:

- Cross-coupling reactions on 2-iodoglycal starting compounds for the formation of C-C, C-N or C-P bonds : (A), (C), (D) (E) and (F).
- Directed C-H functionalisation reactions of the pseudo-anomeric position of C2-amidoglycals (B).



****

For any informations, 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 : For nomination to the French Academy of Sciences

June 15th, 14h
Room 101
T 32-42
Campus P et M Curie
Sorbonne Université

Sason SHAIK (*Institute of Chemistry, The Hebrew University, Jerusalem, Israel*)
Sason.Shaik@mail.huji.ac.il

My Travels Through Science

Abstract. This is a story of my travels through chemistry from being an experimentalist in 1972-3, to becoming a theorist from 1974 to this day. The story mixes science with life events. Among these stories are: (a) the "orbital which has converted me to a theorist"; (b) my decision to study in the US for my Ph.D. with the late Nick Epiotis and his influence on me; (c) my adventures with VB theory, the development of VB diagrams for chemical reactivity, and the questioning of key common paradigms; (d) an adventure with deriving the stereochemical requirements for spin-state crossing in triplet photoreactions, which led in 1993 to the development of the Two-State Reactivity (TSR) concept with Helmut Schwarz; (e) the postdoc time with Roald Hoffmann – What an amazing teacher!; (f) the return to Israel to Ben-Gurion University; (g) the anus mirabilis in Orsay with Philippe Hiberty – great science (the onset of quantitative VB testing of concepts), and a lasting friendship; (h) consolidation of VB theory – bonding and reactivity; (i) the call to join the Hebrew University; (j) becoming the director of the Lise Meitner Center; (k) my adventures with the complexity of nanomachines…

****

****

June 20th, 11h
Auditorium Durand
Building Esclangon
Campus P et M Curie
Sorbonne Université

Florian JAROSCHIK (Institut Charles Gerhardt Montpellier)
florian.jaroschik@enscm.fr

Selective C-F and C-P bond activation processes involving lanthanide metals

Abstract. Lanthanide metals are strong reducing agents with redox potentials $E^0(Ln^{3+}/Ln) \approx -2.2$ V, close to the one of magnesium. The synthetic potential of these relatively easy-to-handle metals is increasingly studied in organic and organometallic chemistry as they provide several key features: (i) variation of reactivity along the series due to the lanthanide contraction; (ii) two or three electron reductions depending on the metals; (iii) generation of strong Lewis acidic species for consecutive transformations. Lanthanide metals have already been employed in the generation of Grignard-type complexes, as radical generators and for the reduction and transformations of carbonyl groups. Furthermore, metallic lanthanides are convenient starting materials for the synthesis of organometallic complexes via redox-transmetallation reactions, avoiding tedious workup often encountered in salt-metathesis reactions.
I will present some recent examples of selective C-P and C-F bond activation using lanthanide metals to access divalent organolanthanide complexes bearing bulky cyclopentadienyl ligands, including the first examples of heteroleptic divalent fluoride complexes. In a second part, the selective C-F bond activation in trifluoromethylated dienes will be discussed providing new fluorine containing building blocks. The fine-tuning of reaction conditions, mechanistic studies and synthetic applications will be outlined.

****

****

June 27th, 11h
Auditorium Herpin
Building Esclangon
Campus P et M Curie
Sorbonne Université

Giovanni MAESTRI (Università di Parma, ITALY)
giovanni.maestri@unipr.it

Atom-economical cascades: cyclizations from strained to medium-sized rings

Abstract. The ever increasing human population all but calls for a similar augmenting pool of commodities. Taking into account the ceiling imposed by sustainable development, it is therefore of the outmost importance to be able to fulfill the needs of functional molecules in the next few decades aiming to produce more by consuming less. Within this framework, the development of synthetic methods that could readily forms complex polycyclic molecular architectures in a time- and cost-savvy fashion is still in high demand.

The lecture will present a selection of recent studies from my research group on the topic. Examples took advantage of various catalytic strategies to convert linear polyfunctional substrates, which could be conveniently prepared in a concise fashion, into elaborated products through the development of ordered cascades that occur with complete atom economy.

The journey will present strategies based on synergic catalysis, in which a transition metal complex or a trinuclear cluster and a carboxylic acid cooperate to trigger the substrate activation. These methods could allow one to access in a concise fashion the core of fused polycycles, such as carbolines and ramonanines that can be found in natural compounds, and to induce the selective deuterium labelling of alkenyl C(sp2)-H bonds using cheap and safe deuterium oxide. A complementary approach involves the use of visible light to elicit complex domino sequences, enabling one to devise original route to the formation of both strained small rings and medium-sized ones.

The synthetic interest that drives these research projects is accompanied by the curiosity to understand their unusual molecular pathways, which are usually addressed combining experiments with DFT modeling. This approach provides not just key hints on their mechanisms but also, quite often, the most intriguing challenges that await to be addressed next.

****