

CulturChem 406

2017-2018

September

Monday September 11th
Auditorium 45B 11h



2

Brigitte Bibal (ISM - UMR 5255, Université de Bordeaux)

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Functional PolyAromatics: a little flexibility in Molecular Recognition and Gold Complexes

Abstract. Our research aims to design modular polyaromatic compounds devoted to catalysis and molecular recognition. In this seminar, we will focus on 9,10-diphenylanthracene and its unique photochemical and photophysical properties. Its switchable function was highlighted within a molecular cage that binds cations in an adjustable fashion. Its ability for energy transfer was also associated to gold complexes. A fast and controlled photoreduction of Gold(III) catalysts was then demonstrated.

Monday September 18th
Auditorium 45B 11h



3

Guillaume Chastanet (ICMCB, Université de Bordeaux)

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Transition de spin photo-induite : développements récents

Abstract. Depuis le début des années 80, la commutation optique de complexes de Fe(II) à conversion de spin a suscité un engouement notable puisqu'elle laissait envisager des processus ultrarapides, à l'échelle de la molécule. Nous verrons que la photocommutation ne se restreint plus aux composés à conversion de spin et que la conception des matériaux doit intégrer de nouvelles contraintes pour donner accès à de nouvelles propriétés. Cela nécessite une bonne compréhension des mécanismes opérant lors de la transition de spin, de la molécule au solide. Nous verrons les récentes évolutions qui en découlent.

Monday September 25th
Auditorium 45B 11h



XX

Cristina Nevado (University of Zurich)

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Cristina Nevado graduated in chemistry at the Autónoma University of Madrid in 2000. In October 2004 she received her PhD in organic chemistry from the same University working with Prof. Antonio M. Echavarren in late transition metal catalyzed reactions. After a post-doctoral stay in the group of Prof. Alois Fürstner at the Max-Planck-Institut für Kohlenforschung (Germany), she joined the University of Zürich as an Assistant Professor in May 2007. In 2011, Cristina was awarded the Chemical Society Reviews Emerging Investigator Award and the Thieme Chemistry Journal Award in recognition of her contributions in the field of synthetic organic chemistry. In 2012 she received an ERC Junior Investigator grant and has been awarded the Werner Prize of the Swiss Chemical Society. In 2013 she became Full Professor at the Organic Chemistry Institute of the University of Zürich. Rooted in the wide area of organic chemistry, her research program is focused on complex chemical synthesis and new organometallic reactions.

October

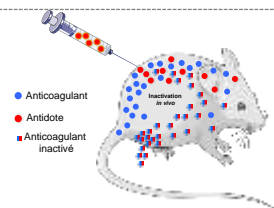
Monday October 2nd
 Auditorium 45B 11h



Alain Wagner (Chimie BioFonctionnelle, UMR 7199, Illkirch)
alwag@unistra.fr - www.biofunctional.eu
Advancing Synthetic Chemistry in Biological Media

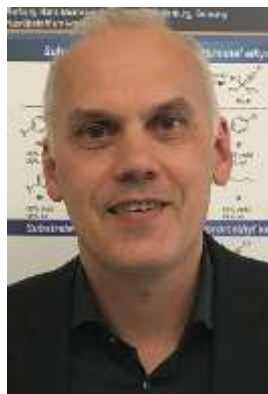
Abstract. Our research focuses on the development of chemical reactions that are compatible with complex biological media. They are qualified as bioorthogonal when they can take place in a complex biological medium without distorting it, or as bio-specific when they touch only a precise part of it.

Taking advantage of imaging and bioanalytical methods, we have developed original chemometric methodologies to figure the bio-reactivity profile of bond-forming and bond-breaking chemical reactions. By applying this methodology, we were able to characterize novel functional groups and reagents that exhibit a precise activation profile and to uncover unexpected biospecificity. Applications to bioconjugation, *in vivo* drug neutralization and chemoselective metabolomic approaches will be described.



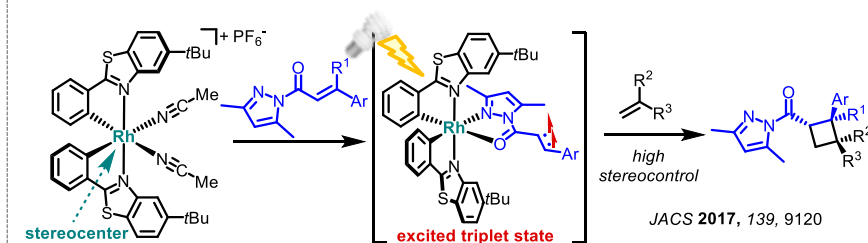
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Monday October 9th
 Auditorium 45B 11h



Eric Meggers (Department of Chemistry, University of Marburg)
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Asymmetric Catalysis Induced by Visible Light: From Free Radical to Excited State Chemistry

Abstract. The lecture will report on our progress to intertwine visible-light-activated chemistry with asymmetric catalysis. An unusual class of catalysts is employed which derive their chirality exclusively from a stereogenic metal center. Bis-cyclometalated chiral-at-metal iridium(III) and rhodium(III) catalysts provide substrate activation and the asymmetric induction, and often simultaneously serve as photoactive species (typically after substrate binding) for photoredox-mediated free radical chemistry or even direct bond forming reactions from photoexcited states.



5

Monday October 16th
Auditorium 45B 11h



6

Colette Boskovic (The University of Melbourne)

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Studies of Lanthanoid Single-Molecule Magnets

Abstract. The slow magnetisation relaxation and quantum tunnelling exhibited by single-molecule magnets (SMMs) may see them as the basis of future molecular spintronics devices or quantum computers. We are presently exploring the development of new lanthanoid-based SMMs that incorporate redox-active ligands. Another focus is elucidation of the crystal field splitting that is responsible for the SMM properties. We use inelastic neutron scattering to determine the crystal field splitting experimentally, which provides an invaluable benchmark for ab initio calculations and other computational approaches.

Monday October 23rd
Auditorium 45B 11h



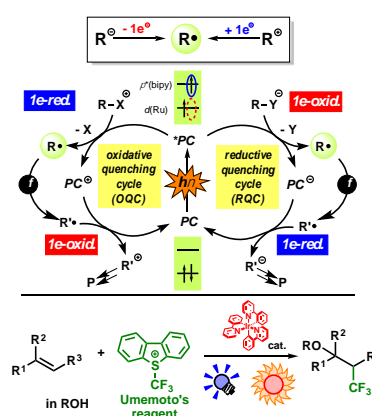
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Munetaka Akita (Tokyo Institute of Technology, Yokohama)

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Photoredox Catalysis: Trifluoromethylation and Beyond

Abstract. Photoredox catalysis mediated by photo-sensitizers (e.g. [Ru(bipy)₃]²⁺ and relevant Ir complexes) has attracted increasing attention as practical, green synthetic chemical processes, because they are visible light-promoted, redox-neutral reaction systems. Organyl radicals can be formally generated by 1e-oxidation and 1e-reduction of anionic and cationic species, respectively. We have demonstrated that the action of the redox functions of the photo-excited catalyst (*PC) to organyl onium and ate species regarded as stabilized forms of



them causes generation of organyl radicals with elimination of the auxiliary groups (X, Y). Further functionalization (f) followed by reverse redox processes leads to a redox-neutral reaction system. Photoredox catalysis via oxidative quenching cycle is in particular effective for tri- and difluoromethylation of olefinic substrates, which is the main topic of the presentation. Electron transfer from the photoexcited metal species to an electrophilic CF₃-reagent such as Umemoto's reagent generates the key ·CF₃ radical intermediate via homolytic bond cleavage (e.g. C-S bond) together with the cationic species of the catalyst. Subsequent addition of the ·CF₃ radical to the olefinic substrate followed by oxidation of the resultant carbon radical intermediate by the cationic metal species gives the carbocationic intermediate, which is trapped by nucleophiles to furnish the coupling products. It is remarkable that the reactions are promoted not only by artificial light sources (e.g. Xe lamp and blue LED lamps) but also by sunlight. This concept can be extended to organyl radicals other than the ·CF₃ radical.

November

Monday November 6th
Amphi 45B 11h



Prof. **Joost Reek** (University of Amsterdam)

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Supramolecular Transition metal catalysis: control of activity and selectivity by second coordination sphere

Abstract. The interface between supramolecular chemistry and transition metal catalysis has received surprisingly little attention in contrast to the individual disciplines. It provides, however, novel and elegant strategies that lead to new tools for the search of effective catalysts, and as such this has been an important research theme in our laboratories. In this presentation I will focus on supramolecular strategies to control activity and selectivity in transition metal catalysis, which is especially important for reactions that are impossible to control using traditional catalyst development..

Monday
November 13th
Auditorium Astier 11h

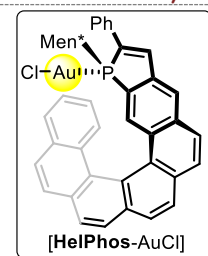


Arnaud Voiturier (CNRS-ICSN, Gif-sur-Yvette)

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New Phospha-helicenes: Synthesis and Applications in Asymmetric Catalysis

Abstract. Over the past few years, helicenes have attracted considerable attention due to their wide potential, notably in materials science. However, molecular scaffolds with helical chirality have been rarely used for building phosphorus ligands and catalysts. In this context, our goal was to access unprecedented chiral auxiliaries for organo- and organometallic catalysis. We have synthesized new phospha-helicenes, where the phosphorus moiety is embedded at the end of the helical structure, following two strategies: the photochemical oxidative cyclization of diaryl olefins and the nickel-catalyzed [2+2+2] cyclootrimerization reaction. The corresponding gold complexes of these phosphahelicenes were isolated, characterized and evaluated in enantioselective enyne, allen-ene and allene-diene cyclizations.



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Monday Nov 20th
Amphi 45B 11h



Prof. **David Vocadlo** (Simon Fraser University)

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Chemical Biology Tools to Perceive and Perturb Carbohydrates and Carbohydrate Processing Enzymes in Living Systems

Abstract: The carbohydrate structures found in every kingdom of life are emerging as a frontier area of chemical biology. I discuss our efforts to create new chemical biology tools for studying these structures and the enzymes that process them within cells and in animal models. Topics will be selected from the synthesis and deployment of; (i) a new family of fluorescence-quenched substrates that permit quantitative imaging of glycoside hydrolase activities in live cells by high content imaging, (ii) the design, synthesis, and creation of potent and selective inhibitors of carbohydrate processing enzymes active in cells and in vivo, and (iii) new chemical genetic methods to map glycosylation to the genome.

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

Lundi 27 Novembre
Amphi 45B

Pr. **Julien Bachmann** (FAU, Erlangen-Nürnberg)
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Turning lead into gold: Materials and nanostructures in electrochemical energy conversion



Abstract. One strategy for minimizing the use of expensive functional materials in energy conversion devices consists in accurately controlling the interface's microscopic geometry. 'Anodic' nanoporous templates and atomic layer deposition yield structured electrode surfaces with a tunable geometry of ordered pores. Their diameter and length are set accurately and varied systematically. Diffusion-limited electrochemical transformations remain unaffected by changes in their length, whereas galvanic current densities observed for slow multielectron transformations increase linearly with the pore length. We increase the electrochemical water oxidation turnover at iron oxide surfaces by three orders of magnitude.

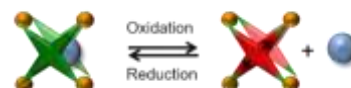
December

Monday December 4th
Amphi 45B 11h



Marc Sallé (MOLTECH-Anjou, UMR CNRS 6200, Univ. Angers)
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Redox-active self-assembled cages

Abstract. While molecular cages are often challenging to prepare through covalent chemistry procedures, the metal-driven self-assembly methodology allows a straightforward access to a wide variety of discrete architectures. The resulting cavities offer promising opportunities for applications in host-guest chemistry. In this context, we have focused our interest in the designing of electron-rich self-assembled discrete cavities. The seminar will be dedicated to this new class of metalla-cages, including recent advances related to their ability to trigger the encapsulation/release process of a guest, through a redox stimulus.



Monday December 11th
Amphi 45B 11h



Jesús Jiménez Barbero (CIC bioGUNE, Spain)
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Breaking the limits in investigating Glycan-Protein Interactions by using NMR

Abstract. Molecular recognition by specific targets is at the heart of the life processes. In recent years, it has been shown that the interactions between proteins (lectins, enzymes, antibodies) and carbohydrates mediate a broad range of biological activities, from fertilization, embryogenesis, and tissue maturation, to pathological processes. The elucidation of the mechanisms that govern how glycans are accommodated in the binding sites of these receptors is currently a topic of interest. Thus, the determination of the structural and conformational factors and the physicochemical features that govern the molecular recognition of these molecules is of paramount importance. This presentation is focused on the application of NMR methods both from the ligand and receptor's perspective (especially HSQC-based chemical shift perturbation analysis and ¹⁹F-based Saturation Transfer Difference) to the study of molecular recognition processes between a variety of polypeptides of biomedical interest and carbohydrate-based molecules, drugs and inhibitors. The use of novel lanthanide-binding tags and ¹⁹F-containing glycomimetics as probes for monitoring interactions from the ligand's point of view will be highlighted. Different glycan receptors, both wild type and mutants, have been used as receptors with the final aim to know and to evaluate the relative importance of polar (hydrogen bonding, electrostatic interactions) and non polar (van der Waals, CH-π) forces in the molecular recognition processes and to design novel molecules with improved binding properties. As examples, the structural and conformational details of the effect of branching in the glycan chain and how this affects its recognition by lectins, enzymes, and antibodies will be shown

Monday December 18th
Amphi 45B 11h

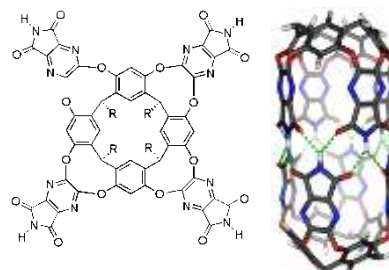


Julius Rebek, Jr (The Scripps Research Institute and Shanghai University)

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Molecular Behavior in a Small Space

Abstract. This lecture describes molecular behavior in synthetic receptors that completely surround their targets: encapsulation complexes. Topics include the new forms of stereochemistry, amplified interactions, chiral spaces and reactivity of molecules confined to a small space. The composition of the capsule and the shape of its space determine what processes occur inside. The basic structure of the capsule is shown below.



January

Lundi 15 Janvier
Amphi 45B

Dr. **Christophe Léger** (BIP, Université d'Aix-Marseille)
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Mechanistic studies of the enzymes that make dihydrogen



Abstract. The enzymes that consume or produce « solar fuels » are large protein complexes that embed inorganic cofactors. Understanding their mechanisms requires a combination of biochemistry, molecular biology, spectroscopy, crystallography, theoretical chemistry and kinetics. As part of kinetics, electrochemistry has become very important in this field. I will illustrate how we use it in Marseille to learn about hydrogenases, the enzymes that make dihydrogen.

Lundi 22 Janvier
Amphi 45B

Dr. **Guillaume Rogez** (IPCMS, Université de Strasbourg)
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Functionalization of layered hydroxides and oxide materials: insertion, grafting, in situ reactions...and microwaves



Abstract. Since the discovery of the outstanding properties of graphene or metal dichalcogenides single layers, research in the domain of functional nanomaterials based on nanosheets and 2D materials has received ever growing attention. In this respect, the organic-inorganic hybrid material approach seems particularly promising to promote multifunctionality within a lamellar material. In this presentation, I will describe different examples of synthetic strategies developed in the group to functionalize two kinds of layered materials, hydroxides and oxides, and some of the properties of the obtained hybrid compounds.

Lundi 29 Janvier

Pr. **Guido Clever** (TU Dortmund)

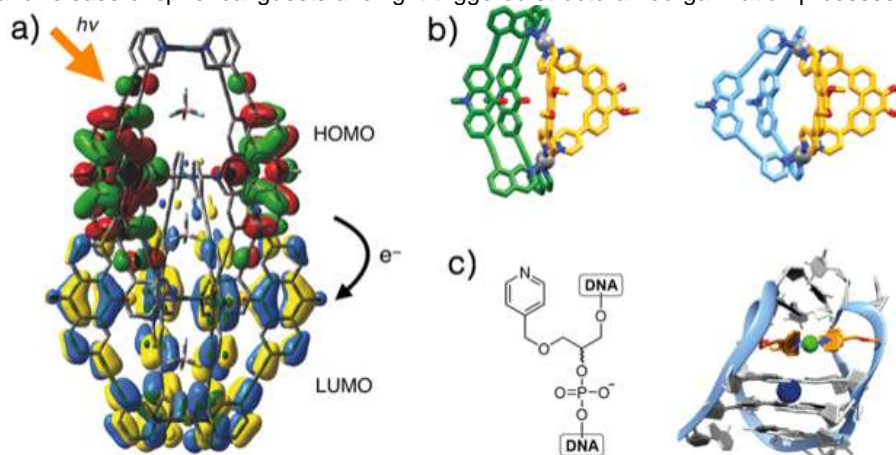
Amphi 45B

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Metal-mediated Quadruplex Assemblies with and without DNA



Abstract. We employ the square-planar metal(pyridine)₄-motif in the self-assembly of quadruply stranded supramolecular architectures based on various organic and DNA-derived ligands. The talk will highlight functional assemblies including reversibly stabilized DNA-quadruplexes and guest-binding coordination cages. A focus will be laid on stimuli-responsive and multifunctional systems. In a series of interpenetrated double-cages, phenomena such as allosteric and triggered guest binding were observed. We further examine photochromic coordination cages based on dithienylethene (DTE) ligands that allow for reversible control over uptake and release of spherical guests and light-triggered structural reorganization processes.



References:

W. M. Bloch, G. H. Clever, *Chem. Commun.* 2017, 53, 8506.

G. H. Clever, P. Punt, *Acc. Chem. Res.* 2017, 50, 2233.

D. M. Engelhard, J. Nowack, G. H. Clever, *Angew. Chem. Int. Ed.* 2017, 56, 11640.

February

Monday February 5th
Amphi Astier, 11h

Laurence Grimaud (Laboratoire PASTEUR, ENS, Paris)
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Reverse Engineering in Metal-Catalyzed Processes



Abstract. Mechanistic studies are of utmost importance for the rationale development of new reactions. Indeed, a better understanding of the molecular processes is still required especially for transition metal-catalyzed reactions, for which the development of new methodologies continues at a fast pace and still takes place by trial and error. The mechanisms of some relevant reactions have been studied by the synergic use of experimental and computational methods. DFT calculations are an invaluable tool to properties of unstable intermediates that drive the reaction and are not usually accessible experimentally. Unfortunately, an initial guess is always needed to apply any computational technique, and this can be confidently drawn only from experimental data, which emerge from the combination of electrochemistry, spectroscopy and conductimetry analyses. This lecture will highlight some of our recent contributions to mechanistic studies of several processes and particularly in the field of transition-metal catalyzed reactions.

Monday February 12th
Amphi Astier, 11h

Boris Vauzeilles (Institut de Chimie Moléculaire et des Matériaux d'Orsay et ICSN, Paris-Saclay)
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Détecter les pathogènes en leurrant leur métabolisme



Abstract. La détection et l'identification rapides de bactéries est un défi majeur de santé publique. L'approche que nous développons repose sur le marquage métabolique de la surface cellulaire. A titre d'exemple, la paroi externe des bactéries dites à Gram négatif est recouverte par une couche compacte de lipopolysaccharides (LPS), qui jouent un rôle dans l'intégrité de la cellule, mais également dans la virulence de certaines souches. Nos travaux récents ont montré que, lorsqu'elles sont métaboliquement actives, les bactéries à Gram négatif peuvent spécifiquement incorporer au sein de leurs LPS un monosaccharide modifié chimiquement par l'introduction d'un groupe *azoture*. Cette fonction indicatrice bioorthogonale peut ensuite être utilisée pour "révéler" les bactéries marquées, en utilisant une méthode de ligation telle que la "click chemistry". Cette approche permet la détection rapide des bactéries pathogènes vivantes. Cette conférence présentera nos principaux résultats dans ce domaine, avec notamment le développement d'une stratégie pour le marquage spécifique de *Legionella pneumophila*, bactérie responsable de la maladie du légionnaire, ou d'une méthode de concentration d'échantillons bactériens.

Monday February 19th
Amphi Astier, 11h

Kevin Bernot (INSA-Rennes, ISCR, Université de Rennes 1)

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Chimie coordination des lanthanides : des molécules-aimants au marqueurs luminescents anti-contrefaçon



Abstract. La chimie de coordination des ions lanthanides permet de synthétiser une incroyable variété de matériaux moléculaires, du plus simple (molécule isolée) au plus élaboré (réseau tridimensionnel de molécules fonctionnelles). Ces concepts seront illustrés par des exemples récents de l'activité de notre équipe dans le domaine des molécules-aimants,¹ des dispositifs photo-commutables,² des précurseurs moléculaires luminescents³ et des marqueurs luminescents anti-contrefaçon.⁴

1) E. Kiefl et al., *ACS Nano* **2016**, 10, 5663. 2) X. Yi et al., *ACS Applied Materials & Interfaces* **2016**, 24, 15551. 3) G. Calvez et al., *Coord. Chem. Rev.* **2017**, 340, 134. 4) O. Guillou et al., *Acc. Chem. Res.* **2016**, 49, 844.

Monday February 26th
Amphi Astier, 11h

Samuel Dagorne (Institut de Chimie, CNRS - Univ. Strasbourg)

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Combining N-heterocyclic carbenes (NHCs) with oxophilic and earth-abundant metal centers: fundamental reactivity and use in homogeneous catalysis



Abstract. The development of earth-abundant, affordable and low toxic metal-based catalysts is of current strategic importance for sustainable catalytic processes. In this context, the organometallics of oxophilic and high-oxidation state metal centers, such as Zn(II) and Al(III), holds a particular interest in catalysis. However, such entities may display a limited hydrolytic stability, prompting our studies on derivatives stabilized by N-heterocyclic-carbenes (which are exceptional σ -donating properties) for improved robustness. In the present seminar, discrete NHC-Zn(II) and NHC-Al(III) species are described along with their reactivity trends. As will be discussed, such rather simple coordination complexes may be involved in various chemical transformations ranging from unusual fundamental reactivity (rearrangement processes), small molecules activation (H_2 , CO_2) and homogeneous catalysis (cyclic esters/carbonates polymerization, CO_2 hydrosilylation catalysis).

Selected refs: *Chem. Commun.* **2010**, 46, 2480; *ChemCatChem* **2014**, 6, 1357; *Chem. Eur. J.* **2015**, 21, 17959; *Organometallics* **2016**, 35, 1726; *Chem. Eur. J.* **2017**, 23, 5509; *Chem. Eur. J.* **2017**, 23, 15908.

March

Monday March 5th

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Dr. Claude-Marie Bachelet (Inserm)

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Chimie et biophotonique : de la chimie moléculaire à l'imagerie subcellulaire

Abstract.

Nous ferons un tour d'horizon des techniques développées en microscopie en lien avec les marqueurs chimiques associés, dans les études du vivant en temps réel, comme approche technologique interdisciplinaire pour l'analyse des mécanismes biologiques.

Monday March 19th

Amphi Astier 11h



Yoshinori Takashima (Osaka University)

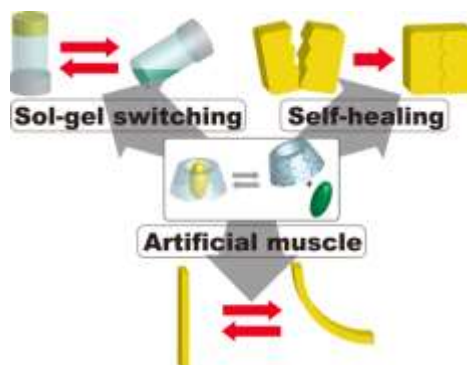
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Stimuli responsive polymeric materials via host-guest interactions

Abstract. Molecular recognition chemistry and supramolecular chemistry have received much attention, owing to their effects on catalytic activity, molecular switches, and materials. Stimuli-responsive supramolecular polymers is relevant not only for biological functions but also for a range of other applications. Our research group has employed cyclodextrins (CDs) as host molecules. In this presentation, I would like to introduce our studies to realize sol-gel switching, self-healing, adhesion control, and contraction-expansion properties through the formation of inclusion complexes with CDs.

References

Nat. Chem. 2011, 3, 34-37; Nat. Commun. 2011, 2, 511; Adv. Mater. 2013, 25, 2849-2853; Macromolecules 2017, 50, 3254-3261; Angew. Chem. Int. Ed. 2015, 54, 8984-8987; Macromolecules 2017, 50, 4144-4150; Nat. Commun. 2012, 3, 1270; Nat. Chem. 2016, 8, 625-632; Chem. 2016, 1, 766-775; Acc. Chem. Res. 2014, 47, 2128.



May

Monday May 14th
Auditorium Astier 11h



Prof. **Ali Tavassoli** (University of Southampton)

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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 femtolitre-sized microfluidic droplets.

Monday 28th May
Auditorium Astier 11h



Dr. **Paul Lusby** (Edinburgh University)

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*Turning Capsule Catalysis Inside Out:
Novel Approaches Utilizing Innately-Polarized Pd₂L₄ Scaffolds*

Abstract. Substrate pre-organization remains the paradigm for bio-inspired catalytic strategies using supramolecular capsule systems. The scarcity of capsule-catalyzed annulation reactions (A+B→C) highlights the limitation of this approach—while co-encapsulation can give significant acceleration, product inhibition frequently halts turnover.^{1,2} In this talk, two novel and distinct methods for realizing capsule-catalyzed annulation processes will be described, both involving the host-guest chemistry of simple Pd₂L₄ assemblies.^{3,4}

1. J. Kang, J. Rebek, *Nature*, **1998**, *385*, 50; 2. M. Yoshizawa, M. Tamura, M. Fujita, *Science*, **2006**, *312*, 251; 3. D. P. August, G. S. Nichol, P. J. Lusby, *Angew. Chem. Int. Ed.* **2016**, *55*, 15022; 4. V. Marti-Centelles, A. L. Lawrence, P. J. Lusby, *J. Am. Chem. Soc.* **2018**, DOI: 10.1021/jacs.7b12146.

June

The « 18èmes Journées de l'École Doctorale de Chimie Moléculaire de Paris-Centre (ED406) » will take place on **Tuesday, June 5th and Wednesday, June 6th, 2018** at the Astier amphitheater, building Esclangon, Campus Pierre et Marie Curie, Sorbonne Université.

Plenary conferences will be given by Mrs **Marie-Odile LAFON** (SATT LUTECHE, Paris), Pr. **Thomas CARELL** (Ludwig-Maximilians-Universität München, Germany), Pr. **Oliver S. WENGER** (Universität Basel, Switzerland) and Pr. **Burkhard KÖNIG** (Universität Regensburg, Germany).

Monday June 11th
T 43-44 salle 317 11h



Matteo Mannini (LaMM, Université de Florence, Italie)

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Developing hybrid architectures embedding Single Molecule Magnets for spintronics

Abstract. The use of magnetic molecule discloses new exciting possibilities for spintronics and quantum computing linked to the individual properties of these molecular units as well as to their interaction with specific surfaces. However, the coupling of molecules with the spin-transport processes is far from trivial. First, the stability of molecules in the device environment has to be validated and, subsequently, the organization of molecules in the desired architectures has to be mastered in order to carefully control the interactions between the substrates and molecular layers. I will overview our activities on the organization of Single Molecule Magnets on surfaces and I will highlight the technological perspectives of this research.

Monday June 18th
Auditorium Herpin 11h



Isabelle Chataigner (Université de Rouen Normandie)

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Dearomatizations of Nitroarenes by additions and cycloadditions

Abstract. Involving arenes in dearomatizing addition and/or cycloaddition reactions is an attractive and convergent approach to construct complex polycycles from easily accessible substrates, however, challenging because of their intrinsic stability. Nitroarenes are interesting substrates in this context, allowing to carry out various dearomatizing reactions when reacted with nucleophilic species, in cycloadditions or annulations for example. Different examples of these transformations will be presented and commented on according to the proposed mechanisms.

Monday June 25th
Auditorium Herpin 11h



Pascale Delangle (CEA Grenoble, France)

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Bio-inspired peptide-like ligands to help understanding metal toxicity, regulation and detoxification

Abstract. Peptides are promising metal-chelating agents, which offer many advantages over synthetic chemical compounds for biological and medical applications. They are made of the same building blocks as proteins and are therefore excellent mimics of biological sites that help predicting high affinity metal binding environments *in vivo*. They are also very attractive water-soluble ligands to design non-toxic chelating agents for medical applications. Two strategies are developed in our laboratory to obtain peptide-like ligands that efficiently mimic metal binding sites in proteins. These chemical architectures are rationally designed to promote the pre-orientation of several coordinating amino acid side-chains towards the metal center. The first design consists in grafting amino acids on chemical scaffolds such as poly-aminocarboxylates via classical peptide coupling reactions to get pseudo-peptides, whereas the second one exploits cyclodecapeptide sequences that induce β -sheet structures. Synthetic organic chemistry is combined to solid-phase peptide synthesis to obtain high purity bio-inspired peptide-like ligands. These two strategies will be discussed for the design of Cu(I) chelators mimicking copper-binding sites found in copper transporters, metallochaperones or metallothioneins and peptide-like ligands for the hexavalent uranyl cation, UO_2^{2+} , which is purely toxic and classified as a hard Lewis acid. We will focus on the rational design of the peptide-like ligands, taking into account the metal coordination properties. The structure of the complexes, their stability and selectivity will be discussed in relation to the biological question.
