culturchem

JANUARY 2025

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January 13th, 11h
Auditorium Herpin
Building Esclangon
Campus P et M Curie
Sorbonne Université

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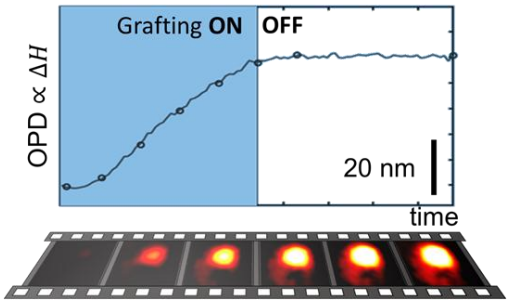
Combining photochemistry, electrochemistry and optics for measuring and controlling chemistry at the nanoscale

Abstract. Carrying out chemical transformations locally, in the micro- and nanoscale, requires the development of specific methodologies, often employing operando strategies. In this seminar, after reviewing some opto-electrochemical methodologies developed in the context of nanoparticles chemistry, I will detail some of our recent efforts to analyze and control surface chemical reactions using photochemical approaches combined with in situ optical monitoring in real time.
Radical-enabled surface modification photochemistry will be used as a guiding line to illustrate how mechanistic analysis can be combined with control methods to achieve attoL precision. Other chemical systems will also be presented to illustrate the versatility of the developed strategies.



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January 20th, 11h
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Phase separation: an effective tool to improve the performance and processability of covalent adaptable networks

Abstract. Vitrimers are chemically crosslinked networks that can rearrange their topology without decreasing their crosslinking density thanks to exchangeable links present in the network. As a result, vitrimers can be potentially reshaped and recycled at will, while displaying the superior properties of crosslinked polymers at service temperature. Very promising materials to create a circular economy of plastics and polymeric materials, vitrimers still display limitations that impact their transition towards industry, such as high viscosity even at elevated temperatures, due to the Arrhenian temperature dependence of the melt viscosity, or moderate creep resistance at working temperatures in the case of low T_g materials.

Although many strategies have been reported to address these issues, it remains challenging to overcome a key tradeoff between improving the processability or the mechanical performance of vitrimers. In this lecture, new strategies relying on phase separation and reactive processing will be presented to jointly improve the processability and the mechanical performance of vitrimers relying on dioxaborolane metathesis, or to recycle blends of polyolefins.

Selected references:

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ii. G. J. M. Formon, S. Storch, A. Y.-G. Delplanque, B. Bresson, N. J. Van Zee, R. Nicolaÿ, *Adv. Funct. Mater.*, **2023**, *33*, 2306065 ; DOI: 10.1002/adfm.202306065
ii. A. Quinteros-Sedano, B. Bresson, N. J. Van Zee, R. Nicolaÿ, *ACS Materials Lett.*, **2024**, *6*, 877 ; DOI: 10.1021/acsmaterialslett.4c00076
v. G. J. M. Formon, J. Jayaratnam, C. Guibert, N. J. Van Zee, R. Nicolaÿ, *Macromolecules*. **2024**, *57*, 8277 ; DOI: 10.1021/acs.macromol.4c01363
v. v. T. Vialon, H. Sun, G. J. M. Formon, P. Galanopoulo, C. Guibert, F. Averseng, M-N. Rager, A. Percot, Y. Guillaneuf, N. J. Van Zee, R. Nicolaÿ, *J. Am. Chem. Soc.*, **2024**, *146*, 2673 ; DOI: 10.1021/jacs.3c12303

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January 23rd, 11h
Auditorium 56B
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Sylvestre BONNET (Leiden University, The Netherlands)
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Molecular excited states in biomimetic and biological environments: photocatalytic and photomedicinal applications

Abstract. Molecules are characterized by well-defined structures and excited states. Usually, the chemical properties of molecular excited states are very different from that of the ground state. By placing these molecules in a biological or biomimetic environment, it is possible to harvest the power of these different excited states for different types of applications, ranging from sensing to solar fuel or medicine. In this presentation, I will describe the different types of excited states of ruthenium polypyridyl complexes, and their applications in photocatalysis and photomedicine.

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January 27th, 11h
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Philippe DAUBAN (Institut de Chimie des Substances Naturelles, CNRS, Université Paris-Saclay)
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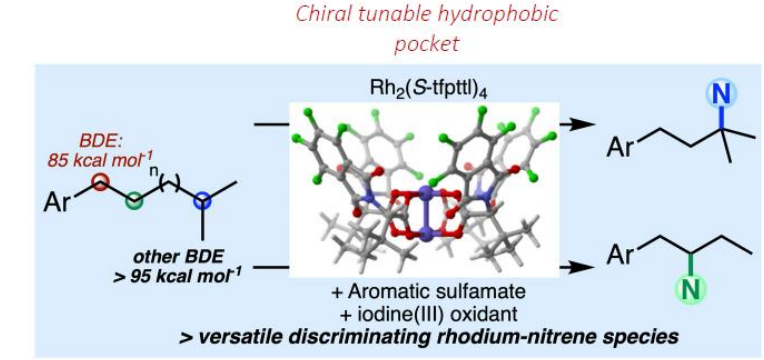
Catalyst-controlled selective C(sp^3)–H amination reactions

Abstract. Catalytic C–H functionalization reactions provide unique opportunities in chemistry by giving a streamlined access to a new molecular space through the late-stage peripheral edition of drugs or materials. The selectivity of these reactions can be tuned according to several strategies, 1) through the design of directed processes, which encompass directing group-based C–H activation protocols or intramolecular processes, or 2) by capitalizing on the electronic/steric properties of organic compounds. Though efficient and selective, these substrate-controlled reactions have limitations with respect to unactivated C–H bonds (BDE > 95 kcal.mol-1) which often remain inaccessible. A solution to go beyond these limitations relies on a third strategy based on the concept of "catalyst-controlled selectivity". In this lecture, we will discuss the results of our recent investigations aimed to design reagents and catalysts for catalyst-controlled selective C(sp^3)–H amination reactions involving highly discriminating rhodium-bound nitrene species.



SUPRAMOLECULAR CATALYSIS
> Non-covalent interactions between the substrate, the nitrene source and the catalyst

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FEBRUARY 2025

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February 3rd, 11h
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Benoit COLASSON (Université Paris Cité)
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Supramolecular control of the properties of metal complexes

Abstract. Supramolecular chemistry appears to be a fruitful strategy for controlling the properties of metal complexes. In this presentation, we discuss an original method to control the second coordination sphere and the environment around a metal center. For instance, a biomimetic model can be assembled with a tris(2-pyridylmethyl)amine (TMPA) ligand-based complex encapsulated in a supramolecular hydrogen-bonded capsule. The same capsule can also be used to encapsulated Cu(I) complexes. The characterization of some of the properties resulting from this design will be presented.

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February 7th, 11h
Corridor 54.55
Room 125
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Jacinto SÁ (Uppsala University, Uppsala, Sweden)
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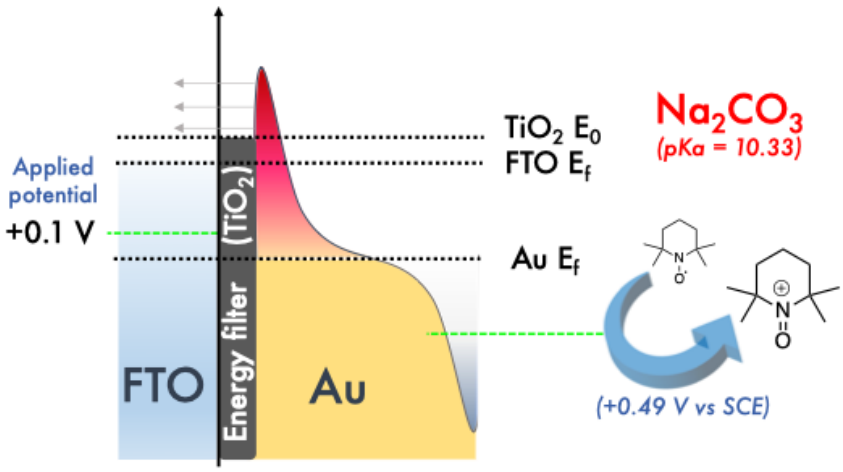
Plasmons: From metal ore to catalyst

Abstract. The urgent need for sustainable chemical production drives the development of innovative technologies for essential compounds, from bulk chemicals to pharmaceuticals. Photoredox catalysis, recognized with the 2021 Nobel Prize in Chemistry, offers a versatile approach for selective transformations under mild conditions. However, traditional molecular photocatalysts face challenges like high costs, low quantum yields, and difficult scalability.

In this seminar, I will present my research group's innovative approach to overcoming these limitations through the development of a novel class of photosystems based on modified plasmonic materials. These materials address current bottlenecks, enabling cost-effective, waste-minimized production processes with enhanced performance. Our strategy transforms gold grains into efficient photoactive systems capable of driving photoredox catalysis. These systems are designed to operate with cutting-edge engineering tools and leverage photo-electrochemical geometries, resulting in significantly improved quantum yields.

Key highlights include simplified product-catalyst separation, continuous flow reaction compatibility, and laser-based characterization techniques to track the behavior of photogenerated carriers. I will also illustrate how these advancements facilitate demanding radical-mediated bond formations, such as C-N bonds, opening doors to more efficient and scalable industrial applications. By the end of this talk, attendees will gain insight into the unique photophysics of plasmonic materials and their potential to revolutionize sustainable chemical synthesis.



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February 10th, 11h
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Thibault CANTAT (CEA, CNRS, Université Paris Saclay)
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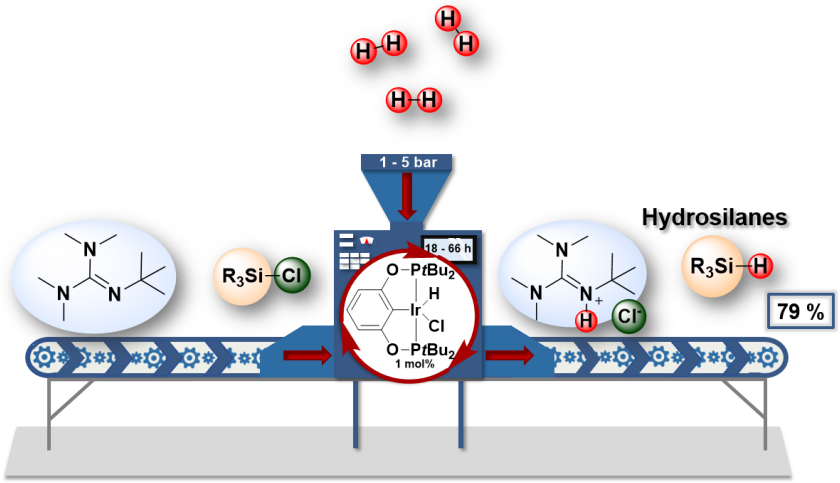
En route to more energy efficient silicon hydrides and their use in the recycling of waste plastics

Abstract. Hydrosilanes are useful compounds for the production of a variety of organosilicon compounds through hydrosilylation of alkenes or dehydrocoupling reactions. They also promote, in mild conditions, the reduction of functional groups such as esters or amides with high selectivity. In comparison with apolar dihydrogen, the couple $E^0(Si(OEt)_{4(l)}/SiH_{4(g}$ (−0.51 V vs. NHE) and the polarized and weaker Si–H bond (BDE_{Si-H} = 95 kcal.mol^{-1} < BDE_{H-H} = 104 kcal.mol^{-1}) offer some thermodynamic and kinetic advantages relevant for the reduction of oxygenated chemical feedstocks that could replace oil in the long run (lignin, plastics and CO_2). Because classical routes for the production of hydrosilanes are energy demanding, alternative catalytic syntheses that would transform Si–X (X = halides, alkoxides) precursors into Si–H are appealing. This endeavor has motivated us to explore the synthesis, use, and recycling of energy efficient surrogates of hydrosilanes, namely silylformates, in hydrosilylation chemistry. In addition, our recent findings in hydrogenolysis routes to hydrosilanes will be presented using transition metal based catalysts as well as metal-free catalysts. Their use in the recycling waste plastics will be discussed with novel catalytic transformations.



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February 13th, 11h
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Jeon LE-RANG (CRPP, Bordeaux)
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Activating sigma-hole interactions: for crystal engineering and tailored properties

Abstract. The ability to understand and to control noncovalent interactions is important in materials science, spanning solution applications (organo-catalysis and anion recognition/transport) to solid-state properties (topochemical reactions and molecular conductors). Among those available in the toolbox of crystal engineering, chalcogen bonding (ChB) has recently entered the growing family of sigma-hole interactions, following the strong developments based on the halogen bonding (XB) interaction over the last 30 years. Nevertheless, harnessing chalcogen bonding (ChB) for crystal engineering remains challenging mainly due to the poor predictability of ChB associated with the presence of two sigma-holes. In this talk, I will discuss different strategies developed in our group that extend from fundamental studies focused on addressing strong directionality in ChB to a demonstration of its application in the design of functional materials with tailored properties.

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February 17th, 11h
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Claire SMADJA (Institut Galien Paris-Saclay)
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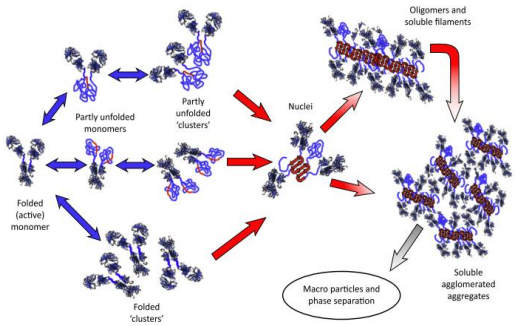
Deep view into analytical strategies to address the quality control of therapeutic monoclonal antibodies

Abstract. Monoclonal antibodies (mAbs) are increasingly developed for the treatment of a variety of autoimmune and inflammatory diseases, as well as cancer. However, mAbs are highly complex molecules, extremely sensitive to their environment. At a hospital, formulated mAbs could be submitted to various stresses during the compounding, storage, and handling stages, which may impact their efficacy and safety. Thus, a careful characterization of mAbs states is required to limit immunogenicity due to mAbs modifications/degradation, such as modification of the conformational state, self-association, or small oligomers' formation. To study the stability of mAbs in the hospital context, two separation methods based on capillary zone electrophoresis (CZE) and size exclusion chromatography (SEC), coupled with native mass spectrometry (MS), will be first presented. CZE-native MS method using a triple-layer coating of polybrene-dextran sulfate-polybrene was developed to analyze stressed Infliximab. The obtained results showed that it was possible to detect and separate native monomers, denatured monomers as well as dimers in a single analysis. Then, an SEC analysis method was coupled simultaneously with MS and a fluorescence detector to detect degraded therapeutic mAbs and biases of conformational changes (e.g., dimerization, denaturation) that may arise during native MS. Finally, a more straightforward approach, which is a combination of image capillary isoelectric focusing (icIEF) and multivariate analysis will be presented. In this talk, the advantages and drawbacks of these three different analytical methods for detecting conformational changes in therapeutic monoclonal antibodies will be discussed.



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February 24th, 11h
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Anaïs PITTO-BARRY (Institut Galien Paris-Saclay, Université Paris-Saclay)
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Strategies for the delivery of inorganics

Abstract. Cancer is projected to claim the lives of up to 24 million individuals worldwide by 2030, with potential costs exceeding 20 trillion euros by 2050 if no additional investments in research and prevention are done.[1] Despite significant advancements in the development of chemotherapy agents combatting cancers, drug resistance and toxicity persist as substantial barriers. Inorganics, boasting a wider range of properties compared to organic drugs, emerge as promising candidates for acquiring specific functionalities,[2] while polymer assemblies are more and more exploited for the delivery of such compounds.[3]
We will present the various strategies we have been working with for the delivery of inorganics such as boron and ruthenium complexes: physical encapsulation into polymeric micelles,[4] chemical binding between inorganics and monomers or preformed polymers,[5] ligand modification on ruthenium complexes.[6] The influence of the prodrug system will be shown on both chemical and biological properties.

Références

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(4) Pitto-Barry, A.; Lupan, A.; Ellingford, C.; Attia, A. A. A.; Barry, N. P. E. *ACS Appl. Mater. Interfaces* **2018**, *10*, 13693-13701.
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MARCH 2025

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March 3rd, 16h
Auditorium Friedel
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Kellie TUCK (School of Chemistry, Monash University, Melbourne, Australia)
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Lessons learnt with Coordination Cages and Lanthanide Complexes: Decoding Host-Guest Chemistry for Catalysis and Analyte Detection

Abstract. For decades, scientists have been captivated by the extraordinary optical characteristics of lanthanide ions, recognising their potential for optical sensing applications. We have pioneered the development of luminescent lanthanide-based complexes tailored for detecting metal ions, nucleotides, and hydrogen sulfide in both aqueous solutions and gaseous states (see Figure 1 a and b).[1,2] The careful design of these complexes ensures supramolecular interactions between host and guest, leading to a luminescence change from 'off' to 'on,' crucial for effective time-gated signal detection. This approach is extremely beneficial for sensing analytes in biological and environmental solutions, eliminating interference from short-lived fluorescence.
Additionally, with our collaborators, our research also explores highly charged coordination cages, probing their host-guest chemistry with small molecules and evaluating their potential to detect and detoxify toxic organophosphorus compounds. These cages have catalytic properties, facilitating hydrolysis reactions in aqueous solutions, due to presence of hydroxide anions that accumulate at the exterior surface of the cage (Figure 1 c and d).[3,4]
The presentation will highlight discoveries in both these areas, with specific emphasis on the fundamental host-guest chemistry underlying the responses observed. The challenges encountered, insights gained and pitfalls encountered along the way will also be discussed.

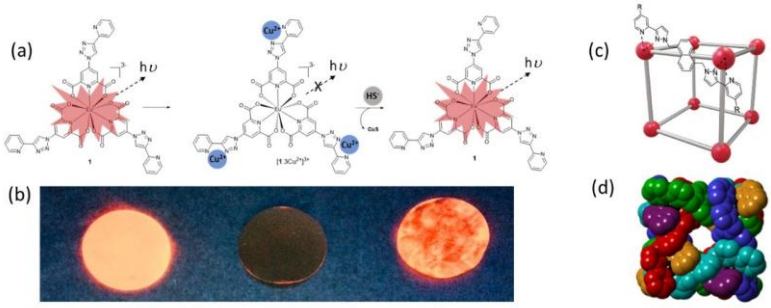

Figure 1. a) the hydrogen sulfide sensing principle of a lanthanide-based sensor; (b) paper discs illuminated with a UV lamp showing the 'on' to 'off' to 'on' of the sensor in the presence of copper(II) ions and hydrogen sulfide; (c) a schematic of the cage; (d) space filling diagram showing the hollow cavity of the cage.

References. 1 P. Mini, M. A. Springer, M. R. Grace, G. H. Dennison, K. L. Tuck, Chem. Commun., 2020, 56, 5605. 2 P. Mini, S E. Walker, M. R. Grace, G. H. Dennison, K. L. Tuck, Dalton Trans., 2023, 52, 12235. 3 J. C. Dorrat, R. J. Young, C. G. P. Taylor, M. B. Tipping, A. J. Blok, D. R. Turner, A. I. McKay, S. Ovenden, M. D. Ward, G. H. Dennison, K. L. Tuck, Dalton Trans., 2023, 52, 11802, and unpublished work. 4 J. C. Dorrat, C. G. P. Taylor, R. J. Young, A. B. Solea, D. Turner, G. H. Dennison, M. D. Ward, K. L. Tuck, Chemistry–A European Journal, 2024, e202400501.

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March 10th, 11h
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Géraldine MASSON (Institut de Chimie des Substances Naturelles, Université Paris-Saclay, Gif-sur-Yvette, France)
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Asymmetric Organocatalysis and Photoredox Catalysis for the Synthesis of Chiral Amines

Abstract. Chiral amines are crucial intermediates in the synthesis of biologically active molecules, such as pharmaceuticals and agrochemicals. Given their significance, there is continuous interest in developing new, efficient, and stereoselective methods for their synthesis.
In this context, we have worked on developing innovative methods for the α,β-difunctionalization of enamides using a synergistic two-step strategy that combines asymmetric organocatalysis with photoredox catalysis. A key aspect of this approach is the use of thiol as a transient reaction partner, which plays a vital role in enabling these transformations and allows for the synthesis of a diverse array of enantioenriched α,β-substituted amines.[1]
Additionally, we successfully applied stereoselective and enantioselective photocatalytic processes to synthesize both α- and β-chiral amino boronic acids. In these reactions, α- and β-amino acids act as ideal linchpins, facilitating selective transformations and achieving high enantioselectivity.[2]
Finally, we report an efficient enantioselective synthesis of α-arylproanamides and α-arylpropionic acids through stereoselective desulfonative radical Truce-Smiles rearrangements.[3]
In this presentation, we will highlight our work on these methodologies, focusing on their application in the synthesis of biologically active compounds and discussing their potential impact on the field.

References :
1) (a) K Bouchet, Y. D.; Varlet, T.; Masson, G. *Acc. Chem. Res*. **2022**, 55, 3265. (b) Naulin, E.; Lombard, M.; Gandon, V.; Retailleau, P.; Elslande, E. V.; Neuville, L.; Masson, G. *J. Am. Chem. Soc.* **2023**, 145, 48, 26504. (c) Varlet, T.; Matišić, M.; Van Elslande, E.; Neuville, L.; Gandon, V.; Masson, G. *J. Am. Chem. Soc.* **2021**, *143*, 11611.
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3) Ma, W.-Y.; Leone, M.; Derat, E.; Retailleau, P.; Reddy, C. R.; Neuville, L.; Masson, G. *Angew. Chem. Int. Ed.* **2024**, e202408154.

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March 17th, 11h
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Anett SCHALLMEY (Institute for Biochemistry, Biotechnology and Bioinformatics, Technische Universität Braunschweig, Germany)
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Novel enzymes for biocatalytic application in cascade reactions and continuous flow

Abstract. Enzymes are powerful catalysts for the provision of a plethora of valuable products in a highly regio- and stereoselective manner. My group is active in this highly vibrant field with a special focus on the identification, characterization and engineering of novel enzymes for application in biocatalytic processes. As an example, we have identified a huge number of novel halohydrin dehalogenases, amongst others, using a tailored database mining approach [1], which has resulted in an impressive number of new applications of these enzymes for the synthesis of a broad range of β- and γ-substituted alcohols. Among these enzymes, halohydrin dehalogenase HheG from *Ilumatobacter coccineus* displays an exceptional substrate scope [2,3] and we have engineered this enzyme to improve its stability [4] and enantioselectivity [5] for biocatalytic application in continuous-flow reactions.
Moreover, we are studying the enzymatic depolymerization of lignin polymer as a renewable source for the selective provision of valuable monoaromatic compounds [6,7]. In this context, we currently make use of an enzyme cascade composed of 4 chemical steps to selectively cleave the β-O-4 arylether bonds present in lignin. By employing a design-of-experiments approach to investigate the impact of individual parameters on product yield, we were able so far to improve the yield of the desired monoaromatic product to several hundred miligrams per liter of reaction.
In another cascade reaction, we have investigated the application of an archaeal glycerolprenylase for the biocatalytic synthesis of different prenyl ethers [8].

References

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Peptidomimetic foldamers adopting β-hairpin or helix conformation inhibit the aggregation of proteins involved in neurodegeneration and type 2 Diabetes

Abstract. The process of amyloid deposition formation is implicated in cell degeneration and in the pathogenesis of more than twenty diseases, such as Alzheimer's and Parkinson's diseases and type 2 Diabetes. Numerous anti-amyloid molecules have been reported over the past 25 years and most of them belong to the class of small molecules or antibodies. However, so far only one of the anti-amyloid drug candidates, Tafamidis, inhibiting transthyretin (TTR) amyloidogenesis, and three antibodies targeting beta-peptide aggregates amyloid ($A\beta_{1-42}$), have reached the clinic. Peptides represent an attractive alternative to small molecules and antibodies as anti-amyloid drugs, thanks to their improved efficacy, selectivity or specificity and potency. However, very few of them have reached the (pre)clinical stages. Peptidomimetic foldamers, bioinspired by the secondary structures of proteins, offer a promising alternative to peptides because they retain the specific side chains of a peptide sequence while having new and improved structural, biological and pharmacokinetic properties. Here I will present our strategies to modulate amyloid protein aggregation, based on the design of peptidomimetic foldamers adopting β-hairpin and helical structures inspired by peptide sequences of the target amyloid proteins or on the physiological chaperone proteins. In particular, β-hairpin mimics built on a piperidine-pyrrolidine β-turn inducer have proved to inhibit $A\beta_{1-42}$,[1] hIAPP, [2] Tau[3] or α-Synuclein[4] aggregation, according to the specific selection of the two peptidic arms. We have also demonstrated that preserving helical conformations of $A\beta_{1-42}$, hIAPP, or α-Synuclein by using 4-amino(methyl)-1,3-thiazole-5-carboxylic acid (ATC)[5] or diazapeptide[6] based foldamers is of promising interest to inhibit their aggregation.

References:
[1] a) *Chem. Sci.* **2017, *8***, 1295; b) *Eur. J. Med. Chem.* **2018**, *154*, 280
[2] a) Front. Cell Dev. Biol. **2021**, 9, 729001; b) *Chem. Eur. J.* **2024**, e202303887
[3] bioRxiv **2024**, doi: https://doi.org/10.1101/2024.10.01.615850
[4] In preparation
[5] *Chem. Eur. J.* **2020**, *26*, 14612
[6] *J. Med. Chem,* **2023**, *66*, 12005

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March 31st, 11h
Auditorium Herpin
Building Esclangon
Campus P et M Curie
Sorbonne Université

Contact:
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Anne DOLBECQ (Institut Lavoisier de Versailles, UVSQ, Université Paris-Saclay)
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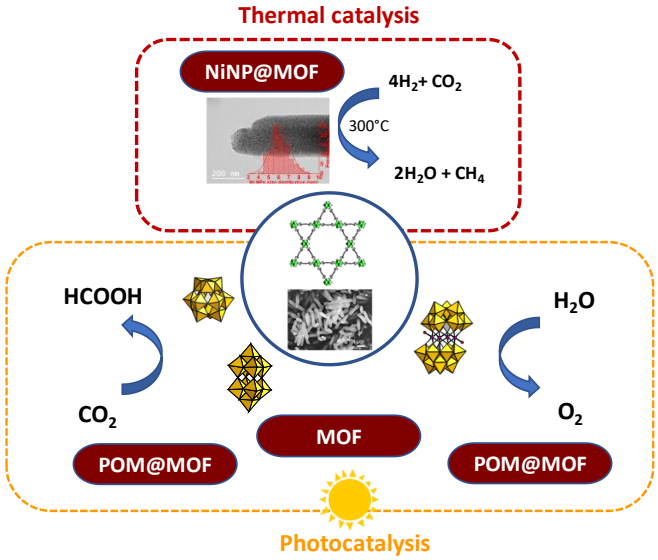
Metal-organic framework composites with polyoxometalates or metal nanoparticles for energy applications

Abstract. Metal-organic frameworks (MOFs) are a large class of porous hybrid organic-inorganic crystalline solids built from the connection of metal clusters with polydentate organic linkers. Composite materials with MOFs can be obtained by immobilization of molecular species, such as polyoxometalates (POMs), or metal nanoparticles (NPs), into the MOF pores, leading to highly efficient catalysts.

This presentation will focus on the synthesis and characterization of composites with porphyrin-based MOFs, POMs or Ni NPs, in the larger context of other researches carried in the field. Their applications for photocatalytic CO_2 reduction, water oxidation or CO_2 methanation will also be described.



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JUNE 2025

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JUNE 2nd, 11h
Auditorium MOISSAN
Chimie Paris Tech – PSL
11, rue P et M Curie

Contact:
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Jeremy MERAD (Université Claude Bernard Lyon 1)
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Photochemical approaches in radical organocatalysis

Abstract. The development of new catalytic systems with enhanced reactivity and selectivity is a cornerstone of modern organic synthesis.
Over the past two decades, both organocatalysis and photoredox catalysis have experienced remarkable advancements, emerging as major fields in molecular catalysis. The use of small organic molecules as catalysts has unlocked diverse opportunities in activation modes and reaction design, particularly in enantioselective synthesis. Simultaneously, photoredox catalysis has proven to be a powerful tool for converting visible light into molecular potential energy. By enabling the generation of catalytic amounts of free radicals from closed-shell substrates, photoredox catalysis excels at orchestrating reactions involving highly reactive open-shell intermediates.

At the intersection of these two domains, we are developing novel catalytic systems that utilize the generation of radical organocatalysts upon visible-light irradiation. Our work explores their synthetic potential and underlying mechanisms. This seminar will showcase some of the synthetic challenges we have sought to address through this approach.

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JUNE 3rd, 11h
Sorbonne Université
Campus P et M Curie
Corridor 42-43
1st Floor, Room Chimie 2

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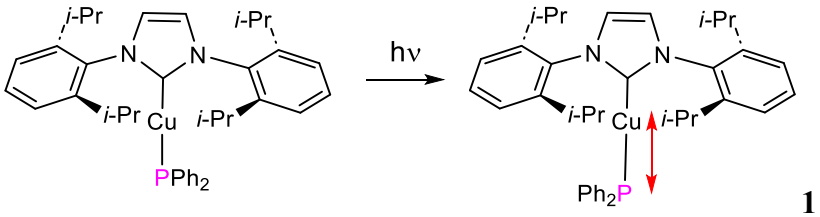
Rory WATERMAN (University of Vermont)
rory.waterman@uvm.edu

Advances in Photocatalytic Hydrophosphination

Abstract. An important challenge for chemists is increasingly efficient routes to element–carbon bonds, as characterized by energetic costs and atom economy, among other factors. Hydrophosphination, or P–C bond formation, has challenges in substrate scope, selectivity, and catalyst activity. In an arc from zirconium to iron to copper, high activity and access to previously inaccessible substrates has been witnessed that addresses several latent challenges. The key to this reactivity has been photoactivation and photocatalysis. In the case of photocatalysis, high activity has been seen in d^0 to d^8 metals. This activity is hypothesized to arise from excitation to a low-lying orbital that has significant M–P antibonding character, weaking that bond to avail faster insertion (**1**). Interestingly, this photocatalysis extends into the s-block, yet simple s-block salts are adequately activating for a nucleophilic hydrophosphination that complex catalysts are not needed for relatively 'unactivated' substates like styrenes (**2**).



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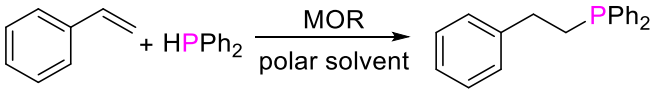

high conversion **2**

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NO SEMINAR : MONDAY JUNE 9th and 16th

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JUNE 18th, 11h
Salle 102
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Campus P et M Curie
Sorbonne Université

Contact:
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Stefan MATILE (Department of Organic Chemistry, University of Geneva, Geneva, Switzerland)
stefan.matile@unige.ch

Translational Supramolecular Chemistry

Abstract. This lecture will summarize current highlights from our interest to translate principles from supramolecular chemistry to create significant function and, at best, approach big questions in science and society from new directions. Particularly hot topics at the moment are scalable electric-field catalysis (EFC) in microfluidic reactors and thiol-mediated uptake (TMU) as an emerging method to penetrate cells.

Our interest in electric field catalysis emerged from the earlier introduction of anion-π interactions, chalcogen bonds and pnictogen bonds to catalysis. Central for the origin of life and predicted to change the way we make molecules, the challenge with EFC is to accelerate and direct the flow of electrons during reactions with external electric fields under scalable conditions that are compatible with sustainable production in chemical industry. We found that this might become possible in microfluidic reactors. Recent progress focuses on organocatalysis at high voltage and carbon nanotubes to combine with anion-π catalysis. Applying lessons from cell-penetrating peptides (CPPs), electrical double layer engineering promises access to organocatalytic microfluidic supercapacitors.

Lessons from CPPs not only direct ongoing research in electric field catalysis but also triggered our interest in thiol-mediated uptake. With initial observations made by Sandrine Sagan and her group at this University, TMU appears upon attachment of disulfide exchangers to substrates of interest, proteins and beyond. It operates by dynamic covalent exchange cascades with cellular thiols and disulfides. With recent reports implying that TMU might be much more important than we all expected to enable and inhibit the entry into cells, including viral entry, we thought time is up to go serious and crack TMU. This starts with understanding the underlying cascade exchange chemistry, continues with pattern generation and photocatalytic microenvironment proteomics to decode exchange networks and identify the involved cellular exchange proteins, and hopefully will end up with traceless TMU tags that solve daily delivery problems in the community.

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JUNE 23rd, 11h
Corridor 54-55
Room 125
Campus P et M Curie
Sorbonne Université

Contact:
Virginie VIDAL
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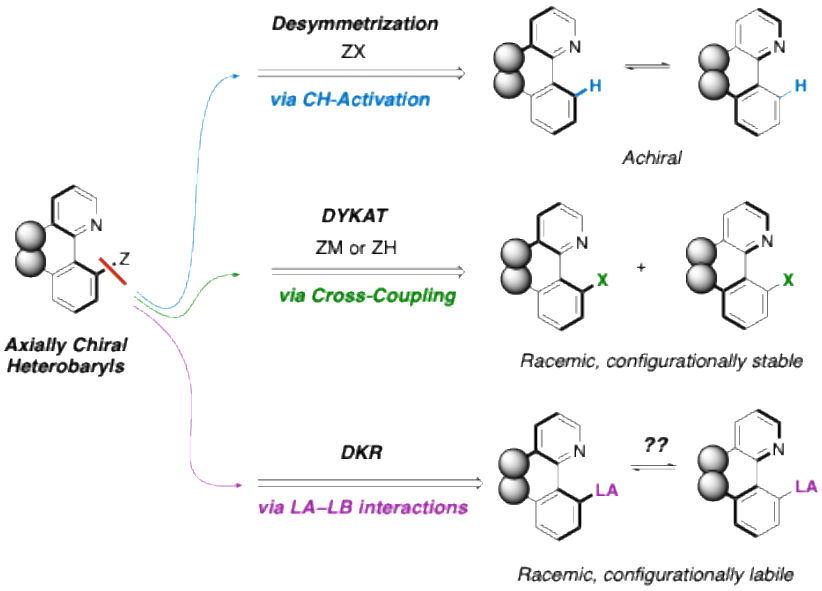
José M. LASSALETTA (Instituto de Investigaciones Químicas, CSIC, Sevilla, Spain)
jmlassa@iiq.csic.es

Dynamization Strategies for Atroposelective Catalysis

Abstract. In the field of asymmetric carbon–carbon and carbon-heteroatom cross–coupling reactions, the synthesis of functionalized, configurationally stable axially chiral heterobiaryls remain as one of the most challenging targets. Well established cross-coupling catalysts fail for the coupling of heterocyclic derivatives, probably due to problems associated with the coordination ability of the substrates, the stability of the required organometallics, and/or the lower configurational stability of the desired heterobiaryls. Considering, however, the high potential that functionalized heterobiaryls hold in the field of asymmetric catalysis, we started a program to explore new strategies based in dynamic kinetic asymmetric C–C[1] and C–X (X = P,[2] N[3]) cross–couplings (DYKAT) from heterobiaryl electrophiles and dynamic kinetic resolution (DKR), either via C–H activation[4] or exploiting transient Lewis acid-base interactions[5]. In this lecture, the collected results and the mechanistic aspects related with these reactions will be discussed.



References:
1. (a) *J. Am. Chem. Soc.* **2013**, *135*, 15730; (b) *Chem. Commun.* **2016**, *52*, 14121; (c) *J. Am. Chem. Soc.* **2018**, *140*, 11067; (d) *Org. Lett.* **2022**, *24*, 3812.
2. *ACS Catal.* **2016**, *6*, 3955.
3. *J. Am. Chem. Soc.* **2016**, *138*, 12053.
4. (a) *Angew. Chem. Int. Ed*. **2018**, *57*, 3777; (b) *ACS Catal.* **2021**, *11*, 4117; (c) *Angew. Chem. Int. Ed.* **2023**, *62*, e202306981; (d) *ACS Catal.* **2023**, *13*, 659; (e) *ACS Catal.* **2023**, *13*, 12134; (f) *Angew. Chem. Int. Ed.* **2024**, *63*, e202409524.
5. (a) *J. Am. Chem. Soc.* **2020**, *142*, 2628−2639; (b) *ACS Catal.* **2023**, *13*, 42−48

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JUNE 30th, 11h
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Daniel MERK (LMU Munich, Chair of Pharmaceutical & Medicinal Chemistry)
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Chemical Tools for Orphan Nuclear Receptors

Abstract. Nuclear receptors are ligand-sensing transcription factors regulating transcription in response to ligand binding. Their modulation enables pharmacological control of gene expression thus rendering the 48 human nuclear receptors as attractive drug targets. However, a significant portion of the nuclear receptor family is still poorly explored and potent, selective and well-characterized ligands are lacking. Using systematic and structure-guided design approaches, microscale library synthesis and machine learning, we develop extensively optimized and highly annotated chemical toolboxes to study orphan nuclear receptor biology and explore their therapeutic potential. Our present main focus lies on the orphan receptors nuclear receptor related 1 (Nurr1), tailless homologue (TLX) and the hepatocyte nuclear factor 4 (HNF4), which hold promise in neurodegeneration (Nurr1, TLX) and metabolic dysfunction (HNF4). Application of recently developed tools in phenotypic settings revealed, for example, neuroprotective potential of Nurr1 activation and involvement of several (orphan) nuclear receptors in autophagy and endoplasmic reticulum stress regulation. Further exploration of these tools and their pharmacological effects may hence open avenues to new therapies in important areas.

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culturchem

JULY 2025

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JULY 7th, 11h
Corridor 54-55
Room 125
Campus P et M Curie
Sorbonne Université

Javier MONTENEGRO (Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), Universidade de Santiago de Compostela, Spain)
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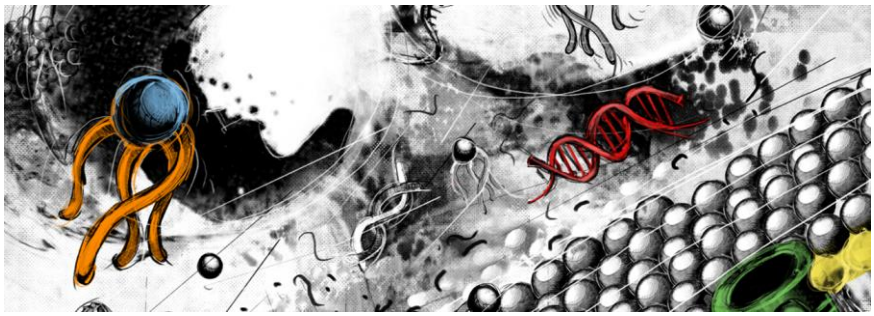
Supramolecular Dynamic Chemistry for membrane transport and Biomimetic Systems

Abstract. Our research group is interested in the application of supramolecular chemistry to understand and manipulate biology. [1,2] Our work philosophy is based in the importance of weak and non-covalent forces to control the shape and the topology of biomolecules, which are governed by the principles described by supramolecular chemistry. These supramolecular lessons can then be applied to control the properties and function of biomolecules. We believe that by modulating the shape we can mimic, control and improve functional behaviour. With focus in supramolecular interactions for artificial membranes and tubular composites, we investigate the construction of synthetic systems for controlling and emulating biology and life-like soft systems. [3-4]



[1] Fuertes, A.; Juanes, M.; Granja, J.R.; Montenegro, J.; Chem. Commun. 2017, 53, 7861–7871.
[2] Lostalé-Seijo, I.; Montenegro, J.; Nat. Rev. Chem. 2018, 2, 258–277.
[3] Priegue, J.M.; Crisan, D.N.; Martínez-Costas, J.; Granja, J.R.; Fernandez-Trillo, F.; Montenegro, J.; Angew. Chem. Int. Ed. 2016, 55, 7492–7495. b) Lostalé-Seijo, I.; Louzao, I.; Juanes, M.; Montenegro, J.; Chem. Sci. 2017, 8, 7923–7931. c) Barba-Bon, A. et al. Nature, 2022, 603, 637–642.
[4] Insua, I.; Montenegro, J.; J. Am. Chem. Soc. 2020, 142, 1, 300-307, b) Méndez-Ardoy, A.; Granja, J.R.; Montenegro, J.; Nanoscale Horizons, 2018, 3, 391-396. c) Méndez-Ardoy, A. et al. Angew. Chem. Int. Ed. 2020, 59, 6902–6908. d) Booth, R., Insua, I., Ahmed, S., Rioboo, A. & Montenegro, J.; Nat Commun. 2021, 12, 6421.

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JULY 9th, 10h30
Auditorium Astier
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From Weak Interactions to Strong Selectivity: Halogen Bonding in Catalyst Design

Abstract. Our research program centers on catalysis—an essential field of chemistry that enables the transformation of simple compounds into complex molecules with significant practical value. We have developed a new strategy that leverages halogen bonding to assemble catalyst backbones through the supramolecular attachment of modular building blocks. These blocks incorporate both the functional groups necessary for metal coordination and the structural motifs required for supramolecular organization.
We have successfully applied these halogen-bonded supramolecular complexes in the catalytic hydroboration of terminal alkynes, [4+2] cycloadditions and hydroalkoxylation reactions.[1] The lecture will cover synthetic approaches to halogen-bonded metal catalysts (M = Rh, Ir, Pt), experimental and computational investigations of halogen bonding,[2] and analysis of the selectivity and mechanistic pathways of the catalytic transformations.

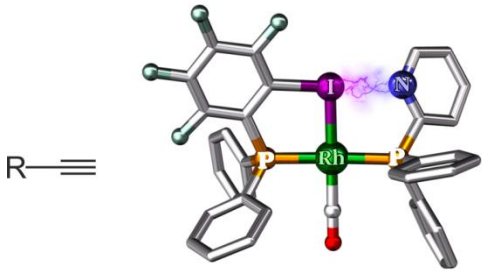

Figure 1: Supramolecular halogen-bond assembled catalysts for Rh-mediated hydroborations.

References

[1] A. Vidal-Ferran *et al.*, *Pure Appl. Chem.* **2019**, *91*, 3-15; *ACS Catal.* **2023**, *13*, 10447-10456 and unpublished results.
[2] A. Vidal-Ferran *et al.*, *Chem. Commun.* **2019**, *55*, 2380-2383 and unpublished results.

Acknowledgements: Financial support from the Spanish *Ministerio de Ciencia, Innovación y Universidades* MICIU/AEI/10.13039/501100011033 under the project PID2020-115658GB-I00 and *AGAUR* under the project 2021 SGR 01107 are gratefully acknowledged.

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JULY 10th, 11h
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Carbon-Negative Generation of Green Hydrogen via Electrolysis of Biomass

Abstract. Climate change and fossil fuel depletion are intertwined global challenges that necessitate urgent action and lead to the sustainability shift towards low-carbon biofuels, renewable energy, and clean hydrogen fuel, as well as green chemicals. High purity hydrogen can be generated from water electrolysis but is hindered by inefficient oxygen evolution reaction (OER) and the possible explosive mixture of oxygen and hydrogen under the condition of partial loading and membrane degradation. There is a widespread effort to replace OER with the more favorable electrooxidation of small organic molecules. Although value-added products can be generated, the production of these organics is process-intensive and costly. Most importantly, they lack the abundance necessary to meet the requirements of a hydrogen economy. Abundant raw biomass with annual production of billions of tons in nature are promising alternatives to these small organics. Significantly, biomass reforming via electrooxidation (to replace OER) could close the carbon cycle and promote a circular economy. However, the complex structure of raw biomass poses challenges, limiting processability. To overcome the low processability of raw biomass, highly efficient pretreatment methods were developed and thoroughly investigated. Herein, fast-growing plant species were featured as promising biomass for reforming due to their rapid carbon fixation within short timeframe. Their fast growth rate also accompanies with a shorter lifespan; hence they release carbon back into the atmosphere only after a short period of storage, rendering advanced carbon storage and utilization crucial. Reforming of biomass from fast-growing plant species not only produces green hydrogen fuels but also sustainable commodity chemicals. (Refs can be found at https://scholar.google.com/citations?user=4sPoVMAAAAAJ&hl=en)

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We wish you a wonderful summer, and look forward to seeing you at the start of the new academic year on September 4 and 5, 2025, for the 24th days of the Ecole Doctorale de Chimie Moléculaire de Paris-Centre.

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