



18th ICC • LYON 2024

DISCOVER

THE YOUNG LAUREATES OF FRENCH CATALYSIS !

THE LAUREATES

AND THEIR CONTACT DETAILS

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Dear colleagues,

It is with great pleasure that I present you this brochure, « Young laureates of French catalysis », which the Catalysis Division of the French Chemical Society has prepared in the context of ICC 2024.

Our goal is to introduce you to young researchers working in French laboratories, who in recent years have been rewarded by national prizes such as the CNRS bronze medal, by prizes awarded by the Division, or by labels of excellence delivered on the occasion of ICC 2024.

What struck me during the preparation of this brochure is in one word, diversity: diversity of disciplines, diversity of backgrounds, diversity of points of view and personal interests. The vitality of French catalysis is expressed here. And, of course, this vitality is also to be found among all the other young talents who are currently developing their work in our laboratories, and whom I encourage you to meet during this congress.

May this document be the starting point for fruitful discussions and contacts, and allow you to better know our laboratories and all those who will contribute to French research in catalysis in the years to come.

Eric Marceau
President of the Catalysis Division of the French Chemical Society

Bronze medal, CNRS, 2024
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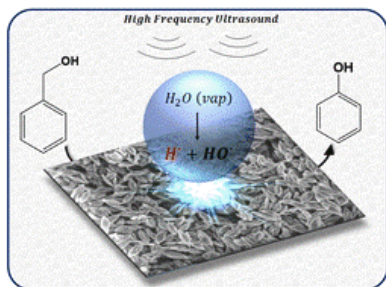
TELL US MORE ABOUT YOUR BACKGROUND

Specializing in heterogeneous catalysis, I honed my expertise in catalytic oxidation reactions throughout my doctoral studies in Chemical Engineering at Nanyang Technological University, Singapore.

Under the direction of Prof. Yanhui Yang and Dr. Armando Borgna, and funded by the prestigious Singapore International Graduate Award from A*STAR Singapore, my research activities focused on the development and investigations of nanometric gold particle interactions with metal oxide supports.

My research centered on unraveling the dynamics of these interactions and their profound impact on catalytic activities, particularly in sugar oxidation reactions.

WHAT IS YOUR RESEARCH ABOUT ?



Having joined as a CNRS Researcher in 2019 at the Institute of Chemistry of Environments and Materials of Poitiers (IC2MP), my professional passion revolves around leveraging ultrasound technology – spanning both low and high frequencies – as an unconventional activation tool in facilitating catalytic reactions that are generally considered sluggish and challenging. I specialize in employing ultrasound for pioneering synthesis of catalytic materials and harnessing its chemical potential for ultrasound-assisted catalytic

conversion of bio-based substrates into industrially relevant platform and commodity chemicals. I am presently the principal investigator of an ERC Starting Grant project aimed at redesigning novel catalytic materials.

Our primary focus lies in controlling the nucleation of cavitation bubbles formed on the surfaces of these novel catalytic materials during ultrasonic irradiation. This allows us to harness the chemical potential of these bubbles towards the activation of small molecules, marking a significant leap in catalytic innovation.

!ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

When I am not immersed in scientific pursuits, I find joy in exploring new destinations and immersing myself in diverse cultures. Exploring the flavors and nuances of wine is a particular passion of mine, perhaps I should explore a career as a wine tasting consultant.

On another note, my research group is continuously seeking vibrant, inquisitive individuals for postdoc and PhD positions as part of our ongoing ERC-funded starting grant. Visit our website for more information on current opportunities.

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| TELL US MORE ABOUT YOUR BACKGROUND

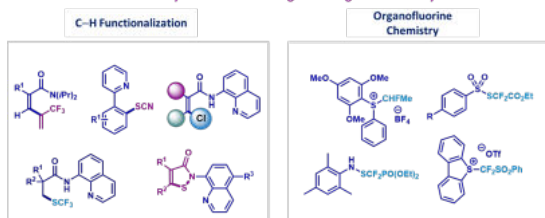
I graduated from the National Graduate School of Chemistry and Chemical Engineering of Clermont Ferrand (ENSCCF), and I obtained my PhD in organic chemistry (2009) at Grenoble University in the group of Dr. A. E. Greene. I pursued first with as a postdoctoral fellow in the group of Prof. F. Glorius at the WWU Münster (Germany), on homogeneous catalysis, and especially on transition metal-catalyzed activation of the C-H bond. In 2011, I joined the group of Prof. Reek at Amsterdam University as an industrial postdoctoral fellow (Eastman). There, I acquired skills in organometallic and supramolecular chemistry applied to hydroformylation, especially in inorganic synthesis. Between 2012 and 2021, I was a CNRS Researcher (Habilitation in 2018) in the “Fluorinated Biomolecules Synthesis” group at the laboratory COBRA and I was promoted senior researcher in 2022.

| WHAT IS YOUR RESEARCH ABOUT ?

My research interest focuses on developing new strategies to access unprecedented organic scaffolds. Cutting-edge methodology developments were achieved for the introduction of fluorinated groups on various scaffolds, by combining organofluorine chemistry and homogeneous catalysis (transition-metal catalyzed C-H bond activation).

In addition, I have been particularly interested in providing the scientific community with efficient and more sustainable synthetic processes (mild reaction conditions, non-noble metals, flow chemistry).

Modern Synthetic Methodologies for Organic Chemistry



In recent years, I naturally turned my attention to emerging fluorinated groups (CF₂FG and SCF₂FG, FG = functional groups) along with sulfur-containing moieties of interest (e.g., SCN), with the elaboration of original electrophilic sources, necessary for the development of these novel transformations.

ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

Besides my interest in research, I actively promote Women in Science through different actions. Indeed, beyond all the major advances made over the years, I strongly believe that one role of a scientist nowadays is to open the field of research to all and to be a key player in Society.

In my opinion, a key point is to stimulate the interest of the younger generation to pursue the actions that have already been carried out, to go beyond, and to promote the curiosity that drives them in science.

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TELL US MORE ABOUT YOUR BACKGROUND

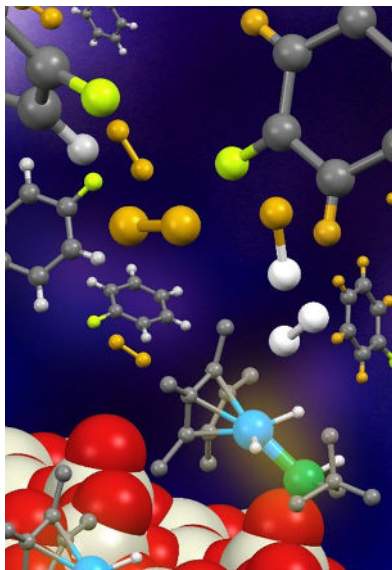
I spent my childhood in the green mountains of Mazamet, in south-western France. I became passionate about molecular chemistry at the start of my undergraduate studies in Toulouse. I then entered the École Normale Supérieure de Lyon (France) and obtained the “agrégation” degree in Chemistry in 2009. I completed my doctoral thesis (2013) at the CEA-Grenoble (France) under the supervision of Marinella Mazzanti, on the coordination chemistry and reactivity of mono- and polymetallic complexes of f-elements (lanthanides and uranium) in very low oxidation states. To this end, I developed two strategies: the use of non-innocent ligands as electron reservoirs, and the use of siloxide ligands to stabilize highly reductive and reactive compounds.

I then joined Professor John Arnold’s group (University of California, Berkeley, USA) from 2013 to 2015 for a postdoctoral stay, during which I diversified my range of metal elements of interest (Co, Nb, Ta, Th), strengthening my expertise in the inert-atmosphere design of highly sensitive organometallic species. In particular, I have studied original activation modes for small molecules, including P_4 , H_2 , PCO^- or N_3^- .

WHAT IS YOUR RESEARCH ABOUT ?

I design, synthesize and characterize innovative organometallic objects for targeted applications in catalysis (homogeneous and heterogeneous). Following recruitment into the CNRS in 2015, I broadened my areas of expertise towards solid-state chemistry and catalysis.

I am currently exploring new synthetic approaches for the preparation of tailored organometallic molecules associating two distinct metal centers at close proximity. Through advanced characterization and modelization of the resulting metal-metal pairs, I wish to advance knowledge regarding the electronic structure of these entities, in relation with their reactivity. These molecules are then used to prepare well-defined and highly dispersed heterobimetallic supported solid catalysts featuring engineered active sites at a molecular level, using Surface Organometallic Chemistry (SOMC) methodologies.



Through immobilization I can achieve metal species having unconventional low-coordinate structures, not achievable in solution and featuring unique reactivity. The aim is to target cooperative mechanisms between two distinct metal centers, in order to promote original chemical reactivity which differs from, and ideally surpasses, that of its two parent metals. I have notably illustrated this concept for the activation of CO₂ and C-H bonds.

One of our recent focus is on catalytic hydrogen isotope exchange reactions. Early metal hydrides on silica and late metal catalysts are well known to perform hydrogenolysis, therefore we were skeptical about the possibility of performing hydrogen isotope exchange with alkanes using D₂. One of our recent achievements, as part of the ERC StG project "DUO", was to discover that the combination of the two metals eliminated this pathway. As a result, the heterobimetallic catalyst is highly selective for C-H activation, without breaking the C-C bonds.

| ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

Participating in the organization of ICC 2024 as a member of the executive committee and coordinator of the young scientists committee has been an exceptional experience and an opportunity to strengthen my network and serve the catalysis community. I hope you enjoy this Lyonnaise edition of ICC 2024 and that the events specially designed for young researchers will be a great success! And after that: well-deserved holidays, hiking the mountains and scuba-diving the ocean!

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| TELL US MORE ABOUT YOUR BACKGROUND

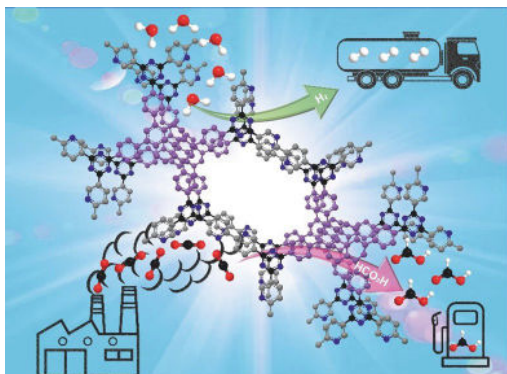
After obtaining a master degree in organic and macromolecular chemistry from the University of Lille, France, I moved to Switzerland to do my PhD from 2003 to 2007 in the group of Prof. Georg Süss-Fink at Neuchâtel University, where I developed molecular organometallic catalysts based on Ru, Ir and Rh in aqueous solution, especially for the transfer hydrogenation of ketones and imines to give an environmentally friendly access to alkaloids via asymmetric catalysis in water.

Then I extended my field of research to other catalytic reactions, such as carbon-carbon coupling, and to self-assembled materials. I joined the group of Prof. Kenichiro Itami from 2007 to 2009 in Nagoya, Japan, as a JSPS postdoctoral fellow, in order to develop new systems (molecular catalysts and/or nanoparticles) able to catalyze the functionalization of heteroarenes via C-H activation under mild conditions, enhancing the cost efficiency of the process.

In 2009, I came back to France to join IRCELYON with Dr. David Farrusseng, in order to develop new catalysts based on Metal-Organic Frameworks (MOFs), expanding the field of applications of these promising porous crystalline materials. Finally, in 2010, I was appointed CNRS researcher at IRCELYON where I am currently developing new catalytic systems confined in the cavities of MOFs and porous organic polymers (POPs), in order to obtain unique selectivities and activities with heterogenized molecular catalysts.

| WHAT IS YOUR RESEARCH ABOUT ?

We are developing new catalytic systems answering current challenges in fine chemicals synthesis and solar fuels production, by unravelling novel molecular catalysts and heterogenizing them within Porous Macroligands, a concept we established for synergistically bridging homogeneous and heterogeneous catalysis.



MOFs and POPs are very appealing platforms for designing Porous Macroligands and exploiting the effect of confinement.

The structuration of molecular species into three-dimensional porous structures allows improving their catalytic activity and selectivity, as we demonstrated for various reactions such as C-H arylation, asymmetric transfer hydrogenation, hydrogen and oxygen evolution reactions, and carbon dioxide photoreduction.

ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

What drives my efforts is that the most important discoveries do not come from chance or serendipity, but from trials and failures which form most of the scientific research, in chemistry like in other fields. To me, being a researcher requires pugnacity and resilience to face failures and to continue looking for unravelling what nature hides from us. The most important is not the final result, which obviously and unfortunately will most of the time not change the world, but the path to reach it which should be full of curiosity, fantasy and imagination. That is how team working and great collaborations can bring you to the best.

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TELL US MORE ABOUT YOUR BACKGROUND

I graduated from Ecole Polytechnique, Palaiseau, in 2008. I obtained my PhD in 2011 from University Pierre & Marie Curie, Paris, for my work on the synthesis and applications of metal phosphide nanoparticles, under the co-supervision of Prof. Clément Sanchez (UPMC) and Dr. Nicolas Mézailles (Ecole Polytechnique). From 2012 to 2013, I was a post-doctoral fellow at Lawrence Berkeley National Lab, Berkeley, California, in the group of Prof. Miquel Salmeron, where I used synchrotron-based in situ spectroscopies (near-ambient-pressure XPS, high pressure XAS) to monitor the surface state of (bi)metallic nanoparticles during catalytic reactions.

In 2014, I joined CNRS in the Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP), associated with Sorbonne Université, CNRS and Collège de France. I work in the team Nano on novel synthetic routes of exotic nanomaterials for energy-relevant challenges. In 2017, I was awarded an ERC Starting Grant to work on small molecules activation at the surface of nanoparticles.

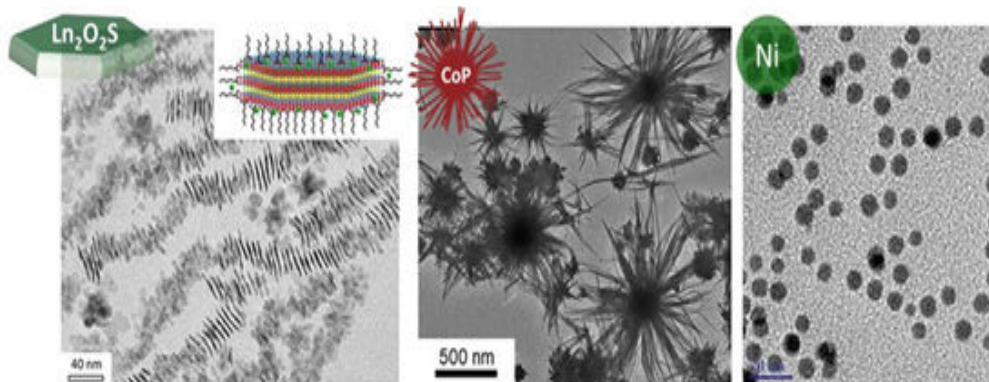
WHAT IS YOUR RESEARCH ABOUT ?

My research in nano-chemistry gives equal importance to core and surface in nanoparticles design. I am leading a research direction on metal oxysulfide nanoparticles. I combine disciplinary and interdisciplinary approaches (with physicists, biologists, etc.), with an emphasis on using synchrotron-based spectroscopies for fundamental understanding of nanoscaled matter behavior. I direct research on the design of nanoparticles (metals, alloys, phosphides, carbides) covered with ligands and the study of their surface reactivity.

My research activity is shared between two main programs: boosting the reactivity of nanoparticles and exploring new compositions and interfaces at the nanoscale. They address the design of synthetic routes for metal alloys, phosphides, carbides and oxysulfides, their structural characterization (including for amorphous phases) and their monitoring in situ using synchrotron radiation, They also question the nature of the interface, with or without organic

ligands, and its dynamic evolution in reactive environment, in the context of small molecule activation and, more recently, for nano-bio interface.

On the long term, my aim is to identify adequate descriptors for matter at the nanoscale in the hope of creating a conceptual breakthrough in nanochemistry.



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Bronze medal, CNRS, 2018
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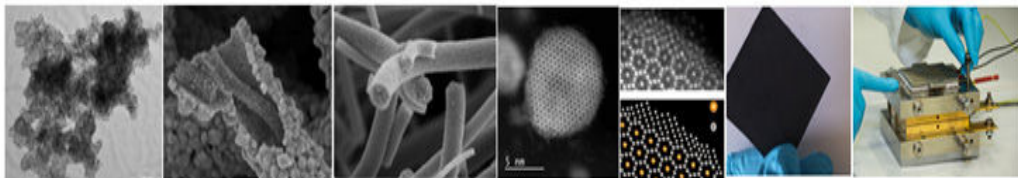
After a master degree in Chemistry at the University of Milan (Italy), a PhD at the Lavoisier Institute of Versailles (France) in collaboration with the French Alternative Energies and Atomic Energy Commission, and postdoctoral fellowships at the Universities of Freiburg (Germany) and Lyon (France), I obtained a position as lecturer at the University of Montpellier in 2009. All these experiences built my expertise in synthesis and characterization of nanomaterials of various morphologies and chemical compositions for a wide range of applications, from magnetic materials and sensing, to catalysis and energy conversion.

My research at the Charles Gerhardt Institute for Molecular Chemistry and Materials was supported in 2013 by a Starting Grant from the European Research Council (ERC), followed by an ERC Proof of Concept Grant in 2019, aiming to develop novel nanostructured materials for fuel cell and water electrolysis applications. In 2017, I was appointed junior member of the Institut Universitaire de France. Since 2021, I have been Professor at the University of Montpellier, and currently I am working for a semester at the University of Nevada, Reno (USA), supported by a Fulbright Scholar Grant.

| WHAT IS YOUR RESEARCH ABOUT ?

My research interests focus on the design and preparation of nanostructured materials for energy conversion and storage applications *via* hydrogen. Current research directions include the development of new electrolyte and electrode materials for proton and anion exchange membrane fuel cells and water electrolyzers, as well as of mitigation strategies against the degradation of these components by modifying their chemical composition, surface chemistry, morphology and nanostructure.

My activity develops around three main axes: the development of reinforced membranes, the preparation and functionalization of catalyst supports, and the synthesis of metal electrocatalysts. Several deposition methods and surface functionalization techniques are developed and used with these goals, including microwave-assisted and electrochemical synthesis, electrospinning, active plasma treatment, and atomic layer deposition. Furthermore, various physico-chemical and electrochemical techniques also *operando* are employed to characterize the obtained materials up to their characterization in fuel cell and electrolysis devices.



| ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

The main motivation to become a researcher is my curiosity and passion for chemical science, which I enjoy sharing being also a teacher. In this work we start from the design of materials, their synthesis and characterization to understand and tune their properties, until their final application in devices, in my case related to sustainable energy: this potential impact of science in technology and society is highly challenging and motivating.

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| TELL US MORE ABOUT YOUR BACKGROUND

I graduated from Ecole Normale Supérieure (Paris, MSc in 2002, “Agrégation de Chimie” in 2003), and obtained a PhD in Inorganic Chemistry in 2006 (Paris VI University), under the supervision of Prof. Michel Che, Hélène Lauron-Pernot and Guylène Costentin, in collaboration with Philippe Sautet (Ecole Normale Supérieure de Lyon).

At that time, I acquired skills in mineral synthesis, spectroscopies, catalytic testing, and computational modelling. This was the beginning of my motivation to explore more deeply the potential offered by ab initio calculations for the modelling of catalytic surfaces relevant to industrial applications.

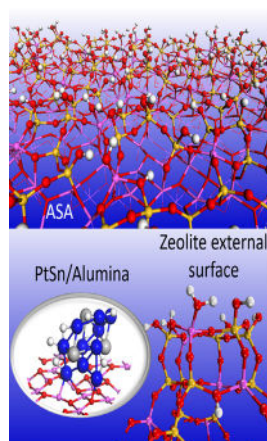
I thus joined IFP Energies nouvelles, first in the Applied Chemistry and Physical-Chemistry division in Rueil-Malmaison (close to Paris), then in 2007 in the Catalysis, Biocatalysis and Separation Division in Solaize (close to Lyon), where I am still working now. My mission consists in applying ab initio calculations in close relation with experimental research programs. The results of my works have been awarded by an HDR (Habilitation à Diriger des Recherches) from Ecole Normale Supérieure de Lyon in 2017, and by several young researcher awards (Edith Flanigen, 2015, Physical Chemistry division of SCF, 2016, DivCat, 2018, French group of zeolites, 2023).

The impact of my research was recognized by my nomination in 2014, as the project leader of the EYRING research program, gathering specialists in various disciplines, with the aim of building kinetic models (for refining, petrochemistry, biomass conversion and pollution abatement) from ab initio calculations. In 2019, I was appointed leader of the FERMI project, devoted to the use of advanced modelling methodologies for chemical reactivity. Since 2023, I have been the coordinator of the collaborative project MAMABIO, in the framework of the B-BEST PEPR.

WHAT IS YOUR RESEARCH ABOUT ?

My research works are devoted to the understanding and prediction at the atomic scale, of the structure and reactivity of realistic heterogeneous catalysts of industrial relevance (such as aluminosilicates and supported metals), for applications in the fields of energy and chemistry. To achieve this goal, Density Functional Theory (DFT) calculations are performed, in strong connection with experimental studies (spectroscopies, reaction kinetics) and kinetic modelling.

When needed, advanced methods (molecular dynamics, and levels of theory higher than DFT) are used. I am very happy and proud to collaborate with many talented researchers from IFPEN and from academic teams in France and abroad.



ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

Being the happy mother of twins, I experience everyday the challenge of combining busy personal and professional lives. This does not prevent me from devoting a significant part of my time to the catalysis community, by organizing events of various sizes, from GECAT (the French annual catalysis event, that I chaired from 2014 to 2017), FCCat (the French Conference on Catalysis, that I co-funded in 2016) and ... ICC 2024 (being vice-chair and secretary of the event you are currently attending). I really hope you will like enjoy this 18th edition in Lyon !

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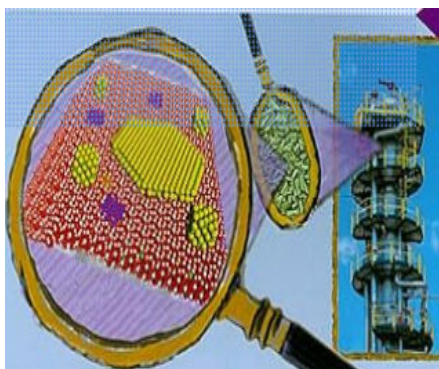
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TELL US MORE ABOUT YOUR BACKGROUND

Following a cycle of study in Caen in an Engineering School in Materials Science and Chemistry (ENSICAEN, 2003), and an academic Master's Degree (Basse Normandie University, France, 2003), I completed my research background with a PhD on fundamental studies on heterogeneous catalysis by transition metal sulfides (IC2MP, University of Poitiers, 2003-2006).

I thus joined IFP Energies nouvelles (Catalysis, Biocatalysis and Separation Division) as a research engineer in 2006, in the field of hydroprocessing catalysts for the refining of fossil fuels and renewable resources. From 2018 onwards, I have had an additional position as R&I project manager for the development of industrial catalysts and processes in this field for IFPEN Business Unit "Energy Products".



WHAT IS YOUR RESEARCH ABOUT ?

Since 2003 during my PhD, and since 2006 at IFPEN, my research activities have been mainly devoted to heterogeneous catalysis by transition metal sulfides for different applications in the energy sector using hydroprocessing technologies: clean fuel chemicals, biofuels and bioproducts from various diversified feedstocks (such as fossil fuels, lipids, bio-oil, lignin). I am involved in various research projects concerning fundamental research on catalysis by transition metal sulfides, but also in leading Research & Innovation hydroprocessing projects for the industrial

development of new catalysts and processes on (bio)fuels, in a context of resources diversification for energy transition.

The impact and relevance of my research at the crossroads of fundamental and applied research has also been recognized by the French scientific community (SCF, Catalysis division) in 2020 by the Young Scientist Award and highlighted by my scientific and technical contributions:

- 32 articles published in peer-reviewed journals, and 1 book chapter
- 39 patent applications,
- 3 invited talks, 8 oral presentations at international conferences.

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TELL US MORE ABOUT YOUR BACKGROUND

By training, I am a bio-science engineer from the University of Louvain (UCLouvain), in Belgium. During my master, I specialized in chemistry, nanobiotechnology, catalysis, and materials chemistry. I did my master degree thesis (2006) and my PhD (2010) under the supervision of Prof. Eric Gaigneaux, in heterogeneous catalysis. I chose to work in this field because I reckoned it was one of the most effective ways to participate to the development of more effective and sustainable practices, in the broad context of “transition”: thus, I was initially working on air pollution remediation.

After my PhD on low-temperature olefin metathesis (2010), I had the chance to embark on a long postdoctoral research associate contract with FNRS. I took this opportunity to spend 1 year in the lab of Prof. Clément Sanchez (Sorbonne Université, Paris) to work on original materials synthesis processes (sol-gel) and then 1 year in the lab of Prof. Nicholas Turner (University of Manchester) to dive into the fascinating world of biocatalysis. Quickly after that (2012), I obtained a PI position at UCLouvain, where I started to teach (physical chemistry, process engineering, biorefinery) and where I started my own research group.

WHAT IS YOUR RESEARCH ABOUT ?

Our main focus is to develop innovative catalysts for sustainable chemistry. We target three main applications: (i) the upgrading of biomass and bio-based platform chemicals (glycerol, lignocellulose and lignin-derived monomers, ethanol, short carboxylic acids, triglycerides, sugars, etc.) to valuable molecules, (ii) CO₂ capture and conversion (hydrogenation), and (iii) greener organic synthesis using enzymes and hybrid catalysis approaches. This latter line of research is probably the most original one. To expand the catalytic toolbox, we combine heterogeneous chemo-catalysts with enzymes, to run cascade reactions in a more effective way. Beyond “hybrid catalysis”, we strive to develop actual “hybrid catalysts”, i.e. solid catalysts that bear both chemo-catalytic and biocatalytic functionalities and that can be recovered and reused. The idea is to leverage the “pros” and mitigate the “cons” of each catalyst, to design

multifunctional catalysts that can synthesize high-value chemicals (e.g. drugs) in an effective way. The concept allows using cheap substrates, having effective co-factor recycling, reaching very high enantioselectivity, avoiding substrate or product inhibition, etc. To do so, we implement ad-hoc strategies to immobilize enzymes into/onto catalytically active solid materials.

| ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

In my research activities, I enjoy being involved in international collaborations and in multi-disciplinary research projects. I also like science communication, social media (find me on X (@deuxbeck) or on LinkedIn !), and all aspects of scientific publishing, as an author, reviewer, editor.

I was recently appointed as an Associate Editor of the new journal Chem & Bio Engineering (ACS), to which I encourage the catalysis community to submit their high-quality papers ! Also, I am the happy father of 3 young kids, who keep me busy outside of the lab. I used to be quite an active sportsman and now I am trying to keep it up despite time constraints. If we meet at a conference somewhere nice, join me for a morning run !

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Filippo Brienza, David Cannella, Diego Montesdeoca, Iwona Cybulska,* Damien P. Debecker*

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Yingrui Zhao, Valentina Girelli, Ovidiu Ersen, Damien P. Debecker,*

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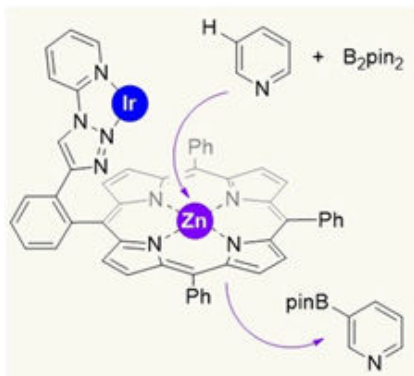
TELL US MORE ABOUT YOUR BACKGROUND

After having studied chemical sciences for 3 years at the University of Valencia (Spain), I was lucky enough to join the École Européenne de Chimie, Polymères et Matériaux (ECPM) in Strasbourg and also obtained a MSc degree. During that time, I enjoyed the expertise of superb professors that strongly stimulated my curiosity in research and I decided to carry out PhD studies with Dominique Matt and Dominique Armspach in the area of metallocyclodextrins. This was a fantastic experience to discover the power and uniqueness of ligand design, coordination chemistry and homogeneous catalysis. Then, I pursued with a Rubicon-funded postdoc position in the group of Joost Reek (Amsterdam) to explore metal-catalyzed processes in confined spaces.

This followed a short research period in Nagoya in the group of Takashi Ooi dealing with ion-paired catalysis. These two postdoctoral periods definitely expanded my horizons from both scientific and personal points of view. In 2015, I obtained a CNRS researcher position in the Rennes Institute of Chemical Sciences, and I joined the Organometallics Materials and Catalysis team that provided a stimulating and optimal environment.

WHAT IS YOUR RESEARCH ABOUT ?

My research work is devoted to homogeneous metal catalysis, and it is mainly focused on the introduction of weak interactions in the secondary coordination sphere of the catalysts, similar to the action mode of enzymes, but for purely artificial systems. Beyond well-known hydrogen bonding or ion-pairing, we exploit weak coordination chemistry for selecting and pre-organizing substrates by remote control, and we have applied this concept to challenging iridium-catalyzed C-H bond functionalizations with spectacular reactivities and selectivities. In parallel to that, we have disclosed that rather simple iron- and cobalt-porphyrins are excellent catalysts for selective Wacker-type oxidations of olefins into ketones, which is a major discovery for replacing the scarce palladium-based catalysts currently used in the industry.



Our overarching research strategy not only combines catalyst design and exploitation, but we have also deciphered reaction mechanisms in order to circumvent undesired pathways and to design superior catalysts by rational understanding. Lastly, we have established successful collaborations for the utilization of our non-noble metal-based complexes for the sustainable production of hydrogen under electrocatalytic conditions. As such, our research spans a wide domain from transition metal catalysis for fine-chemicals, to green chemistry applications, with an emphasis on supramolecular and bio-inspired catalysis.

| ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

By far, the most exciting part of my job is to train the highly engaged students and researchers at any levels (postdoc, PhD, MSc) that I have been lucky to supervise while witnessing their evolution towards very skilled scientists. I am really pleased of our regular scientific discussions and our facing together of the challenges associated to our research.

I am also really excited for having established some collaborations in France and abroad in order to complement our expertise and I am looking forward to our next projects together.

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[5] "Markovnikov-Selective Cobalt-Catalyzed Wacker-Type Oxidation of Styrenes into Ketones under Ambient Conditions Enabled by Hydrogen Bonding" N. Abuhafez, A. W. Ehlers, B. de Bruin, R. Gramage-Doria, *Angew. Chem. Int. Ed.* 2024, 63, e202316825.

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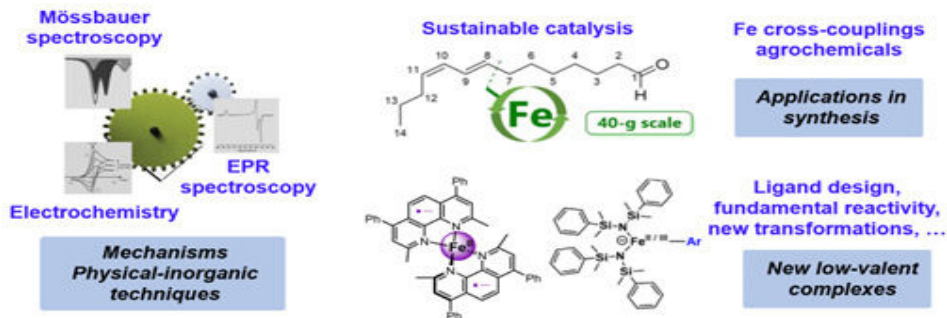


| TELL US MORE ABOUT YOUR BACKGROUND

I completed my graduate studies in 2012 under the guidance of Anny Jutand, at the Ecole Normale Supérieure de Paris, where I learnt how to decipher the mechanism of transition-metal-catalyzed cross-couplings using cyclic voltammetry as an investigation tool. I moved afterwards for a postdoctoral stay in Vancouver, at the University of the British Columbia in the group of Peter Legzdins, where I explored the reactivity of tungsten nitrosyl complexes in alkane C-H activation processes, a position funded by the DOW Chemicals company.

I moved back to France in 2014 and was appointed as a CNRS Fellow in the group of Thibault Cantat (CEA Saclay), to work on the use of CO₂ and of its analogues (formic acid, methanol, CO) as valuable C1 building blocks. In 2019, I moved back to Paris, at Chimie ParisTech – PSL (i-CLeHS), in team Catalysis, Synthesis of Biomolecules and Sustainable Development, directed by Virginie Vidal. I have been devoting my research activities ever since to the development of original reactive iron complexes, the understanding of their structural properties, and their application in catalysis.

WHAT IS YOUR RESEARCH ABOUT ?



My main research focus is to build bridges between the coordination chemistry of reactive, low-valent iron systems and their use in catalytic applications, with a strong interest in mechanistically-driven design of new catalysts. To do so, we use a combination of physical-inorganic techniques such as Mössbauer and EPR spectroscopies, as well as multinuclear NMR experiments. Once the elementary reactivity patterns of our complexes have been deciphered and well-understood, their potency in catalysis is investigated.

This approach, carried out in a constant dialog with an in-depth analysis of the mechanisms at play in those transformations, also leads us to discover new catalytic patterns, that we further apply to the synthesis of organic scaffolds of interest.

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| TELL US MORE ABOUT YOUR BACKGROUND

In 2016, I obtained a double degree from Bordeaux University and the engineering school ENSCBP (now ENSMAC), both in chemistry and chemical physics. I did a Ph.D. at IRCELYON (Research Institute on Catalysis and Environment of Lyon), under the supervision of Eric Puzenat, Christophe Geantet, Pavel Afanasiev and Luis Cardenas. I worked on transition metal sulfides co-catalysts supported on TiO₂ for the photoconversion of alcohol [1], [2].

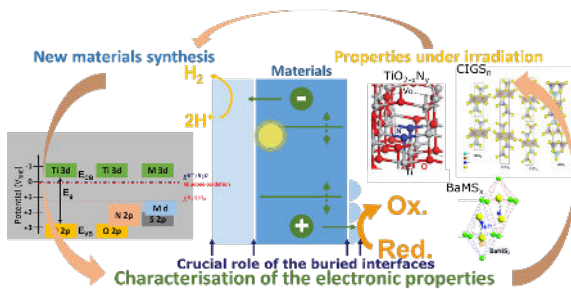
I also started using UV Photoelectron Spectroscopy (UPS) to measure energy levels, especially the valence band edge of nanopowders, in order to discuss possible charge carrier transfers at heterojunctions [2].

I perfected this expertise by joining the Surface Science Laboratory at TU Darmstadt. I learned how to combine different photoelectron spectroscopies (XPS, UPS, SPES) to probe not only chemical properties but also electronic properties. I measured the valence band and conduction band position of single materials [3], and I have probed band bending and interface energetics of heterojunctions. For such purpose, I performed interface experiments into cluster tool and I developed Tapered Cross Section Photoelectron Spectroscopy (TCS-PES) to study buried interfaces of multi layers architecture (e.g. photoelectrodes or solar cells) [4], [5].

Finally, I joined the Institut des Matériaux de Nantes Jean Rouxel, first as a post-doc and then as a research scientist. I learned how to prepare thin-film materials by magnetron sputtering and plasma-enhanced chemical vapor deposition, such as Au nanoparticles on TiO₂ or N-doped TiO₂ thin films, for photo(electro)catalytic applications.

| WHAT IS YOUR RESEARCH ABOUT ?

I now apply my expertise in photoelectron spectroscopy, photocatalysis and materials science to the development of new photo(electro)catalysts for the production of solar fuels. I am convinced that photocatalysis offers a clear advantage over photovoltaic – electrolysis coupling due to its simplicity.



A simpler process leads to the production of local solar fuels favouring energy independence and limiting the carbon footprint of the overall process. I am focusing my research on the oxidation half-reaction. I am currently working on the photoconversion of glucose that generates H_2 and high value-added

molecules (e.g. arabinose, erythrose). As the electrochemical potential of glucose oxidation is closer to the one of the proton reduction, the potential difference that needs to be provided to the system is much less than the 1.23 V required for the water-splitting. Therefore, the band gap of the involved semiconductors can be narrowed to maximize the solar irradiation. I am doing band gap engineering of oxysulfides, oxynitrides and chalcogenides – based photocatalysts.

[ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

As a citizen, I am doing my best to have the lowest environmental impact (e.g. flying less, cycling 95% of the time, zero waste, vegetarian). I considered leaving academia to pursue a more impactful career path, such as planting trees, working on a farm, or engaging in political activism, but the opportunity to become an independent researcher with the flexibility to pursue and advance my own research ideas, and change things from the inside, was a key factor in my decision to remain in the scientific community.

I am very interested in the “Labos 1point5” initiative. Thanks to their calculator, colleagues and I have estimated the carbon footprint of my laboratory and are now discussing the various actions that could be taken to reduce it. As a scientist, I am also very interested in developing new materials and new solar fuel production approaches that take into account not only climate change but also the other 8 planetary boundaries (“Earth beyond six of nine planetary boundaries”, Science Advances, 2023).

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TELL US MORE ABOUT YOUR BACKGROUND

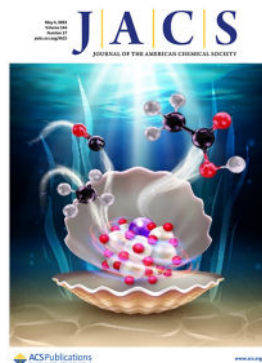
I received my MSc (2006) and PhD (2009) degrees from Moscow State University in the field of zeolite catalysis. I was then a postdoctoral researcher in the Department of Chemical Engineering at the Eindhoven University in the Netherlands, working on biomass conversion. Afterwards, I received a permanent position as a CNRS researcher in 2013 in the Energy group of the UCCS laboratory in Lille, working in C1 chemistry and mainly focusing on Fischer–Tropsch synthesis.

In 2016, I have moved to the “mirror laboratory” Eco-Efficient Products and Processes Laboratory in Shanghai (E2P2L), which is a joint laboratory between CNRS and Solvay, where I performed biomass valorization by reactions of amination, oxidation, etherification and hydrogenation.

At the end of 2019, I returned to Lille where I have been in charge of team CEMOP (Catalysis for energy and platform molecules synthesis), focusing on the valorization of small molecules (CO_2 , CO, CH_4 , N_2 ...) to platform molecules and fuels.

WHAT IS YOUR RESEARCH ABOUT ?

My research focuses on the transformation of small molecules (e.g. CO_2 , CO, CH_3OH , CH_4 , H_2O , N_2 , etc.) into high value-added platform molecules and alternative fuels. Small molecules are generally the most abundant raw materials in carbon reserves derived from fossil resources, such as methane, or from anthropogenic activity, such as CO_2 , and are also well-known greenhouse gases. CO and CH_3OH are considered to be important intermediate molecules. At the same time, water is used as a source of hydrogen, and nitrogen is a valuable resource for ammonia synthesis.



Thus, all these small molecules are today considered as one of the most important potential sources for the synthesis of fuels and platform molecules widely used in industry, such as syngas, methanol, formic and acetic acid, light olefins, aromatics, etc. The originality of our work lies in the fact that we are working simultaneously on the development of new catalysts, on the understanding of the mechanism of catalytic reactions, and on the process development and coupling. Each of these directions complements the other to ultimately provide new approaches for the synthesis of target molecules.

We currently use 3 modes of molecule activation: traditional thermocatalysis, photocatalysis and electrocatalysis. These modes are used separately or in combination with each other. The advantage is that the use of one of the modes allows us to better understand the reaction mechanism and the role of active sites, and to use this knowledge for other approaches.

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TELL US MORE ABOUT YOUR BACKGROUND

After obtaining my chemical engineering degree at ENSEEG-PHELMA (Grenoble, France), I went to Edinburgh (UK) for a 6-month internship at Heriot-Watt University. I really enjoyed my stay, the laboratory, and the research themes, so it is with pleasure that I pursued a thesis under the supervision of Prof M. Keane. My PhD focused on the enhancement of catalytic processes through optimization of heterogeneous catalysts and control of the reaction conditions. The results demonstrated the viability of Au supported on molybdenum nitride and carbide as catalysts for the gas phase hydrogenation of nitroarenes. I defended my thesis in 2012, for which I received the McFarlane Prize.

Then, I conducted my first postdoctoral position in industry at Sasol Technology (St Andrews, UK). The aim of my project was the development of a process for converting biomass-derived glycerol into acrylates as value-added chemicals relevant to Sasol's chemical portfolio. My second postdoctoral position was at the University of Liverpool with Prof M. Rosseinsky. My work focused on the synthesis of novel non-noble metals supported on mixed oxides for the hydrogenation of 5-hydroxymethyl furfural in liquid phase.

I then returned to France in 2015, when I was recruited as a research fellow at the CNRS. I joined the IRCELYON laboratory and more particularly the C'Durable team which focuses on sustainable chemistry. Overall, my research deals with the synthesis, characterization and study of new materials, and correlation between their structure and their catalytic performance.

WHAT IS YOUR RESEARCH ABOUT ?

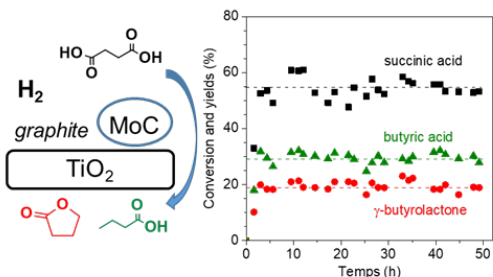
My research projects focus on the design of heterogeneous catalysts for the transformation of biosourced molecules in a liquid medium, via hydrogenation, hydrogenolysis, oxidation and dehydrogenation reactions. I have been particularly interested in the transformation of succinic acid, polyols and cellulose. Materials stable in a hydrothermal environment (e.g. TiO_2 , ZrO_2 , activated carbon) are used as supports. The use of noble metals (e.g. Au, Pd, Pt, Rh)¹ is generally necessary to achieve good yields of desired products. However, due to the cost and the rarefaction of some of these metals, I am trying to develop processes with transition metals (Cu, Co, Mo, W)^{2,3,4,5} in metallic form^{2,5}, oxide, or even carbide⁴ and nitride³.

I particularly specialized in the study of the synthesis parameters of catalysts on their physicochemical and catalytic properties.

One of my studies focused on optimizing the synthesis of molybdenum carbides supported on TiO_2 .⁴ The synthesis parameters of small nanoparticles (< 5 nm) of cubic phase MoC mainly affected the degree of carburization, i.e.

Mo/C ratio. The catalysts were active in the transformation of succinic acid to γ -butyrolactone and, more remarkably, butyric acid. We were able to show that MoC/ TiO_2 is stable for 50 h for the hydrogenation of succinic acid in a continuous reactor.

Acceptor-free alcohol dehydrogenation is an extremely interesting reaction from a green chemistry point of view. We have notably worked on cobalt catalysts. A conversion of around 70% associated with high selectivity (98%) was obtained with Co/ TiO_2 for the dehydrogenation of 2-octanol. Extensive characterization made it possible to evaluate the intrinsic properties of the materials. To understand their performance in the dehydrogenation of mono-(1-octanol, 2-octanol) and polyalcohols (octanediol) having primary and secondary hydroxyl groups, experimental and theoretical approaches were linked. For Co unsupported nanoparticles, the shape, type of exposed metal facets, and thickness of the ligand layer protecting the nanoparticles were analyzed. By combining all the results, it was possible to show that the quantity and nature of the ligand are the main factors guiding the activity of the catalyst.⁵



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| TELL US MORE ABOUT YOUR BACKGROUND

Born in Ithaca, NY (USA) from French parents, I studied at the Ecole Normale Supérieure de Lyon (ENS de Lyon, France), where I obtained my Bachelor Degree (Licence) in Chemistry in 2010. Then, I pursued a Master degree at the same institution, which led me to perform a research internship in the groups of Prof. Curtis Berlinguette and Prof. Simon Trudel at the University of Calgary (UofC, Canada) during which I studied the electrocatalytic properties of amorphous metal oxides for the oxygen evolution reaction.

After obtaining my Master degree in Chemistry in 2012, I joined the research group of Prof. Kevin Sivula at the École Polytechnique Fédérale de Lausanne (EPFL, Switzerland) where I performed my doctoral research. This research primarily consisted in developing and studying metal oxide and metal chalcogenide semiconductors as novel visible-light absorbers. These materials were then employed as photoelectrodes in photoelectrochemical cells for solar hydrogen production. For this work, I obtained my Ph.D. diploma in 2017.

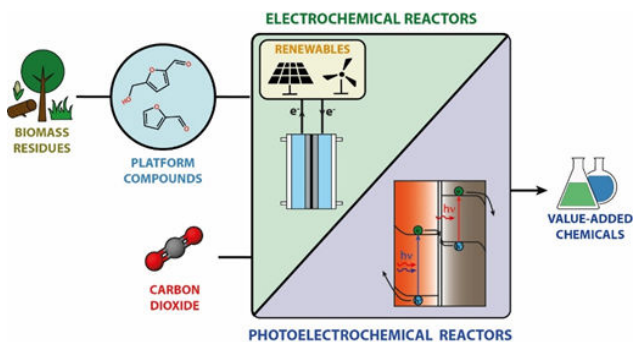
I then joined the group of Prof. Omar Yaghi at the University of California, Berkeley (USA), where I studied the electrocatalytic and water-harvesting properties of metal-organic frameworks, between 2017 and 2019.

After returning to France, I joined the Centre National de la Recherche Scientifique (CNRS) in 2020. Since then, I have been developing my research activities at IRCELYON and taken an active part in the French and European community as independent researcher.

| WHAT IS YOUR RESEARCH ABOUT ?

The current interests of my research group can be organized along the following axes:

- a. Electrocatalytic valorization of biomass-derived platform molecules
- b. Electrocatalytic valorization of carbon dioxide
- c. Material development for photoelectrochemical applications
- d. Design and implementation of operando approaches for (photo)electrocatalytic systems



These activities are conducted in the context of the energy transition and the defossilization of the chemical industry. The philosophy of our research consists in developing a fundamental understanding of the mechanisms of charge generation, transport and transfer inside the materials and at their interface with a reactive medium, which we then use to

elaborate and build lab-scale functional devices. This work is supported by a strong expertise in electrochemistry and photoelectrochemistry, as well as emerging operando approaches conducted in the lab or at synchrotron facilities.

A selection of the materials we are currently investigating and integrating in functional devices include:

- Copper-based electrocatalysts for the reductive valorization of furfural towards 2-methylfuran
- Nickel and manganese-based electrocatalysts for the oxidative valorization of 5-HMF towards DFF and FDCA
- Metallic, molecular and hybrid electrocatalysts for the reductive valorization of CO₂ towards methanol, ethylene and propanol
- Quaternary oxysulfide materials as photoabsorbers for photoelectrochemical applications

These research activities are funded through several national and European programs, and are integrated with the research work of many talented scientific collaborators around the world.

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| TELL US MORE ABOUT YOUR BACKGROUND

Following initial studies at the École Normale Supérieure de Lyon, from which I graduated in 2003 in physical sciences (with an option in chemistry), I obtained a Master graduate degree and a PhD at the University of Strasbourg under the supervision of Dr. Michel Pfeffer. My research work focused on the synthesis of chiral cyclometallated complexes of ruthenium and their applications in catalysis. I subsequently carried out two post-doctoral stays: with Professor Jan-Erling Bäckvall at the University of Stockholm (Sweden) on dynamic kinetic resolution, then with Professor Gerhard Erker at the University of Münster (Germany) in the field of Lewis-Frustrated Pairs.

In 2009, I was recruited as associate professor within the team Organometallics: Materials and Catalysis at the Rennes Institute of Chemical Sciences (ISCR) of the University of Rennes 1. In 2016, I was appointed Junior Member of the Institut Universitaire de France (IUF). In 2017, I was promoted to full professor at the Paul Sabatier University in Toulouse. I conduct my research work on homogeneous organometallic catalysis within a laboratory of the French National Research Centre (CNRS) - the Laboratory for Coordination Chemistry (LCC).

| WHAT IS YOUR RESEARCH ABOUT ?

My current research work is mainly focused on the development of new molecular catalysts based on abundant 3d transition metals, such as iron, nickel, cobalt, and manganese. Catalytic applications focus on reduction processes in the broad sense (hydroelementation, hydrogenation, dehydrogenation, hydrogen transfer, hydrosilylation, hydroboration and hydrogen borrowing) and direct activation of C-H bonds. The main objective of my work is thus to promote new reactivities and/or selectivities based on readily available and inexpensive metal catalysts in the context of sustainable chemistry. Applications range from fine chemicals to more applied solutions to current challenges, such as the recycling of plastics by reductive depolymerization, or the use of methanol as a source of C1 carbon in organic chemistry.

| ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

As a professor, rightly called a "lecturer-researcher" in French, I enjoy both facets of this rich profession. Confronting an idea with experience, trying to understand an unexpected result, participating in our own way in finding solutions to societal challenges, but also training, exchanging, and finally seeing students grow in the lab and at university are two motivations for getting up every morning - and two satisfactions some evenings.

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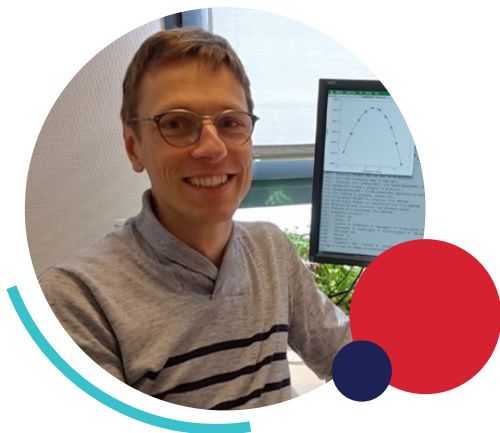
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| TELL US MORE ABOUT YOUR BACKGROUND

I have studied chemistry at the University of Basel, Switzerland, reaching a Master diploma in 2008. Out of the diverse fields of chemistry practiced during my studies, it was computational chemistry that attracted me the most for pursuing a PhD. I decided to move to the Ecole Polytechnique Fédérale de Lausanne, Switzerland, to do my PhD under the supervision of Clémence Corminboeuf.

Working on the development of dispersion corrections to density functional theory, their application and the characterization of electron delocalization in organic compounds, I finished my thesis in 2012. With the intention to move towards more fundamental developments, I joined the group of Weitao Yang at Duke University, USA, for a post-doc. Unexpectedly, I there got also exposed to the modelling of electrocatalytic reactions. This prepared me for my second post-doc at the "Laboratoire de Chimie", Lyon, France, where I fully embraced the topic of modelling heterogeneous electro-catalysis, first under the guidance of Philippe Sautet and, since 2016, as an independent CNRS researcher.

My current research is driven by method development for a better understanding of (electrified) solid/liquid interfaces and collaborations with experimental colleagues to better understand and, in fine, tune electrocatalysts.

| WHAT IS YOUR RESEARCH ABOUT ?

I am a computational chemist, who is most interested in the atomistic details of chemical systems. This implies most of the time the use of electronic structure methods such as density functional theory, but, sometimes, more approximate methods, such as force fields, are more appropriate, especially for the description of solvents.

My research activity around catalysis can be summarized in two broad categories: (i) method developments for treating solid/liquid interfaces, including the effect of the electrochemical potential and (ii) applications to electrocatalysis, with a focus on reaction mechanisms.

The challenge in the first aspect is the delicate balance between model accuracy and realism (from perfect mono-crystalline surfaces to nanoparticles, from vacuum to explicit solvent, influence of the electrochemical potential etc). For the collaborations with experiments, it is most important to come-up with simple enough models that explain the experimental observations and provide complementary insights through the atomistic scale picture. Beyond monometallic catalysts, I have the opportunity to study alloys, sulfides, oxides and other materials. I appreciate this broad range of catalysts that also goes together with various reactions (e.g., CO₂ reduction, oxidation of water or organic molecules, hydrogen evolution etc.). This variety stimulates both the theoretician and the chemist in me.

| ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

I particularly enjoy the collaborative aspect of my work. On the one hand, I like finding technical solutions through discussions with colleagues and students. On the other hand, the collaborations between theory and experiments drive most of my curiosity and make my work particularly pleasant.

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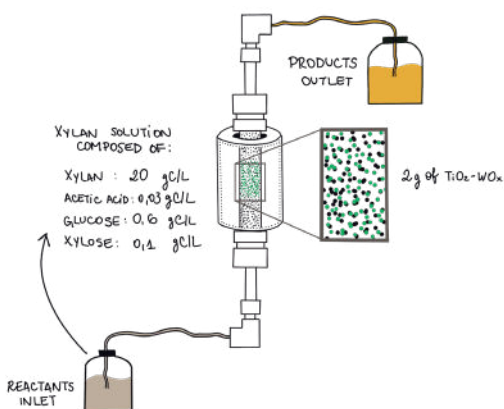


TELL US MORE ABOUT YOUR BACKGROUND

I have a university background in chemistry with a master's degree in green chemistry at the University of Strasbourg. I started a PhD in 2009 at IFPEN in collaboration with the University of Poitiers on the topic of catalysis for biomass valorization, and I defended my thesis in 2012. I pursued the topic of catalysis for biorefineries with a post-doctoral stay in Portugal in 2013. After two further postdoc experiences in academia (at IRCELYON) and industry (at Firmenich in Switzerland), I joined CNRS in 2016 as a researcher in the LGPC team, which later merged into lab CP2M.

WHAT IS YOUR RESEARCH ABOUT ?

My research projects are at the crossroads of biomass chemistry, heterogeneous catalysis and chemical engineering. Biopolymers derived from lignocellulose (e.g., lignin) have a complex structure and composition, with wide variations in monomer composition, type of inter-unit bonds and polymeric structure, depending on the biomass source and extraction process. The depolymerization of these materials is important for their valorization in biorefineries. I am therefore studying the reactivity of these biopolymers in the presence of solid catalysts (mixed oxides, supported metals) in continuous multiphase reactors, as well as the reactivity of the corresponding monomers (e.g., sugars from hemicelluloses).



The aim is to understand the reactions involved in these transformations in order to improve the design of future biorefinery processes. I am also studying the transformation of biosourced monomers and polymers in industrial effluents (such as black liquor) and the transformation of synthetic polymers (plastics).

| ANYTHING MORE PERSONAL YOU WOULD LIKE TO TELL US ?

One of my favorite aspects in my job is accompanying PhD students on their journey and seeing them become researchers. I think the new generation of students and PhD candidates can bring us new ideas and a different approach to the world.

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