XV International School of Organometallic Chemistry

Camerino, Italy

4 - 7 September 2025

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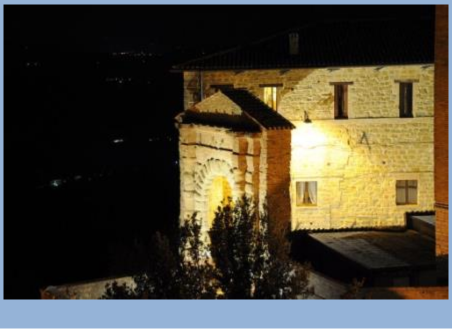

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Organometallic Chemistry beyond the future

The ISOC series is the most important school on organometallic chemistry at the European level, organized by Camerino University under the auspices of the Interdivisional Group of Organometallic chemistry of the Italian Chemical Society. The aim is to encourage the presence of young researchers and Ph.D students both from University and Industry, including those not directly involved in organometallic research projects, in order to bring together young researchers and distinguished European scientists as a contribution to the important goal of increasing the transfer of knowledge at a high level between different European countries and different generation of scientists.

Organometallic compounds continue to have a tremendous impact on modern organic synthesis and are nowadays commonly employed as catalysts for the production of fine chemicals, pharmaceuticals and advanced materials. The XV edition of ISOC will deal not with fundamental principles and there use in novel applications, but also with the role of organometallic chemistry in finding solutions to many of the major societal challenges in the 21st century: from the development of sustainable energy solutions to the mitigation of climate change, from the synthesis of effective therapeutics to the production of new materials ranging from novel polymers to nanomaterials, from the generation of industrial feedstocks to the remediation of the environment.

The scientific community is increasingly being stimulated to tackle problems of practical interest and the society will undoubtedly rely on advances made in the field of organometallic chemistry in the development of improved sustainable chemical transformations.

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TIMETABLE ISOC 2025

Thursday 04 September	Friday 05 September	Saturday 06 September	Sunday 07 September
	7:45-8:45 **Breakfast**	7:45-8:45 **Breakfast**	7:45-8:45 **Breakfast**
9:00-14:40 **Registration**	9:00-10.20 (PL3) **Prof. Joseph Dyson** *Catalytic transformation of natural and synthetic waste into value-added chemicals*	9:00-10:20 (PL7) **Prof. Luca Pignataro** *Two strategies for exploiting base metals in homogeneous catalysis*	9:00-10:20 (PL11) **Prof. Elena Fernandez-Gutierrez** *Catalytic activation of organoboron compounds for strategic and selective construction of target compounds*
	10:20-10.40 **Coffee Break**	10:20-10:40 **Coffee Break**	10:20-10:40 **Coffee Break**
	10:40-12.00 (PL4) **Prof. Alessandro Bismuto** *Exploring Heavy Pnictogens: From low-valent compounds to luminescence*	10:40-12:00 (PL8) **Prof. Antonio Zanotti -Gerosa** *Homogeneous hydrogenation catalysis in the fine chemicals industry: how to develop industrially viable and sustainable processes?*	10:40-12:00 (PL12) **Prof. Matthias Driess** *Cooperative Low-Valent Silicon Atoms in Small Molecule Activation*
	12:00-12:30 **Elsevier Presentation**	12:00-12:30 **Riccardo Porta (Flamma S.p.A.)** *The Grignard Reagents in the Pharmaceutical Industry*	12:00-12:30 **Flash-presentations**
	12:30-14:40 **Lunch**	12:30-13:00 **Silvia Panzeri (Olon S.p.A.)** *Taming the reactivity of a powerful reducing agent: lab optimization and pilot plant scale-up*	12:30-14:40 **Lunch**
		13:00-14:40 **Lunch**	
	14:40-16:00 (PL5) **Prof. Jeanne Crassous** *Organometallic Chemistry of Helicenes*	14:40-16:00 (PL9) **Prof. Didier Bourissou** *Expanding the Chemical Space of Gold thanks to Ligand Design*	14:40-16:00 (PL13) **Prof. Christopher Teskey** *Cobalt hydride catalysis under the spotlight*
15:00 -15:30 **Opening Ceremony**			
15:30-16:50 (PL1) **Prof. Holger Braunschweig** *Turning Boron Chemistry on its Head: The Unusual Reactivity of Boron in Low Oxidation States*	16:00-17:20 (PL6) **Prof. Sonja Herres-Pawlis** *Tailored catalyst design for the synthesis and the recycling of bioplastics*	16:00-17:20 (PL10) **Prof. Christian Hartinger** *Bioorganometallic Chemistry: Organometallic Drugs and Drug Candidates*	16:00 -16:30 **Closing Ceremony**
16:50-17:10 **Coffee Break**			17:10-19:40 **Old town tour**
17:10-18:30 (PL2) **Prof. Cristina Nevado** *A journey towards mechanistic understanding in organometallic chemistry*			
	17:30-18:20 **Flash-presentations**	17:30-18:20 **Flash-presentations**	
	18:20-19:40 **Poster Session**	18:20-19:40 **Poster Session**	
20:00 **Welcome Cocktail**	20:00 **Dinner**	20:00 **Dinner**	20.00 **Social Dinner**

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Prof. Alessandro Bismuto

University of Bonn, Bonn, Germany

"Exploring Heavy Pnictogens: From low-valent compounds to luminescence"

Biography: Alessandro was born and grew up in Southern Italy (Naples). He obtained his Bachelor and Master degree at the University of Naples (Federico II) working under the Supervision of Prof. Francesco Ruffo. In 2014, he moved to Scotland (United Kingdom) where he started his doctorate studies on the CRITICAT CDT (Doctoral Training in Critical Resources) programme. During that time, he worked under the supervision of Dr Stephen Thomas and Dr Michael Cowley on main group catalysis at the direct interface between inorganic and organic chemistry. In 2017, he was awarded a Research Mobility grant from Royal Society of Chemistry to undertake a research placement at the University of California, Berkeley, with Prof. John Hartwig, to study the mechanism in Ir-catalysed borylation reactions. In 2018, he moved to Switzerland to join the group of Prof. Bill Morandi as post-doctoral researcher at ETH Zürich. During the time in Switzerland he has worked on transition-metal chemistry, developing novel catalytic cycles, and studying their mechanism. After starting an independent career at the Institute of Organic and Biomolecular Chemistry (University of Göttingen), Alessandro was appointed Junior Professor (tenure track) at the Institute of Inorganic Chemistry (University of Bonn) in May 2023.

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Prof. Didier Bourissou

University of Toulouse III, Toulose, France

"Expanding the Chemical Space of Gold thanks to Ligand Design"

Biography: Didier Bourissou studied chemistry at the Ecole Normale Superieure in Paris and obtained a PhD degree from Paul Sabatier University in 1998 under the supervision of G. Bertrand. He then worked with F. Mathey and P. Le Floch at the Ecole Polytechnique in Palaiseau as a research associate. He was appointed as a CNRS junior researcher in 1998. Since 2006, he holds a senior scientist position (Directeur de Recherche) at the CNRS and from 2006 to 2018, he has been Associate Professor at the Ecole Polytechnique in Palaiseau. He is Director of the Laboratory of Fundamental and Applied Heterochemistry at the University Paul Sabatier in Toulouse since 2011. His research interests concern new bonding situations and reactivity patterns arising from the main group elements, the transition metals and their interplay. He has pioneered ambiphilic ligands in the mid 2000's and developed the concept of acceptor ligands. Part of his research also deals with non-innocent pincer complexes and unusual behavior of the coinage metals, in particular gold. He is also interested in biodegradable polymers (ring-opening polymerization, organic and dual catalysis, drug delivery systems).

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Prof. Holger Braunschweig

University of Wuerzburg, Wuerzburg, Germany

"Turning Boron Chemistry on its Head: The Unusual Reactivity of Boron in Low Oxidation States"

Biography: Braunschweig is head and chair of Inorganic Chemistry at the University of Würzburg, as well as managing head and founding director of our newly established research center ICB - institute of sustainable chemistry & catalysis with boron. He obtained his PhD and Habilitation with Prof. P. Paetzold (RWTH Aachen). He was post-doc with Prof. M. F. Lappert at Sussex and held a position as Reader at Imperial College, London. He carried out seminal work on metal boron complexes, boron heterocycles, and boron-boron multiple bonds. His work was published in over 720 publications, the majority of which appeared in first ranking journals. His discoveries have been highlighted in a wide range of outlets, including New Scientist, The Times of London, Science, Nature, Nature Chemistry, Chemical and Engineering News, Chemistry World, Spektrum, Chemie in unserer Zeit, and Angewandte Chemie. He was awarded the Gottfried Wilhelm Leibniz award (2009), the RSC Main Group Chemistry Award (2014), and received the Arduengo, Steinhofer, Bruker, and ScotCHEM named visiting lectureships. He is a member of the Bavarian Academy of Sciences, the German National Academy of Sciences (Leopoldina), the North Rhine-Westphalian Academy of Sciences, and the DFG advisory panel for molecular inorganic chemistry.

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Prof. Jeanne Crassous

CNRS-University of Rennes, Rennes, France

"Organometallic Chemistry of Helicenes"

Biography: She received her PhD in 1996 from the Ecole Normale Supérieure de Lyon (ENS Lyon) on 'The Absolute Configuration of Bromochlorofluoromethane (CHFClBr)' under the supervision of Prof. André Collet. After a one-year postdoctoral period studying 'The Chirality of Fullerenes' in Prof. François Diederich's group (ETH Zurich, Switzerland), she received a CNRS researcher position at the ENS Lyon in 1998 and then she joined the ISCR in 2005. She is currently coordinating a French national network (GDR CHIRAFUN, Chirality and multifunctionality) and a European ITN Project (HEL4CHIROLED, Helical molecules for Chiral OLEDs). She is member of the Editorial Board of Chirality and ChemPhysChem journals (Wiley). In 2020, she received the National Prize of the Organic Chemistry Division of the French Chemical Society (DCO-SCF). In 2023, she was awarded the CNRS Silver Medal. She is also a Member of the European Academy of Science (EurASc) and a Chemistry Europe Fellow. She is dealing with many fields of chirality (heteroatomic and organometallic helicenes, chiral π-conjugated systems and assemblies, fundamental aspects of chirality). She is studying chiroptics (electronic and vibrational circular dichroism, circularly polarized luminescence) for potential applications in optoelectronics and spintronics. Jeanne Crassous is a CNRS Research Director at the 'Institut des Sciences Chimiques de Rennes'(ISCR). She is currently active for the French Chemical Society as an elected member of the DCO-SCF executive board (2021-2024).

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Prof. Joseph Dyson

EPFL-Lausanne, Lausanne, Switzerland

"Catalytic transformation of natural and synthetic waste into value-added chemicals"

Biography: Paul Dyson joined the Institute of Chemical Sciences and Engineering at the EPFL in 2002 where he heads the Laboratory of Organometallic and Medicinal Chemistry and between 2008 and 2016 chaired the Institute. He has won several prizes including the Werner Prize of the Swiss Chemical Society in 2004, the Award for Outstanding Achievements in Bioorganometallic Chemistry in 2010, the Centennial Luigi Sacconi Medal of the Italian Chemical Society in 2011, the Bioinorganic Chemistry Award of the Royal Society of Chemistry in 2015, the European Sustainable Chemistry Award of the European Chemical Society in 2018 and the Green Chemistry Award from the Royal Society of Chemistry in 2020. He is also a Clarivate Highly Cited Researcher and has an H-index >110 (web of science and google scholar). He was elected a Fellow of the Royal Society of Chemistry in 2010, a Fellow of the European Academy of Science in 2019 and a life-long fellow of the American Association for the Advancement of Science in 2020. Over the years he has held visiting professorships at the University of Bourgogne, University of Pierre et Marie Curie, University of Vienna, University of Rome Tor Vergara, Chimie Paristech and Shangai Jiao Tong University. Since 2016 he has been Member of the Council of the Division of Mathematics, Natural and Engineering Sciences at the Swiss National Science Foundation. Between 2016-2021 he has been Member of the Council of the Division of Mathematics, Natural and Engineering Sciences at the Swiss National Science Foundation. In 2021 he was appointed Dean of the Faculty of Basic Sciences.

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Prof Matthias Driess

Technical University of Berlin, Berlin, Germany

"Cooperative Low-Valent Silicon Atoms in Small Molecule Activation"

Biography: Matthias Driess was born in 1961 in Eisenach, Thuringia. He received his Diplom in chemistry in 1985 and completed his PhD in 1988 at Heidelberg University. While at Heidelberg, he also studied philosophy and wrote his final thesis on "Über den logischen Empirismus von Rudolf Carnap und die Einheit der Wissenschaften" (On the logical empiricism of Rudolf Carnap and the unity of the sciences). After working as a postdoctoral fellow with Professor Robert West in Madison, Wisconsin, U.S.A., for a year, he returned to Heidelberg in 1989, completing his Habilitation in inorganic chemistry there in 1993 with a thesis about silicon and phosphorus in unusual coordination. After three more intellectually stimulating years in Heidelberg, he was appointed professor for inorganic chemistry at Ruhr University Bochum in 1996. In 2004, Matthias Driess moved to Technische Universität Berlin, where he heads the Chair of Inorganic Chemistry / Metalorganic Chemistry and Inorganic Materials at the Institute of Chemistry. He was spokesperson for the UniCat Cluster of Excellence from 2007 to2018. Since 2019, he has been co-spokesperson of the successor Cluster of Excellence Unifying systems in Catalysis, UniSysCat. Professor Driess was made a member of the German National Academy of Sciences Leopoldina in 2012 and has been an Ordinary Member of the Berlin-Brandenburg Academy of Sciences and Humanities BBAW since 2014. He has been a member of the European Academy of Sciences since 2020.

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Prof. Elena Fernandez-Gutierrez

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ROVIRA i VIRGILI

University of Rovira i Virgili, Tarragona, Spain

"Catalytic activation of organoboron compounds for strategic and selective construction of target compounds"

Biography: Elena Fernández received her degree in chemistry at the University of Barcelona in 1991. She did PhD studies in catalytic hydroformylation of sugars with Prof. S. Castillón and Prof. A. Ruiz (1991-1995) and she moved to Oxford University (UK) (1995-1997) for a postdoctoral position with Prof. John M. Brown where her studies culminated with an approach towards the first catalytic asymmetric hydroboration-amination reaction. Elena accepted in 1997 a lecturer position at the University Rovira i Virgili, becoming part of the permanent staff in 2000 and Full Professor in 2019. She received the Award on Excellence of Research in Organometallic Chemistry 2014 and the Award on Excellence of Research in Chemistry 2017, both from the Spanish Royal Society of Chemistry. She is Distinguished Professor at the URV from 2018. Her current scientific campaign is aimed to generate knowledge and awareness about activation modes of borane reagents to be used in selective organic synthesis of multifunctional compounds. She has contributed to several seminal articles, reviews and book's chapters, highlighting the edition of two books on Synthesis and Applications of Organoboron Compounds for Springer (2015) and Advances in Organoboron Chemistry toward Organic Synthesis for Science of Synthesis-Thieme (2019).

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Prof. Christian Hartinger

University of Auckland, Auckland, New Zealand

"Bioorganometallic Chemistry: Organometallic Drugs and Drug Candidates"

Biography: I received my PhD in Chemistry in 2001 under the supervision of Bernhard Keppler at the University of Vienna. After a period at the University of Vienna, I joined Paul Dyson's group at the EPFL in Switzerland in 2006 as a Schrödinger Fellow. I returned to Vienna in 2009 to finish my habilitation. In 2011, I accepted a position as Associate Professor at the University of Auckland and was promoted to Professor in 2016.

I have received national and international recognition with the Society of Biological Inorganic Chemistry Early Career Award 2016, the NZ Institute of Chemistry's premier award, the Maurice Wilkins Centre Prize for Chemical Science, in 2016, the NZAS Hill Tinsley Medal in 2017, the Morrison Medal of the Australian and New Zealand Society for Mass Spectrometry in 2019, and I was elected a Fellow of the Royal Society of New Zealand in 2021, among others.

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Prof. Sonja Herres-Pawlis

University of Aachen, Aachen, Germany

"Tailored catalyst design for the synthesis and the recycling of bioplastics"

Biography: Franc Meyer earned his Ph.D. with Peter Paetzold at RWTH Aachen (1993, boron chemistry) and was a postdoc with Peter Armentrout at the University of Utah (gas phase guided ion beam studies). On returning to Germany, he completed his Habilitation at the University of Heidelberg in 2000 and became Professor of Inorganic Chemistry at the University of Göttingen in 2001. He is a member of the Göttingen Academy of Sciences, the Royal Physiographic Society in Lund, and the German National Academy of Sciences Leopoldina. His group's research focuses on the activation of small molecules and on cooperative effects in bimetallic and multimetallic complexes, with particular interests in bioinorganic chemistry, bioinspired catalysis and magnetic nanoswitches.

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Prof. Cristina Nevado

University of Zurich, Zurich, Switzerland

"A journey towards mechanistic understanding in organometallic chemistry"

Biography: Cristina Nevado was born in Madrid, where she graduated in chemistry at the Autónoma University in 2000. In October 2004 she received her PhD from the same university working with Prof. Antonio M. Echavarren thereafter joining the group of Prof. Alois Fürstner at the Max-Planck-Institut für Kohlenforschung (Germany) as a post doctoral associate. In May 2007 she started her independent career as an Assistant Professor of Organic Chemistry at the University of Zürich. In 2011, Cristina was awarded the Chemical Society Reviews Emerging Investigator Award and the Thieme Chemistry Journal Award in recognition of her contributions in the field of synthetic organic chemistry. In 2012 she received an ERC Junior Investigator grant and in 2013 was awarded the Werner Prize of the Swiss Chemical Society and was directly promoted to Full Professor. In 2019, she received the Royal Society of Chemistry Award in Organometallic Chemistry and in 2020 the Excellence Research Trajectory Award of the Royal Spanish Chemical Society (RSEQ) as well as the Margaret Faul Women in Chemistry Award. Among her many contributing roles to the community, Cristina is currently Senior Associate Editor for ACS Central Science, Organic Syntheses and Science of Synthesis. Rooted in the wide area of organic chemistry, her research program is focused on complex chemical synthesis and new organometallic reactions.

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Prof. Luca Pignataro

University Of Milano, Milano, Italy

"Two strategies for exploiting base metals in homogeneous catalysis"

Biography: Luca Pignataro completed his PhD at the University of Milan with Prof. Franco Cozzi in 2006. After postdoc periods in the group of Prof. David Leigh (University of Edinburgh) and Prof. Cesare Gennari (University of Milan), he became Researcher (2012) and then Associate Professor (2019) at the University of Milan. His current research interests are in the fields of homogeneous catalysis (base metal catalysis, supramolecular catalysis, enantioselective catalysis, light-driven reactions), and targeted delivery of drugs (small molecule-drug conjugates for anti-tumor therapy).

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Prof. Christopher Teskey

Technical University of Braunschweig, Braunschweig, Germany

"Cobalt hydride catalysis under the spotlight"

Biography: Christopher J. Teskey carried out his undergraduate studies in Natural Sciences at the University of Cambridge and then, in 2012, began his PhD with Prof. Michael F. Greaney at the University of Manchester. After graduating in 2016, he was awarded an EPSRC Doctoral Prize Fellowship to stay at the University of Manchester for a further year. Following this, in 2017 he moved to the University of Vienna, Austria to take up a postdoctoral researcher position in the group of Prof. Nuno Maulide as a Lise Meitner Research Fellow of the FWF (Austrian Science Fund). From March 2019 to October 2023, he led a Junior Research Group at the Institute of Organic Chemistry at RWTH Aachen, Germany funded by a Liebig Fellowship from the Fonds der Chemischen Industrie. From November 2023, he has been a Professor of Organic Chemistry at the TU Braunschweig where he holds a Niedersachsen-Impuls-Professorship.

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Prof. Antonio Zanotti -Gerosa

Johnson-Matthey, United Kingdom

"Homogeneous hydrogenation catalysis in the fine chemicals industry: how to develop industrially viable and sustainable processes?"

Biography: Antonio Zanotti-Gerosa studied in Milano, Italy, completing his PhD in organometallic chemistry in 1994 (Prof. S. Maiorana). His academic experience includes secondments to Imperial College (Professor S.V.Ley), University of Bonn (Prof K.H. Doetz) and Nagoya University (Professor R. Noyori) and post-doctoral research at the University of Lausanne (Professor C. Floriani). Since 1997 he has been working on industrial applications of homogeneous catalysis. In 2003 he joined Johnson Matthey and, as R&D Director, he is now leading the JM chemocatalysis group in the Cambridge laboratories.

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PL 1, September 4, 15:30 - 16:20

Turning Boron Chemistry on its Head: The Unusual Reactivity of Boron in Low Oxidation States

Prof. Dr. Holger Braunschweig

Institute for Inorganic Chemistry, Institute for Sustainable Chemistry & Catalysis with Boron , Julius-Maximilians-University of Würzburg, Würzburg, Germany
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Boron is found in the earth's crust in its +3 oxidation state, and – despite over 200 years of research and development – every consumer application of boron is based on that same oxidation state. Tricoordinate boron(III) is usually electron deficient, strongly Lewis acidic, strongly electrophilic, and mildly oxidising, while all of these properties can essentially be neutralized without changing the oxidation state of the boron (i.e. by adding nucleophilic anions, Lewis bases etc.).

However, this paradigm is on the verge of changing. We and many other groups have long been working on developing the chemistry of boron in its lower oxidation states, from +2 to 0. In marked contrast to boron(III), low-oxidation-state boron compounds can be electron rich, Lewis basic, nucleophilic, and strongly reducing, but in some cases also highly ambiphilic (both Lewis basic and acidic at the same atom).

This lecture will take the audience on a trip through boron's history, from its early applications (e.g. borosilicate glasses, detergents, and enamels) to the properties of boron(III) compounds, to our work on low-oxidation-state boron molecules such as oxoboranes (B≡O), diborenes (B=B), diborynes (B≡B), borynes (B≡C) and borylenes (RB:).[1] The highly unusual and potentially useful reactivity of these species will also be highlighted, particularly the reactivity of metallomimetic boron "superambiphiles" with small molecules such as H_2, CO, alkynes, olefins and even N_2.[2]

[1] (a) H. Braunschweig, K. Radacki, A. Schneider, *Science* **2010**, *328*, 345; (b) H. Braunschweig, R. D. Dewhurst, K. Hammond, J. Mies, A. Vargas, K. Radacki, *Science* **2012**, *336*, 1420; (c) H. Braunschweig, A. Damme, R. D. Dewhurst, A. Vargas, *Nature Chem.* **2013**, *5*, 115; (d) H. Braunschweig, R. D. Dewhurst, F. Hupp, M. Nutz, K. Radacki, C. Tate, A. Vargas, Q. Ye, *Nature* **2015**, *522*, 327; (e) M. Michel, S. Kar, L. Endres, R. D. Dewhurst, B. Engels, H. Braunschweig, *Nature Synth.* **2025**, *4*, 869.

[2] (a) M.-A. Légaré, G. Bélanger-Chabot, R. D. Dewhurst, E. Welz, I. Krummenacher, B. Engels, H. Braunschweig, *Science* **2018**, *359*, 896; (b) M.-A. Légaré, M. Rang, G. Bélanger-Chabot, J. I. Schweizer, I. Krummenacher, R. Bertermann, M. Arrowsmith, M. C. Holthausen, H. Braunschweig, *Science* **2019**, *363*, 1329; (d) M.-A. Légaré, G. Bélanger-Chabot, M. Rang, R. D. Dewhurst, I. Krummenacher, R. Bertermann, H. Braunschweig, *Nature Chem.* **2020**, *12*, 1076.

PL 2, September 4, 17:10 - 18:30

A journey towards mechanistic understanding in organometallic chemistry

Prof. Dr. Cristina Nevado

University of Zurich, Zurich, Switzerland.

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PL 3, September 5, 9:00 - 10:20

Catalytic transformation of natural and synthetic waste into value-added chemicals

Prof. Dr. Paul J. Dyson[a]*

[a] Institut des sciences et ingénierie chimiques, École polytechnique fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland, CH-1015 Lausanne, Switzerland.

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Interest in the transformation of waste materials into valuable products has intensified in recent years with a slow, but steady transition towards a circular economy. We have worked on the development of catalysts that transform complex renewable (polymeric) feedstocks into bulk chemicals[1] or high-value chemical products.[2] In this lecture, I will describe the progression of our research from simple model compounds, through to purified and well-characterized biopolymers, i.e. cellulose and lignin, and eventually to heterogeneous biomass containing waste streams. More recently, we have turned our attention to the valorisation of waste synthetic polymers, including polyolefins,[3] polyamides,[4] polyurethanes (Figure 1)[5] and PVC,[6] and our studies in this area will also be highlighted.

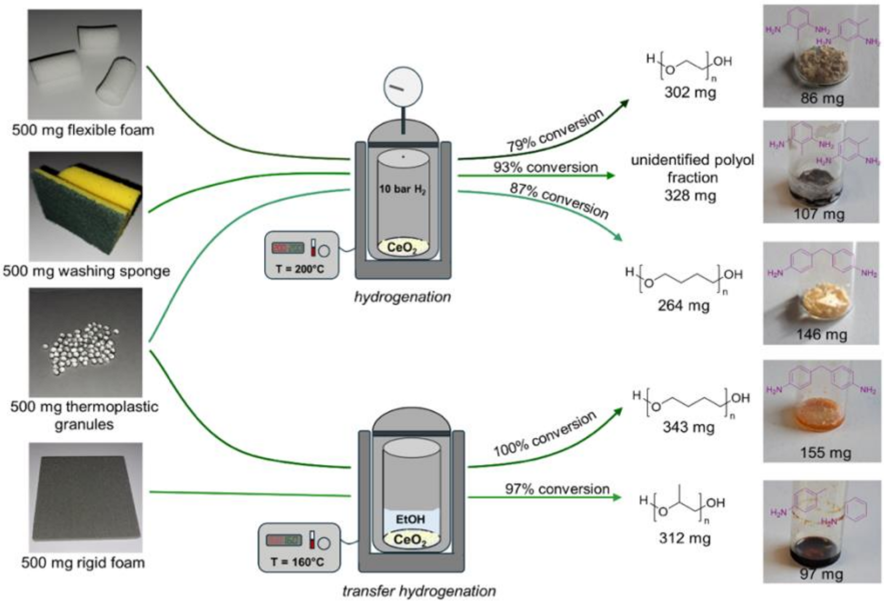

Figure 1. Conversion of commercial PU products using CeO_2 via both hydrogenation and transfer hydrogenation pathways.

[1] M. Liu, B. Han, P. J. Dyson, *Angew. Chem. Int. Ed*., **2022**, e202209093 (1 – 8).
[2] M. Liu, P. J. Dyson, *Nature Commun*., **2023**, *14*, 2830 (1 – 7).
[3] W.-T. Lee, A. van Muyden, F. D. Bobbink, M. D. Mensi, J. R. Carullo, P. J. Dyson, *Nature Commun*., **2022**, *13*, 4850 (1 – 13).
[4] X. Wu, W.-T. Lee, R. C. Turnell-Ritson, P. C. L. Delannoi, K.-H. Lin, P. J. Dyson, *Nature Commun*., **2023**, *14*, 6524 (1 – 11).
[5] X. Wu, R. C. Turnell-Ritson, P. Han, J.-C. Schmidt, L. Piveteau, N. Yan, P. J. Dyson, *Nature Commun*., **2025**, *16*, 4322 (1 – 10).
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PL 4, September 5, 10:40 - 12:00

Exploring Heavy Pnictogens: From Low-valent Compounds to Luminescence

Prof. Dr. Alessandro Bismuto[a]*

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The chemistry of light main group elements has been widely investigated with singular electronic and bonding motifs.[1] In contrast, heavy pnictogens are still underexplored.[2] Due to the large number of electrons available, the energy gap between their orbitals is considerably lower than that of lighter main-group elements. This allows them to span several oxidation states, mimicking transition metal reactivity. In addition, the ability of antimony and bismuth to expand its valence shell (hypervalency) can lead to materials with unusual electronic properties. Heavy pnictogens show thus high potential to merge the benefits of both main-group and transition metal properties to unveil new applications in several fields such as catalysis and optoelectronics (Figure 1).[3-4]

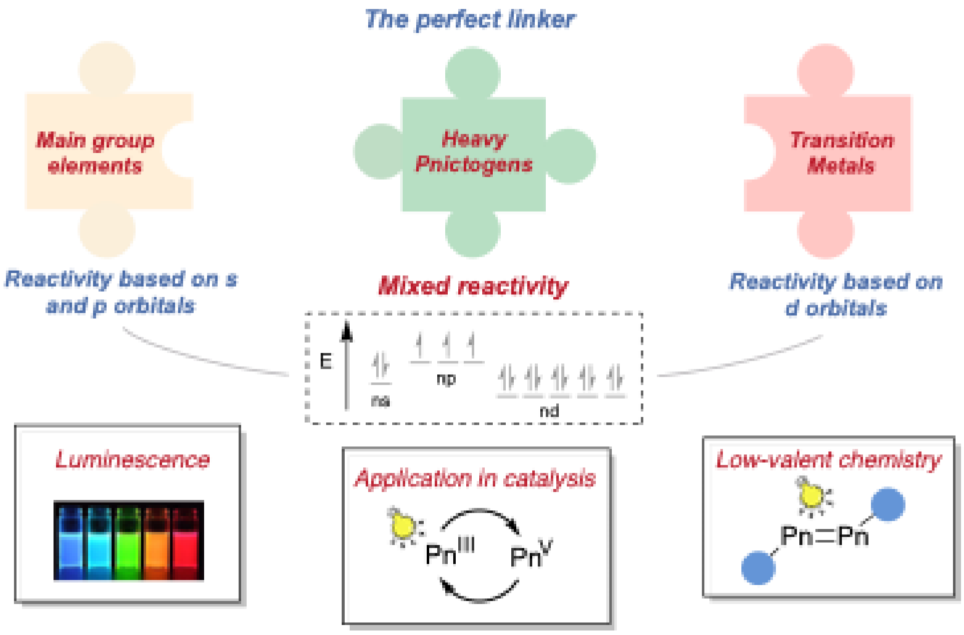

Figure 1. Heavy Pnictogen Chemistry.

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PL 5, September 5, 10:40 - 12:00

Organometallic Chemistry of Helicenes

Prof. Dr. Jeanne Crassous

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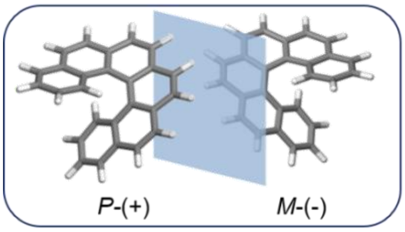
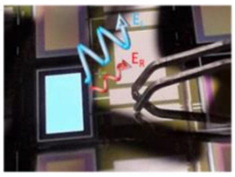
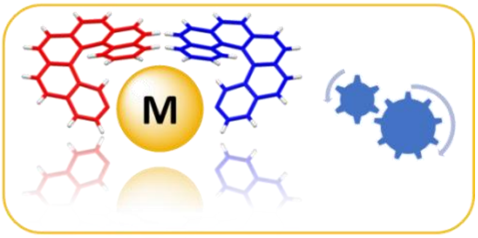
Ortho-fused aromatic rings form helically shaped chiral molecules such as carbo[6]helicenes, that wind in a left-handed (*M*) or a right-handed (*P*) sense.[1] The helical topology combined with extended pi-conjugation provide helicenes with peculiar properties such as strong photophysical and chiroptical properties (high optical rotation values, intense electronic circular dichroism and circularly polarized emission). The molecular engineering of helicenes using organometallic and heteroaromatic chemistries offers a convenient way to tune the properties of these helically shaped pi-ligands. Indeed, their combination with metallic or organic assembling units leads to chiral materials with appealing properties (circularly polarized phosphorescence, magnetochirality, spin selectivity) for applications in materials science (Circularly Polarized OLEDs, Chiroptical Switches, Spintronics). I will present a set of representative examples.[2,3]







[1] a) Dhbaibi, K.; Favereau, L.; Crassous, J. *Chem. Rev.* **2019**, *119*, 8846; b) Crassous, J.; Stará, I. G.; Starý, I. (Eds.). *Helicenes - Synthesis, Properties and Applications,* Wiley, **2022**.

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PL 6, September 5, 16:00 - 17:20

Tailored Catalyst Design for the Synthesis and the Recycling of Bioplastics

Prof. Dr. Sonja Herres-Pawlis [a*]

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*sonja.herres-pawlis@ac.rwth-aachen.de

Plastics are integral to modern life, but conventional petroleum-based materials have created severe environmental problems. Their persistence in nature threatens ecosystems worldwide. Completely abandoning plastics is unrealistic, so the focus is on sustainable alternatives and effective recycling strategies. A leading candidate is polylactide (PLA), a bioplastic derived from renewable resources such as corn or sugar beets. PLA combines the performance of common plastics with the benefit of biodegradability under microbial conditions. Its life cycle is nearly CO_2-neutral because the degradation products, CO_2 and water, are reused by plants. Industrially, PLA is made from lactide, the cyclic diester of lactic acid, through ring-opening polymerization (ROP). This method allows precise control over molecular weight and stereochemistry, making it superior to simple polycondensation. The standard industrial catalyst is stannous octanoate ($Sn(Oct_2)$), but its toxicity raises concerns: residual catalyst in PLA is released during biodegradation. To enable PLA's large-scale use, safe and efficient catalyst alternatives are needed.

For more than a decade, we have developed non-toxic catalysts based on earth-abundant metals such as iron and zinc. Central to their approach is the use of guanidine ligands, which strongly influence catalytic activity and polymerization control. Guanidines are versatile donors that can be tuned by incorporating additional functional groups, such as oxygen or nitrogen donors, leading to hybrid guanidines. The choice of ligand and counterion governs not only reactivity but also polymer properties like molar mass and microstructure. Through systematic design, we developed an iron hybrid guanidine complex with superior activity compared to $Sn(Oct_2)$. This breakthrough enabled the controlled synthesis of PLA as well as a variety of copolymers, expanding the potential applications of bioplastics. The iron complex is robust under industrial conditions, offering both safety and efficiency. Subsequently, zinc-based catalysts were introduced, including bisguanidine and hybrid guanidine variants. These catalysts match or exceed the performance of stannous octanoate while avoiding toxicity, representing promising candidates for future large-scale PLA production. The unique advantage of guanidine-based ligand systems is their modularity: by altering donor groups or electronic environments, catalytic properties can be finely tuned. This flexibility has led to a family of catalysts that balance high activity, selectivity, and environmental compatibility. For example, bisguanidine ligands create strong chelating environments around zinc centers, while hybrid guanidines introduce additional coordination points that allow fine adjustment of catalyst stability and polymerization control. Such designs demonstrate how fundamental coordination chemistry can drive innovation in sustainable polymer synthesis.

Beyond synthesis, these catalysts are also effective in chemical recycling. We have shown that PLA and other bio-based polyesters can be depolymerized via alcoholysis, producing lactates. These compounds serve either as valuable green solvents (e.g., ethyl lactate) or as intermediates that can be recycled back to lactide. Unlike mechanical recycling, which reduces material quality, this method allows true circularity without degradation of polymer properties. The development of guanidine-based iron and zinc catalysts provides both safe production methods for PLA and efficient chemical recycling pathways. This dual functionality represents a major step toward a circular plastics economy, where renewable resources, biodegradable materials, and sustainable catalysis work hand in hand.[1]

[1] https://www.bioac.ac.rwth-aachen.de/cms/bioac/forschung/forschungsfelder/~jtwj/lactidpolymerisation/?lidx=1

PL 7, September 6, 09:00 - 10:20

Two strategies for exploiting base metals in homogeneous catalysis

Prof. Dr. Luca Pignataro[a*]

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Replacing precious metals (PMs) with first-row transition metals (commonly referred to as 'base metals', BMs) represents a key objective in the pursuit of economically and environmentally sustainable catalytic processes. However, the use of BMs presents significant challenges due to their fundamentally different reactivity compared to noble metals, which still underpin the majority of current homogeneous catalytic methodologies. Whereas PMs typically operate through two-electron mechanistic pathways, BMs more readily engage in single-electron transfer processes, often involving radical intermediates. Additionally, low-valent BM complexes tend to be highly sensitive to air and moisture and are frequently difficult to characterize using standard spectroscopic techniques.

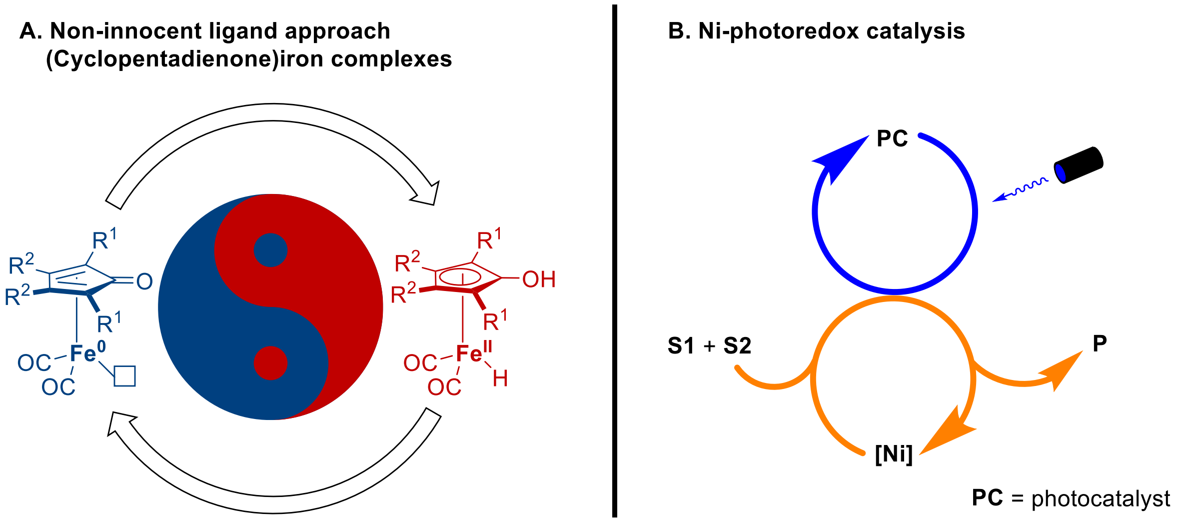

Figure 1

This lecture will explore the use of (i) non-innocent ligands and (ii) metallaphotoredox catalysis as strategies to harness the reactivity of BMs for valuable catalytic transformations, including hydrogen transfer and cross-coupling reactions. These two approaches will be illustrated through examples involving (cyclopentadienone)iron complexes (Figure 1 A)[1] and nickel-photoredox catalysis (Figure 1 B),[2] drawing on both literature precedents and original research from the speaker's group.

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PL 8, September 6, 10:40 - 12:00

Challenges in homogeneous catalysis in industry

Prof. Dr. Antonio Zanotti Gerosa

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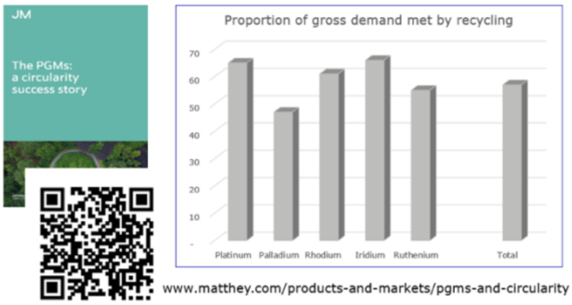
The development of efficient industrial processes using homogeneous catalysts must consider two fundamental parameters: cost and sustainability. To explain and exemplify this, two topics will be discussed:
The current and future availability and sustainability of Platinum Metal Group (PGMs) catalysts, including the carbon footprint of primary and secondary metal and the extent of metal recycling [1] (figure 2). This subject is relevant to the discussion about the replacement of PGM-based catalysts with Earth Abundant Metal (EAMs)-based catalysts.



www.matthey.com/products-and-markets/pgms-and-circularity

Figure 1

The application of asymmetric transfer hydrogenation in the synthesis of complex chiral alcohols and amines [2]. Despite being a thirty years old technology, it remains a workhorse in industry thanks to its wide scope and robustness. Both economics and sustainability much depend on the level of optimization of the process, as some simple carbon footprint models of the catalytic step can demonstrate (figure 2).

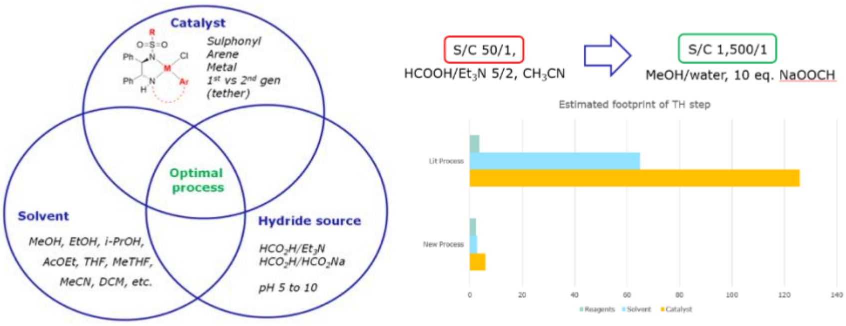


Figure 2

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PL 9, September 9, 14:40 - 16:00

Expanding the Chemical Space of Gold thanks to Ligand Design

Prof. Dr. Didier Bourissou
Laboratoire Hétérochimie Fondamentale et Appliquée (LHFA), CNRS/Université de Toulouse, 118 route de Narbonne, 31062 Toulouse cedex 9, France.
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The research activities in my group are focused on the design of bifunctional ligands for applications in organic and organometallic chemistry. We are particularly interested in new highly reactive species and new chemical transformations. Very fundamental in nature with thorough structural/bonding analyses and mechanistic investigations, our studies aim at developping (catalytic) reactions complementary to those currently known.

In this lecture, I will focus on gold chemistry, where ligand design proved to be extremely powerful and to open completely new chemical space (Figure 1). Special interest will be given to ligands triggering challenging transformations, Au(I)/Au(III) cycling in particular.[1] The stabilization and applications of « activated » and reactive gold complexes such as π-allyl[2] and carbene[3] complexes will also be presented.

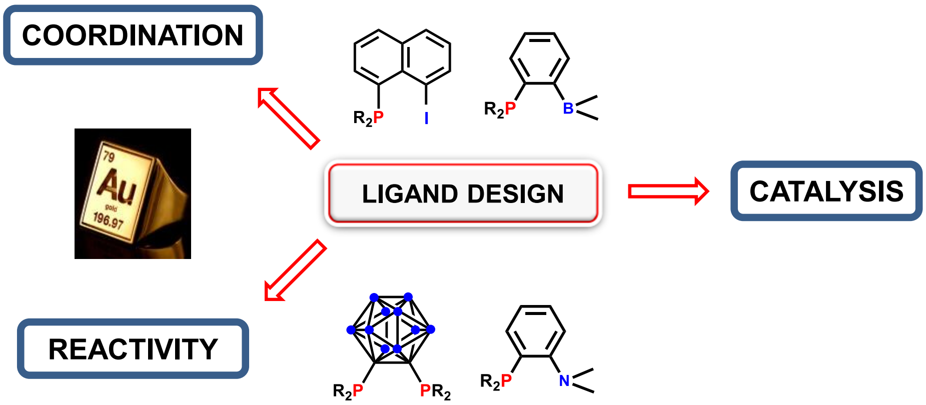

Figure 1

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[2] a) Rodriguez, J.; Szaloki, G.; Sosa Carrizo, E. D.; Saffon-Merceron, N.; Miqueu, K.; Bourissou, D. *Angew. Chem. Int. Ed.* **2020**, *59*, 1511; b) Rodriguez, J.; Holmsen, M.; García-Rodeja, Y.; Sosa Carrizo, E. D.; Lavedan, P.; Mallet-Ladeira, S.; Miqueu, K.; Bourissou, D. *J. Am. Chem. Soc.* **2021**, *143*, 11568; c) Rodriguez, J.; Vesseur, D., A.; Tabey, A.; García-Rodeja, Y.; Miqueu, K.; Bourissou, D. *ACS Catal.* **2022**, *12*, 993; d) Holmsen, M. S. M.; Vesseur, D.; García-Rodeja, Y.; Miqueu, K.; Bourissou, D. *Angew. Chem. Int. Ed.* **2023**, *62*, e202305280.

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PL 10, September 6, 16:00-17:20

Bioorganometallic Chemistry: Organometallic Drugs and Drug Candidates

Prof. Dr. Christian Hartinger

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Organometallic compounds are widely used in industry, mostly as catalysts or as reagents in organic synthesis. Beyond these roles, we can also find organometallics in nature and in the last decades they have found their way into the clinic. This has resulted in the coining of the term bioorganometallic chemistry by Gerard Jaouen in 1985.[1] In this lecture, I will provide an introduction in this interdisciplinary field. I will discuss examples of organometallic compounds in nature, followed by a summary of the development of organometallics with medical applications (Figure 1). A range of organometallic structural motifs will be covered before focusing on more recent studies with half-sandwich structures. I will discuss concepts we use in anticancer metallodrug design, as well as chemical biology and metallomics strategies to interrogate their modes of action, in particular their interactions with proteins.[2,3] These topics will be complemented by a discussion of the unexpected reactivity and behavior of organometallics in the presence of biomolecules.3,4 Such insights will provide us with a roadmap for the design of more specific anticancer metallodrugs and unlock previously untapped opportunities for developing novel therapeutics for a range of diseases.

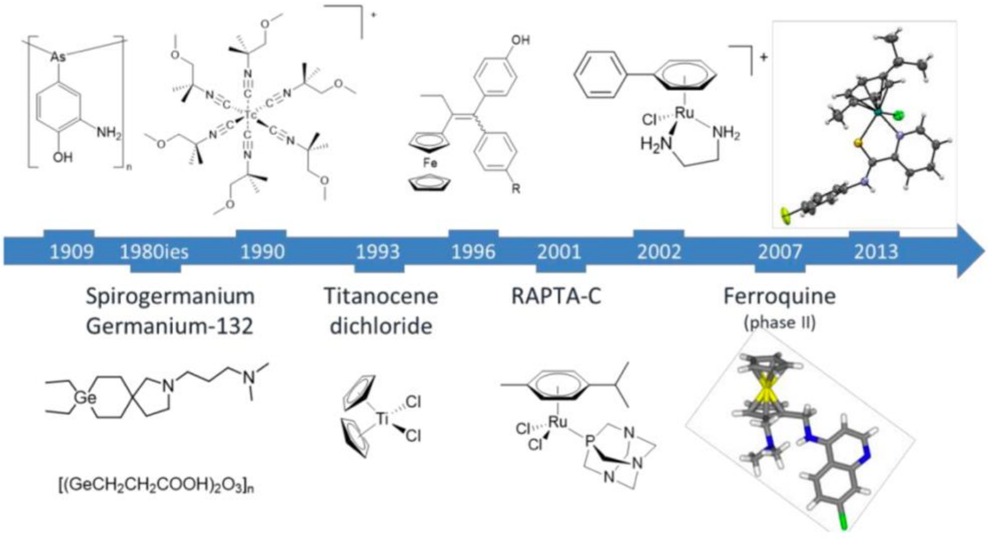

Figure 1

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[4] Lovett, J. H.; Lai, B. P.; Bloomfield, H. O.; Baker, A. T.; Sullivan, M. P.; Hartinger, C. G.; Harris, H. H. *Chem. Sci.*, **2025**, *16*, 11347.

PL 11, September 7, 09:00 – 10:40

Catalytic activation of organoboron compounds for strategic and selective construction of target compounds

Prof. Dr. Elena Fernández

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The progress of boron sources highlights their importance as pilars of organoboron chemistry, however the intrinsic ways to convert them into reactive species is not trivial. Experimental and theoretical studies have devoted deep efforts to generate new knowledge about activation modes of B-B and B-C-B reagents. The synthetic strategies covers transition-metal catalysis, as well as transition-metal-free approaches,[1,2] and in the case of *gem*-diborylalkanes the activation via deborylative or deprotonative pathways, gives access to very reactive α-boryl carbanions.[3,4] Strategic bond formation through homologation-functionalization tactics is presented, aimed to expand the divergent synthesis of complex molecules and drugs (Figure 1).[5,6]

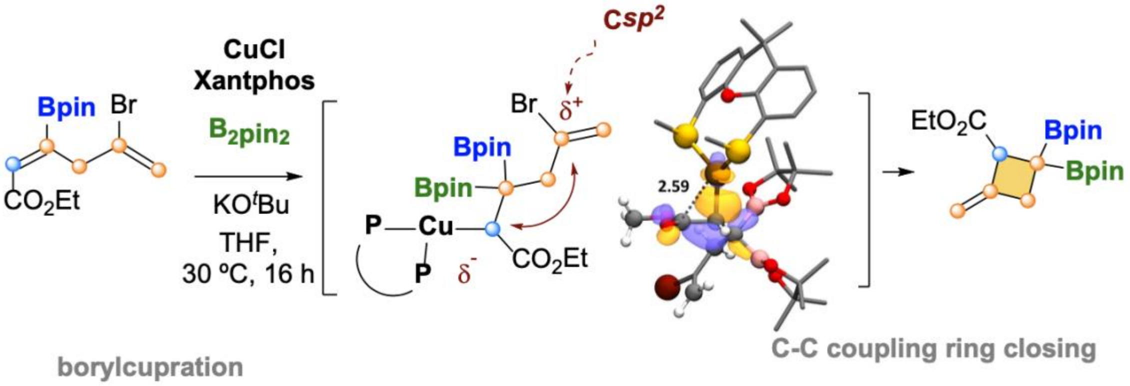

Figure 1

[1] Fernández, E. (ed) Advances in Organoboron Chemistry towards Organic Synthesis, Science of Synthesis, Thieme: Stuttgart, **2020**.
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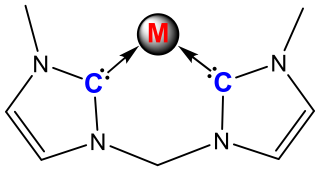
PL 12, September 7, 10:40 – 12:00

Cooperative Low-Valent Silicon Atoms in Small Molecule Activation

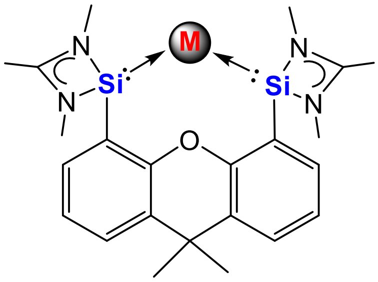
Prof. Dr. Matthias Driess

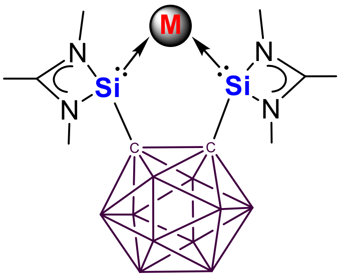
Technical University of Berlin, Department of Chemistry: Metalorganics and Inorganic Materials, Secr C2,
Strasse des 17. Juni 135, E-mail: Matthias.driess@tu-berlin.de

Replacement for noble metals by earth abundant non-metals is a longstanding challenge in small molecule activation and catalysis. In my talk I will address the research question how to tame a single subvalent silicon to serve as an active site in small molecule activation, homogeneous catalysis and stabilizing unusual low oxidation states of heavy main group metals. In fact, silicon, the second most abundant element of the earth crust, provides unexpected opportunities to mimic transition-metals in small molecule activation if it is in a low oxidation state (+2, +1 and 0). Notably, silylenes, the congener of carbenes bearing divalent silicon, show a precious metal-like reactivity and are competent in selective carbon-heteroatom bond activation of organic substrates and even pave the way to organosilicon triplet diradicals.[1] Over the last few years, we have demonstrated that the reactivity of silylenes can be significantly enhanced towards very stable small molecules such as carbon monoxide if two silylene moieties are placed in close proximity in the same molecular entity, giving rise to metal-free cooperative bond activation. Additionally, silylenes are much stronger donor ligands towards transition-metals than phosphines and carbenes that pave the way to more efficient chemoselective metal-mediated catalysis and stabilizing unusual oxidation states. [2-7] Some of these intriguing features of bis-silylenes will be discussed as well.



M = Main-group elements,
transition-metals





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PL 13, September 7, 14:40 – 16:00

Cobalt hydride catalysis under the spotlight

Prof. Dr. Christopher J. Teskey

Institute of Organic Chemistry, Technische Universität Braunschweig, Hagenring 30, 38106 Braunschweig, Germany.

*christopher.teskey@tu-braunschweig.de

Hydrofunctionalisation represents a powerful approach for transforming simple unsaturated substrates into complex three-dimensional molecules. Achieving this requires precise control of regiochemistry and chemoselectivity, which can be facilitated by metal hydride catalysis. This lecture will highlight how structurally distinct cobalt hydrides can promote hydrofunctionalisation with contrasting selectivities *via* divergent mechanistic pathways. Visible-light irradiation can be harnessed to modulate selectivity[1,2] and also unlock new modes of reactivity,[3-6] thereby expanding the synthetic toolbox of cobalt-catalysed organic transformations.

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Poster 1-FP

Photooxygenation of p xylene catalyzed by Fe(III) pyclen complexes: an insight into the magnetic and spectroscopical properties of the catalysts.

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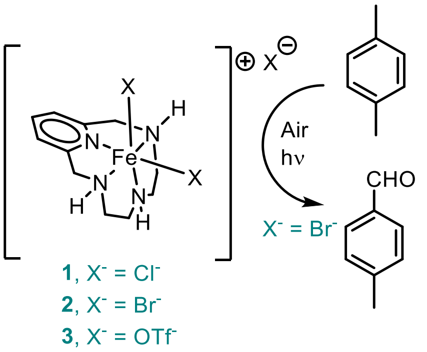
Iron complexes have long been studied in oxidative transformations as biomimetic models of enzyme active sites. In this context, while many examples of iron-mediated oxidation of organic compounds under thermal activation have been reported, the photochemical activation of iron complexes is a less explored field.[1] We report herein the synthesis and detailed characterization of a series of [Fe(III)(X_2)pyclen]X complexes (X = Cl, Br, OTf; pyclen = 3,6,9-triaza-1(2,6)-pyridinacyclodecaphane, complexes 1–3, Figure 1), relevant to the selective photocatalytic oxidation. Structural analysis, Mössbauer spectroscopy, magnetization studies, and UV-vis absorption spectroscopy combined with DFT calculations were employed to investigate their properties. Notably, the complexes display extended absorption into the visible range, attributed to ligand-to-metal charge transfer transitions involving the pyclen and halide/triflate ligands. Evidence suggests that light absorption can promote homolytic cleavage of the Fe–X bond, particularly for X = Cl and Br. Inspired by these findings, the photochemical behavior of the complexes under visible light irradiation (up to 415 nm) was explored for the aerobic oxidation of p-xylene. The nature of the halide ligand was found to influence the reactivity: the bromide complex (2) promoted the selective formation of p-tolualdehyde via a hydrogen atom transfer (HAT) mechanism, while the chloride (1) and triflate (3) analogs showed negligible activity. These results not only demonstrate the catalytic potential of photochemically activated iron complexes but also provide a foundation for future studies aimed at developing sustainable, light-driven oxidation processes.



1, $X^- = Cl^-$
2, $X^- = Br^-$
3, $X^- = OTf^-$

- ☐ Additive free
- ☐ White Light
- ☐ Under air
- ☐ Room temperature
- ☐ High selectivity

Figure 1

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Poster 2

Synthesis of Nylon 6,6 With Pyrene Chain-End for Compati-Bilization with Graphite and Improvement of Thermal and Mechanical Properties

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Nylon 6,6 (PA66) is valued for its mechanical strength, chemical resistance, and thermal stability. To enhance its performance in applications such as automotive and aerospace, it is commonly reinforced with graphite, which provides a high strength-to-weight ratio and excellent thermal conductivity[1–3]. However, poor adhesion between graphite and the PA66 matrix limits composite effectiveness. In order to tackle thisdrawbacks, in this work pyrene-functionalized PA66 (PA66py) was synthesized via interfacial polycondensation (Scheme 1)[4–6]. The pyrene end group promotes π–π stacking interactions with graphite, improving filler dispersion and matrix compatibility. Composites were prepared by ball milling, facilitating graphite exfoliation and uniform distribution. X-ray diffraction (XRD) showed a slight increase in graphite interlayer spacing (from 0.340 to 0.343 nm), indicating polymer intercalation. Thermogravimetric analysis (TGA) revealed enhanced thermal stability, while differential scanning calorimetry (DSC) showed increased crystallinity in PA66py composites, unlike standard PA66, which exhibited disrupted crystal structures. Atomic Force Microscopy (AFM) confirmed more uniform mechanical properties and better interfacial adhesion in PA66py composites, attributed to π–π interactions. Overall, pyrene functionalization significantly improves PA66–graphite compatibility, enhancing thermal, structural, and mechanical performance. This approach is promising for developing high-performance, lightweight composites and can be extended to other polymers and carbon fillers such as graphene and carbon nanotubes.

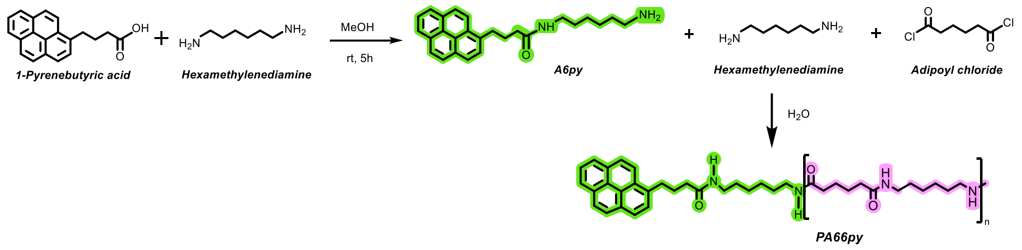

Figure 1: Synthesis of PA66py.

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Poster 3-FP

Direct Reduction of Atmospheric CO_2 by Copper Complexes

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Given our long-term dependence on carbon-based products and the need to reduce CO_2 emissions, it will be crucial to capture carbon in the form of dilute CO_2 from the atmosphere and transform it into useful molecules. However, the current technologies for the direct capture of CO_2 from the air (DAC) are being developed separately from those for CO_2 conversion.[1] Thereby, in order to create an integrated reactive CO_2 capture system and producing sustainable molecules with the highest frugality, we are developing molecular catalyst capable of converting this CO_2 in very dilute environments.

Our strategy is to directly reduce dilute CO_2 from the atmosphere trough a reaction of hydrosilylation, accelerated by the addition of a catalyst. In this reaction, the CO_2 can be selectively reduced at different oxidation states by using hydrosilane as reductant, due to their attractive thermodynamic and kinetic properties.[2] Previously described as highly active for this reaction, the [(dppbz)CuH] catalyst has been reproduced and studied in presence of different hydrosilanes.[3] While working with CO_2 gradually diluted in inert gas (100% → 5%), we have been able to achieve high and fast conversion of the CO_2 with a tunable selectivity at different levels of reduction. (**Figure 1**)

In future work, we will further study this reduction at even lower concentration of CO_2 (≈ 430 ppm) and in the presence of additional constraints, such as the oxygen.

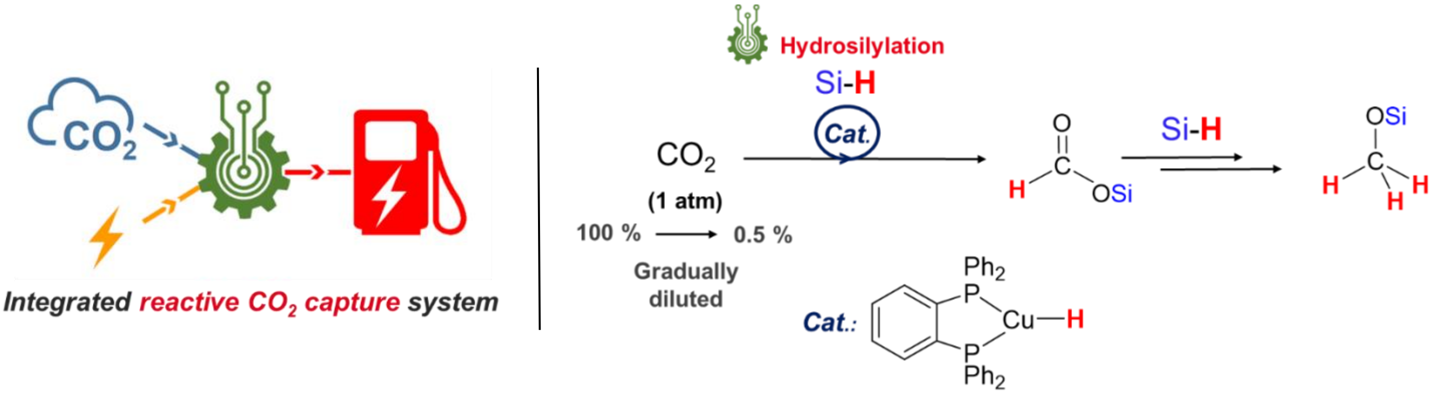

Figure 1: Direct reduction of CO_2 with hydrosilane catalyzed by [(dppbz)CuH].

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Poster 4

Improving the selective synthesis of 2,5-bishydroxymethylfuran: scale up and sustainable solutions

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The biorefinery approach aims to sustainably produce key chemical building blocks from biomass rather than relying on fossil-based resources. Due to the complex nature of biomass feedstocks, a wide variety of valuable chemicals can be obtained. Among these, 5-hydroxymethylfurfural (HMF) has emerged as a crucial platform molecule. One of its most valuable derivatives, 2,5-bis(hydroxymethyl)furan (BHMF), is gaining attention for its versatility in applications such as biodiesel additives, non-ionic surfactants, polymer precursors, and flavoring agents. The catalytic conversion of HMF to BHMF was successfully carried out under mild conditions using Shvo’s catalyst in a hydrogen atmosphere, yielding over 99% in both conversion and selectivity. Additionally, a new iron-based catalyst demonstrated rapid and complete HMF conversion within 20 minutes at moderate conditions (toluene, 90 °C, 5 bar H_2). Building upon these advancements, we have established a scalable and efficient process for producing BHMF, notable for its excellent catalyst recyclability and use of greener solvents like anisole.

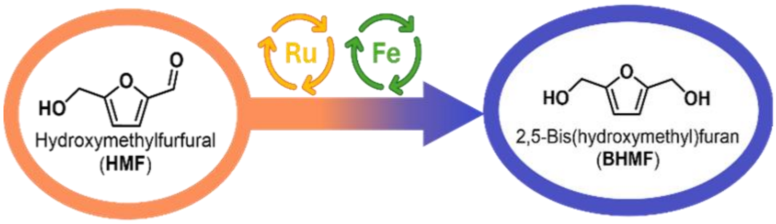

Figure 1: HMF conversion to BHMF

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Poster 5

Synthesis and Characterization of new Potential TADF Photocatalysts

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The use of organic dyes in photoredox catalysis represents one of the fields in which photocatalysis must still unfold its potential. In the last 10 years, thanks to the pioneering work of Zeitler[1] and Zhang,[2] donor-acceptor cyanoarenes have emerged as an asset for photoredox catalysis, due to their modular structure which allows the easy tuning of their photoredox properties. In a study on a Ni-catalytic, visible light-promoted C-N cross-coupling,[3] we found that one of the best performing photocatalyst, commercially available 3DPA2FBN, was also producing two by-products, identified by HPLC-MS analysis as deriving, respectively, from loss of one and two HF molecules.

In this work, we successfully isolated the two products (**1** and **2** in Figure 1) as new potential visible light-absorbing photocatalysts and managed to assess an optimized method to synthesize them. NMR and XRD studies showed that each of these products is obtained as a single regioisomer, whose structure was fully elucidated. The photophysical properties of **1** and **2** were determined by electrochemical and spectroscopic techniques. Their catalytic activity was preliminarily assessed in several types of reactivity.

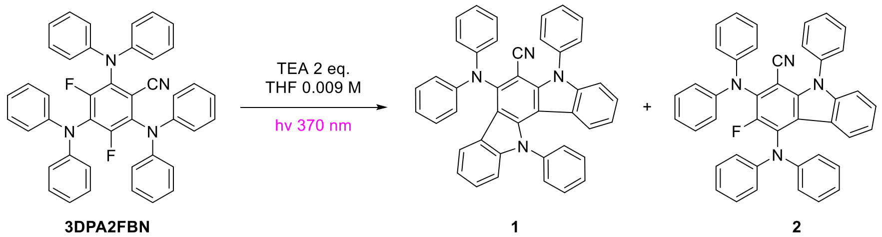

Figure 1. Synthesis of new potential TADF photocatalysts.

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Poster 6

Synthesis of Copper(II) β-Diketonate Complexes and their Catalytic Applications in Ullmann-Type Coupling Reactions

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Miriam Caviglia,[a] Maura Pellei,[a] Carlo Santini,[a] H. V. Rasika Dias,[b] Enrico Marcantoni,[a]
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The Ullmann reaction has attracted considerable interest due to its broad applicability in the formation of new aryl C–C and C–heteroatom bonds, including C–N, C–O, C–S, C–P, and C–Se.[1] Conventional Ullmann protocols typically employ copper catalysts, either in their commercially available forms or as newly synthesized complexes; however, these reactions often require harsh conditions to proceed efficiently. Consequently, there is ongoing interest in developing new copper-based catalytic systems that can operate under milder conditions. Among the various ligands investigated, β-diketones have gained considerable interest due to their strong chelating ability and their effectiveness in stabilizing metals in various oxidation states. In this study, we present the synthesis of a series of Cu(II) complexes supported by different β-diketonate ligands (Figure 1).

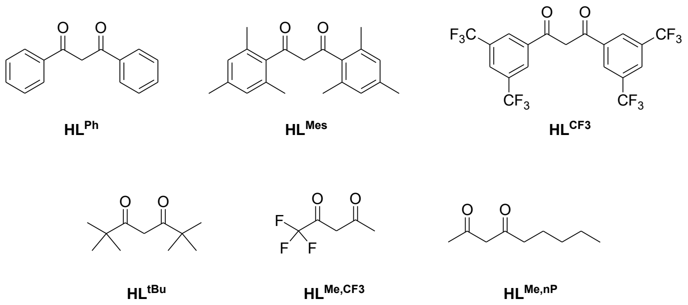

Figure 1. Molecular structures of β-diketone ligands.

All copper complexes were fully characterized in both solution and solid state and subsequently evaluated as catalysts in Ullmann-type C–O coupling reactions for the synthesis of diaryl ethers, using bromobenzene and 2-naphthol as starting materials. Various reaction conditions were explored, including variations in solvent, base, and reaction time. Additionally, microwave irradiation was employed to improve reaction efficiency. All copper(II) β-diketonate complexes exhibited good catalytic activity, with the complex bearing the L^{Ph} ligand emerging as the most effective, achieving a yield of 88%. In addition, various phenol and aryl bromide derivatives were tested using $[Cu(L^{Ph})_2]$ as the catalyst, resulting in moderate to good yields.[2]

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Acknowledgements: Unione Europea – NextGenerationEU (NGEU PNRR, D.M. n. 630/2024 M4C2 I3.3)

Poster 7

Monocarbonyl Ruthenium Catalysts for Aldehyde and Ketone Reduction in Water

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Water represents the ideal solvent, as it is non-toxic, non-flammable, inexpensive, and abundant, contrary to most organic solvents employed in homogeneous catalytic processes, which pose significant environmental, health, and safety concerns. Since the introduction of water-soluble phosphines in the 70's as ligands, water attracted a great deal of interest and begun to be studied for many important catalytic reactions, such as hydrogenation (HY) and transfer hydrogenation (TH), mainly mediated by Rh(III), Ir(III), and Ru(II) catalysts.[1-3] Monocarbonyl diphosphine ruthenium(II) catalysts have proven to be efficient in the reduction of aldehydes and ketones in both HY and TH reactions in ethanol and 2-propanol, respectively.[4] Herein, we present a study of the catalytic activity in water or water-modified media (e.g., H_2O/2-propanol) of [Ru(OAc)(CO)(NN)(PP)]OAc (NN=ampy, en; PP=dppe, dppb) complexes in HY, as well as in TH using formate and formic acid as hydrogen sources (Figure 1).

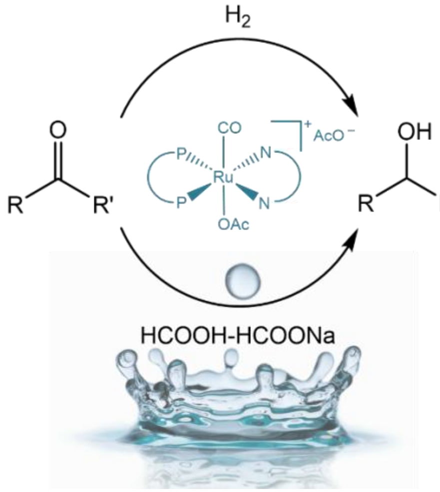

Figure 1

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Poster 8-FP

Highly Active and Recyclable Rhenium Catalysts: A New Heterogeneous Platform for Polyol Deoxydehydration

M. E. Casacchia,[a*] A. Di Giuseppe,[a] M. Crucianelli,[a] N. d'Alessandro,[b] L. Tonucci,[b] A. Mascitti,[b] E. Rombi,[c] M.G. Cutrufello,[c] F. J. Platero,[c] A. Ruggiu,[c] S. Piccinin,[d] C. F. Pauletti [d,e]

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[b] Department of Engineering and Geology, University of Chieti-Pescara, Viale Pindaro, 42, Pescara, Italy.
[c] Dipartimento di Scienze chimiche e geologiche, Università di Cagliari, Monserrato (CA), Italy. [d] CNR-IOM Trieste, Basovizza (TS), Italy. [e] Department of Physics, University of Trieste, Via Alfonso Valerio, 2, Trieste, Italy.
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The transition from petrochemical-based resources to renewable biomass is a key objective in sustainable chemical production. Biomass-derived polyols are promising feedstocks for light olefins, essential intermediates in the polymer and fuel industries. However, their selective deoxygenation remains challenging due to the hydrophilicity of polyols, the reliance of deoxydehydration (DODH) reactions on expensive rhenium-based catalysts, and the harsh reaction conditions typically required. [1–3] This research, arising from a national research project (PRIN) collaboration, focuses on the design of cost-effective, environmentally benign, and industrially scalable heterogeneous rhenium-based catalysts for DODH. Rhenium was supported on a range of metal oxides—including SiO_2, Nb_2O_5, CeO_2, ZrO_2, and mixed oxides such as SiO_2–Nb_2O_5 and CeO_2–ZrO_2—prepared via soft-template (ST), hydrothermal (HT), and alcoholthermal (AT) methods. Extensive catalytic screening using diethyl tartrate as a model substrate enabled the identification of the most efficient materials. Through systematic optimization of temperature, reaction time, and solvent choice, the Re/SiO_2–Nb_2O_5 ST catalyst emerged as the most active and robust system, delivering high yields under significantly milder conditions (130–170 °C). The optimized protocol also ensured excellent recyclability across multiple cycles and proved effective with structurally diverse diol substrates. These findings underscore the critical role of support composition and synthesis methodology in tuning catalytic performance. Overall, this work delivers a practical and scalable DODH protocol, offering a valuable step forward in the catalytic conversion of renewable feedstocks into high-value-added chemicals within a circular economy framework.

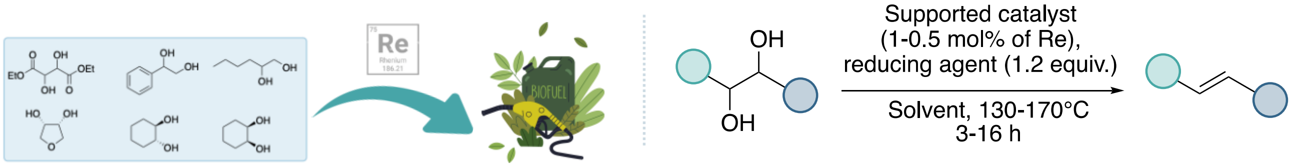

Figure 1: General description of the project

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Poster 9-FP

Iron-Based Eutectic Mixtures in Organic Synthesis: Recent Progress and Future Directions

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Over the past decade, a variety of acidic deep eutectic solvents have emerged as effective and sustainable alternatives to volatile organic compounds (VOCs) in several organic transformations.[1] Within this framework, Lewis acidic deep eutectic solvents (LADESs) based on iron salts are particularly attractive, as iron is an earth-abundant, low toxicity transition metal with excellent redox properties.[2] In this communication, we present several applications of iron-based DESs, including: *a*) the Meyer-Schuster rearrangement of propargylic alcohols at room temperature and under aerobic conditions (Figure 1a);[3] *b*) the oxidation of secondary alcohols (Figure 1b);[4] and *c*) the synthesis of amides and arylsulfonamide derivatives (Figure 1c).[4] Notably, we recently demonstrated the efficacy of a $FeCl_3 \cdot 6H_2O$/glycerol eutectic mixture (3:1 mol/mol) as a highly effective medium for the Ritter reaction of aliphatic and aromatic secondary and tertiary alcohols with both aliphatic and aromatic nitriles. The protocol is operationally simple, scalable, and generally proceeds at 40 °C within 4 h, affording the corresponding amides in yields of up to 98% through straightforward crystallization (Figure 1d). The eutectic mixture can be effectively reused for up to eight consecutive cycles. The robustness and sustainability of the method were further demonstrated through the multigram-scale synthesis of the drug Chlodantane under these conditions (Figure 1d).

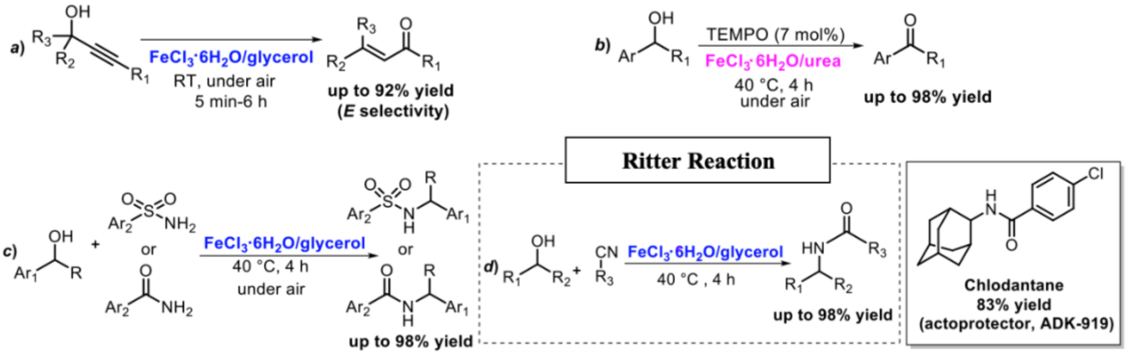

Figure 1. Representative examples highlighting the efficacy of the $FeCl_3 \cdot 6H_2O$-based eutectic mixture as a sustainable reaction medium in organic transformations (a–d).

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Poster 10

New findings on [$Fe_2Cp_2(CO)_4$] toward the development of potential electrocatalysts for H_2 production

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The sustainable generation of molecular hydrogen (H_2) plays a fundamental role in achieving a carbon-neutral economy, and the electrochemical H_2 generation represents an efficient strategy for storing renewable energy.[1] Although platinum remains the benchmark catalyst, its rarity and high cost have driven the search for earth-abundant alternatives.[2] Nature's [FeFe]-hydrogenases (Figure 1A), found in anaerobic microorganisms, efficiently catalyze H_2 formation[3] and have inspired the development of synthetic mimics.[4]

A promising starting material is [$Fe_2Cp_2(CO)_4$] (**Fp_2**, Cp = η^5-C_5H_5), a commercially available and cost-effective compound. Recently, the **Fp_2**-derived complex [$Fe_2Cp_2(CN)(CO)_2(\mu$-$CNMe_2)$] (**FeCN**) has demonstrated catalytic activity for H_2 evolution starting from acetic acid in acetonitrile,[5] encouraging further screening of related complexes. With a view to air-stable and sufficiently water-soluble catalysts, various cationic complexes bearing a bridging thiocarbyne ligand have been developed (Figure 1C).[6]

In this work, recent findings on both known and newly synthesized complexes based on the Fe_2Cp_2 core will be discussed in the context of theoretical investigations and spectroelectrochemical studies.

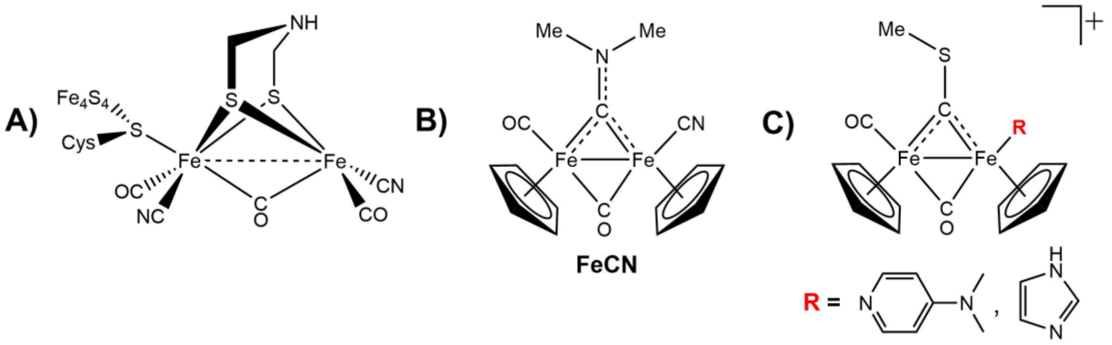

Figure 1: Structures of the active site of [FeFe]-Hydrogenase (A), diiron aminocarbyne cyanide complex (B), electrocatalytically-active cationic thiocarbyne complexes (C).

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Poster 11

Tri- and Di-Nuclear Palladium Complexes Stabilized by Bridging η^2-C=N Coordination of Ar-Bian Ligands

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Ar-BIAN (bis(arylimino)acenaphthene) Schiff bases are well-known ligands for both transition and main group metals due to their rigid structure, which ensures optimal geometry for chelation and enhances compound stability against hydrolysis and central C–C bond cleavage. In the absence of other ligands, the treatment of the $Pd_2(dba)_3$ with Ar-BIAN type ligands results in the unprecedent isolation of a trinuclear palladium complex which represents the first example of a structurally characterized Pd(0) compound stabilized solely by nitrogen ligands. X-ray crystallography reveals that each palladium atom is coordinated in a standard κ^2-*N,N* chelating mode to an Ar-BIAN ligand and in an η^2 coordination to the C=N double bond of a neighboring Ar-BIAN ligand. This unique bonding motif links three Pd(Ar-BIAN) units into a cyclic trimeric structure (Figure1, left).

Additionally, a mixed-valence dinuclear Pd complex was isolated, featuring a $[Pd(Ar\text{-}BIAN)]^0$ fragment bridged to a $[Pd^{II}(Ar\text{-}BIAN)X_2]$ unit via a similar η^2 coordination of the iminic bond (Figure1, right).

These findings highlight an unusual mode of palladium stabilization via η^2(C=N) bridging in both trimeric and dinuclear complexes supported exclusively by Ar-BIAN ligands.

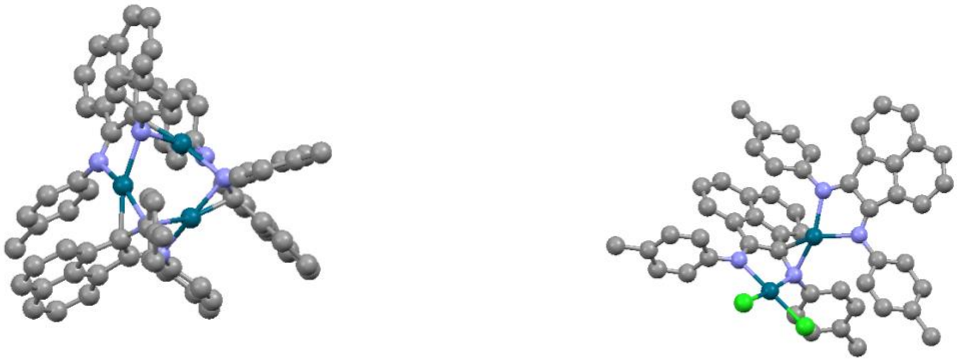

***Figure 1**: X-ray structure of $[Pd(Tol\text{-}BIAN)]_3$ (left) and $[Pd(Tol\text{-}BIAN)]_2Cl_2$ (right)*

Overall, the trinuclear complex has a propeller shape, with the six aryl rings divided into two inequivalent groups. Other complexes have also been obtained showing unusual structures and their synthesis will be described.

Poster 12-FP

Copper(I) phosphane complexes with boron-phenylated poly(3-(CF_3)pyrazolyl)- and poly(6-(CF_3)-2-pyridyl)-borates: structural and antiproliferative insights

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Scorpionate-type ligands, especially poly(pyrazolyl)borates, have enabled significant advances in metal complex design by offering tunable steric and electronic properties.[1,2] Recently, their poly(2-pyridyl)borate analogues have emerged as robust, highly donating scaffolds with different steric profiles, owing to their B-C linkages and six-membered donor rings.[3] Fluorinated variants are particularly attractive for applications in catalysis and medicinal chemistry, where CF_3 groups can enhance both stability and biological activity.[4] In this study, we report the synthesis and full characterization of a series of copper(I) phosphane complexes supported by B-phenylated ligands bearing CF_3-substituted pyrazolyl or pyridyl arms. By varying the number of phenyl substituents on boron, we modulated the steric and electronic environment around the metal center. Notably, mono-substituted analogues featuring mono(pyrazolyl)- and mono(pyridyl)-borate ligands exhibit unusual coordination behavior. Despite containing only a single N-donor, both complexes adopt a pseudo-κ^2 coordination mode via an interaction between the copper(I) center and the ipso carbon of a phenyl ring on the borate ligand. As a result, the copper centers display an essentially trigonal planar geometry, rather than the linear arrangement utilizing only the donor nitrogen site of the scorpionate (Figure 1). Preliminary biological studies against human cancer cell lines revealed promising antiproliferative activity for selected complexes.

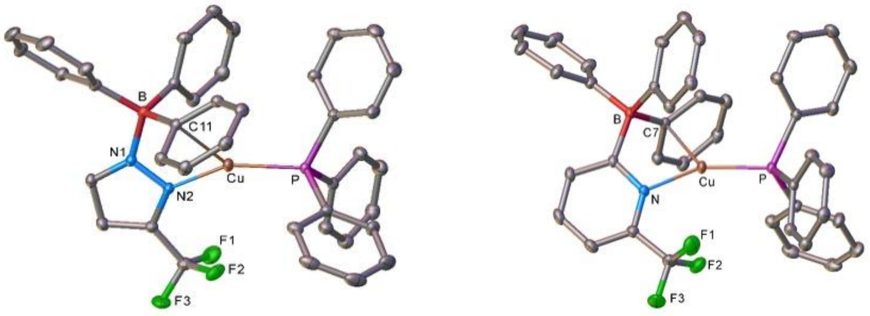

Figure 1. Crystal structure of $[Ph_3B(3\text{-}(CF_3)Pz)]Cu(PPh_3)$ (left) and $[Ph_3B(6\text{-}(CF_3)Py)]Cu(PPh_3)$ (right).

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Poster 13

Autoinductive Effects in Zinc-Catalyzed Alkylation of Benzaldehyde Mediated by Simple Chiral *β*-Amino Alcohol Ligands

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The design of chiral catalysts presents a fundamental challenge due to the intrinsic complexity of catalytic systems, which often limits the effectiveness of approaches solely based on mechanistic and structural principles. Consequently, the development of asymmetric reactions commonly begins with an empirical exploration of well-known privileged chiral structures, assuming that the active catalytic species exists as a monomer. However, since Kagan's 1986 identification of catalyst aggregation and "Non-Linear Effects" (NLEs),[1] it has been shown that chiral structure alone is not always predictive of the system's overall behavior, adding further intricacies to the mechanistic interpretation of asymmetric catalysis.[2,3]

In our study, we investigated in detail the mechanism of the enantioselective diethylzinc addition of benzaldehyde in the presence of the first chiral β-amino alcohol ligands (Figure 1) that had been used for this reaction, published in 1984 by Oguni and co-workers.[4] Our work was achieved through a combination of non-linear effect studies and other related studies such as the variation of the catalyst loading. It has been demonstrated that these catalytic systems are in fact considerably more complex than was previously assumed. In particular, the self-induction phenomena in the reaction demonstrate that the reaction generates higher enantiomeric excesses with a lower catalyst loading and overall, these enantioselective reactions are part of Systems Chemistry.[5]

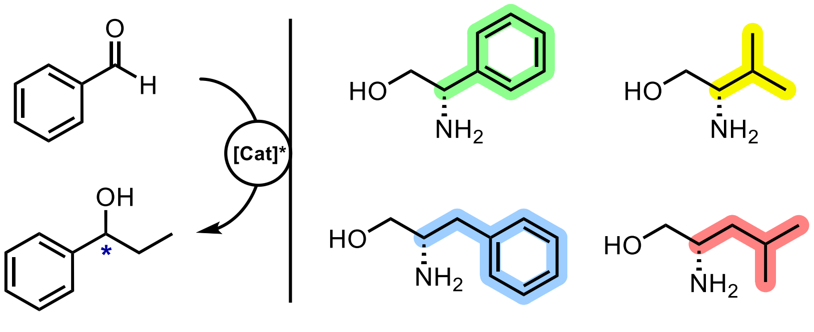

Figure 1. General scheme of the catalytic reaction and molecular structure of the chiral ligands used.

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Poster 14

SABRE of [1-^{13}C]Pyruvate: Ligand design for better hyperpolarization and catalyst separation

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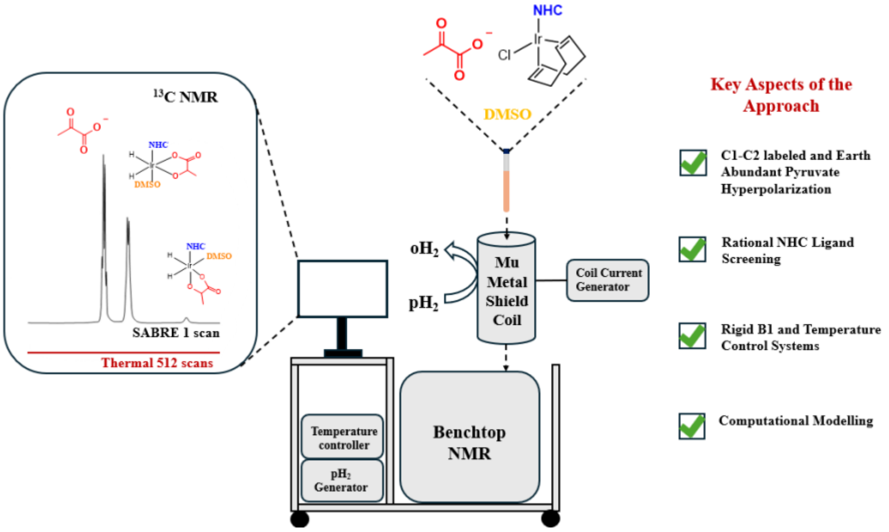
SABRE (Signal Amplification By Reversible Exchange) enhances NMR sensitivity by transferring polarization from parahydrogen to target molecules via their reversible coordination to an iridium catalyst. Among all the candidate molecules, [1-^{13}C]pyruvate stands out as a key probe for metabolic imaging, enabling real-time monitoring of cellular metabolism.

We present a systematic investigation of SABRE hyperpolarization of [1-^{13}C]pyruvate-h$_3$ using a series of Ir–NHC catalysts. In addition to the benchmark IMes ligand,[1,2] we explore sterically and electronically diverse ligands. Furthermore, we introduce novel fluorinated NHCs bearing mono- and difluorinated alkyl chains, designed to preserve hyperpolarization efficiency while enabling more effective post-polarization catalyst removal. Carbon polarization levels exceeding 3% are achieved using 50% parahydrogen, corresponding to over 10% under full enrichment. Experimental results indicate that polarization efficiency is primarily governed by exchange kinetics rather than spin–spin couplings. This observation is corroborated by a reduced-dimension Liouville-space kinetic model, which accurately reproduces the experimental temperature dependence.



Key Aspects of the Approach

- ☑ C1-C2 labeled and Earth Abundant Pyruvate Hyperpolarization
- ☑ Rational NHC Ligand Screening
- ☑ Rigid B1 and Temperature Control Systems
- ☑ Computational Modelling

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Poster 15-FP

Synthesis of Organobismuth(III) Bis(arylselenolates) from Bismuth(I) Precursors: Toward Luminescent Main-Group Compounds

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Luminescent compounds, especially phosphorescent ones, are of great interest due to their various applications. Transition metal complexes with strong spin–orbit coupling (SOC), such as those of platinum, iridium, and gold, have shown promising luminescent properties but suffer from high cost and low abundance. Bismuth, by contrast, is earth-abundant, low in toxicity, and possesses the highest SOC among non-radioactive elements, yet its luminescent complexes often display only weak, ligand-centered emission. Starting from this background and from recent studies reporting some phosphorescent organobismuth(III) bis(arylthiolates)[1] we decided to synthesize some novel organobismuth(III) bis(arylselenolates) trought the oxidative addition of diselenides to organobismuth(I) species generated *in situ* (Figure 1), and to test their optical properties.

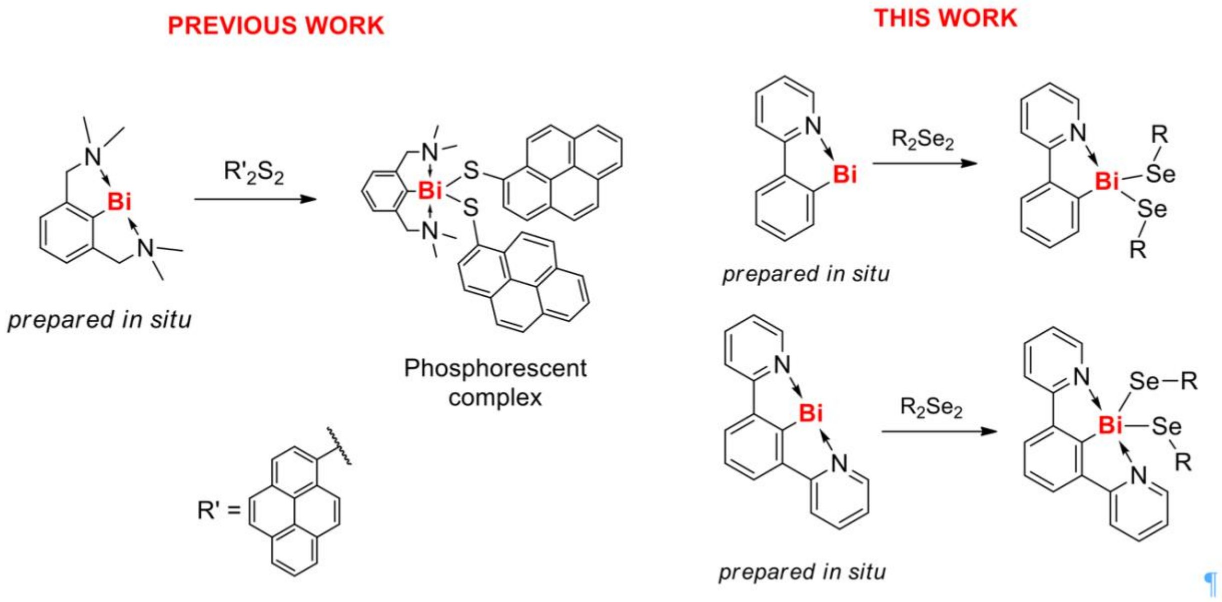

Figure 1

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Poster 16-FP

Comprehensive investigation of a highly reduced Fe_6C carbonyl cluster: a pathway towards nitrogenase cofactor modeling

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A renewed interest in Iron carbide carbonyl clusters was boosted by the recent discovery of the presence of a Fe carbide cluster within the active site of the Fe-Mo cofactor of the enzyme nitrogenase.[1] We conducted a comprehensive investigation of the redox chemistry and reactivity of the highly reduced cluster $[Fe_6C(CO)_{15}]^{4-}$.[2] IR-SEC analysis and DFT calculations enabled us to unravel the nature of the intermediates involved and the mechanism of its substitution reaction.[3] The aim was to discover the experimental conditions for the functionalization of the $\{Fe_6C\}$ cage without fragmentation, possibly through a broad-scope and robust reaction. Exploring $[Fe_6C(CO)_{15}]^{4-}$ oxidative reactivity, particularly in the presence of organo-sulphur compounds, we successfully obtained CO substitution to yield novel tri-anionic clusters of general formula $[Fe_6C(CO)_{14}(SR)]^{3-}$. L-Cysteine, the protein fragment bound to the natural enzyme active site, was introduced as ligand, enabling the synthesis of a chiral $\{Fe_6C\}$ cage cluster, which can act as possible model compound for the Fe-Mo cofactor. The chiral behaviour was confirmed by both experimental and simulated VCD analysis, which also revealed an unprecedented case of ligand-to-cluster chirality transfer.

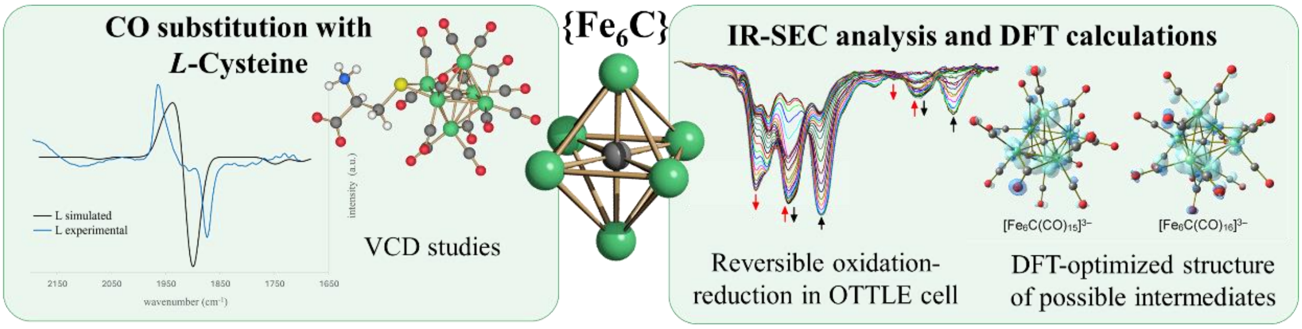

Figure 1. Computational and electro-spectrochemical studies of $[Fe_6C(CO)_{15}]^{4-}$.

Acknowledgements: Funding by C_3, Center for Chemical Catalysis, is heartily acknowledged.

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Poster 17

Polymerization of 1-vinylcyclohexene (VCH) and (*S*)-4-isopropenyl-1-vinyl-1-cyclohexene (IVC) and its copolymerization with linear terpenes mediated by titanium complexes with [OSSO]-type ligands

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The production of plastics from renewable resources to reduce reliance on fossil fuels is particularly appealing.[1] Among natural substances, terpenes include a wide family of compounds characterized by a common isoprenoid unit, and their structural variety contributes to their potential as monomers.[2] This study investigates the versatility of two titanium complexes with [OSSO]-type ligands (catalysts **1-2**), activated by methylalumoxane (MAO), in the polymerization of the 1-vinylcyclohexene (VCH), chosen as a model monomer. Complex **2**, characterized by cumyl substituents, provided a regio- and stereo-regular homopolymer. Furthermore, the stereoselective polymerization was extended to the (*S*)-4-isopropenyl-1-vinyl-1-cyclohexene (IVC),[3] a bio-based monomer synthetized from the perillaldehyde,[4] that differs from the VCH only for the presence of an additional isopropenyl group. Finally, the copolymerization of IVC with two linear terpenes, β-myrcene and β-ocimene, was accomplished, obtaining notable copolymers from sustainable sources.

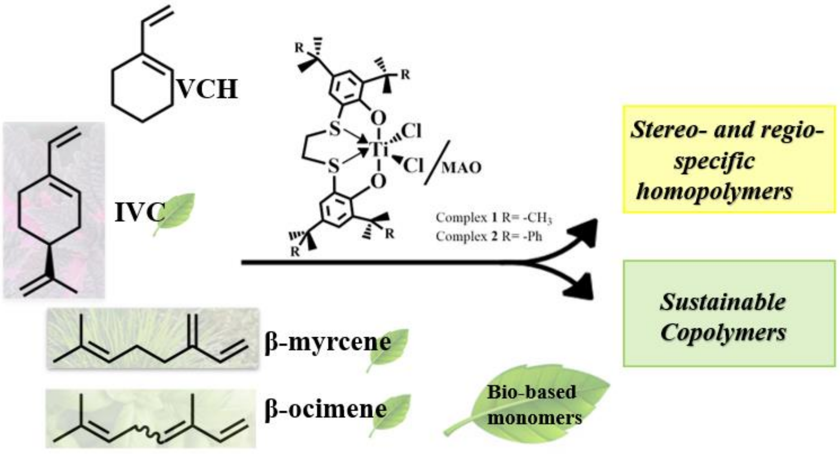

Figure 1. (Co)polymerization of conjugated dienes promoted by [OSSO]-type catalysts.

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Poster 18

Bifunctional nickel-photoredox catalysts for C-O cross coupling reactions

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Our research group recently reported a bifunctional approach to Ni-photoredox catalytic C-O cross-coupling. Connecting a donor-acceptor cyanoarene photocatalyst to a bipyridine ligand leads to photocatalysts **1a-b** (Figure 1), featuring an improved catalytic activity compared to the corresponding dual systems, as a crucial step of the catalytic cycle is turned from intermolecular to intramolecular.[1]

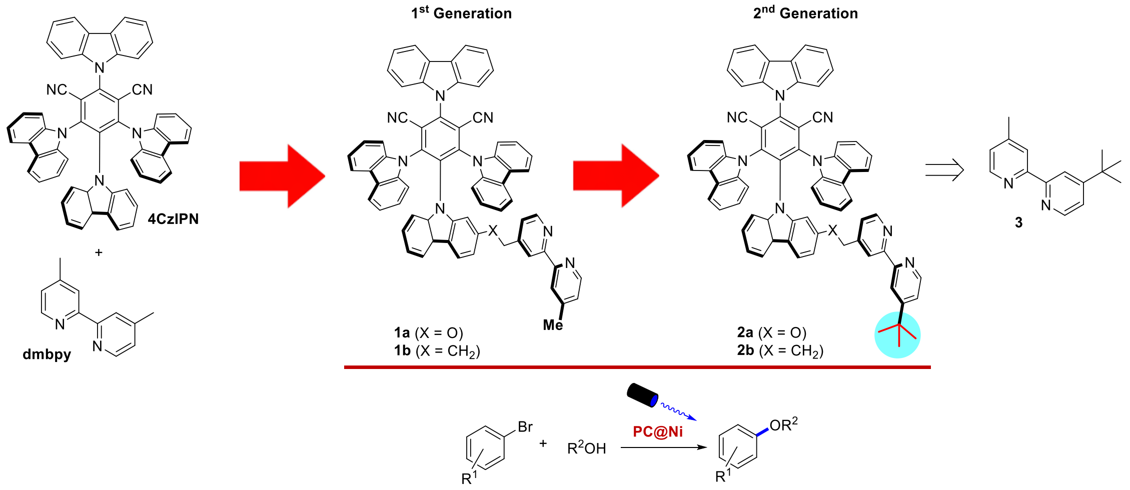

Figure 1. First- and second-generation bifunctional photocatalysts for C-O cross-coupling reactions.

In the dual catalytic system, 4,4'-bis-*tert*-butyl bipyridine is the ligand giving the best results (in combination with 4CzIPN), and for this reason we decided to introduce a *tert*-butyl substituent on the bipy moiety of our bifunctional system, expecting a beneficial effect on catalytic activity. The synthesis of the 2nd generation bifunctional photocatalysts **2a-b** involved 4-*tert*-butyl-4'-methyl-2,2'-bipyridine (**3**) as key intermediate – a previously unreported compound whose preparation turned out to be challenging. Several attempts to forge the pyridine-pyridine bond by cross-coupling were made, but bipyridine **3** was obtained in very low yield at best. For this reason, we opted for a different approach consisting in the construction of one of the pyridine ring according to the methodology reported by Ciufolini and co-workers.[2] Preliminary tests in Ni-photoredox C-O cross-coupling at low catalyst loading confirm that the second-generation systems **2a-b** display the expected improvement in terms of activity.

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Poster 19-FP

Synthesis of Pd(II) complexes via Mechanochemistry Route

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Mechanochemistry, which involves chemical reactions driven by mechanical forces,[1] is aligned with green chemistry. Organometallic mechanochemistry remains relatively unexplored, and only recently key organometallic complexes have been synthesized via this method.[2] Despite the widespread use of Pd(II) complexes in catalysis[3,4] and medicinal chemistry,[5] their mechanochemical synthesis and application have received limited attention.

In this study, the focus was on the synthesis of Pd(II) complexes via mechanochemistry from commercial halogenated and halogen-like Pd(II) precursors and commercial ligands. The synthesized complexes have the following structures: $[Pd(COD)X_2]$ with 1,5-cyclooctadiene; $[Pd(N\frown N)X_2]$ and $[Pd(N\frown N'\frown N)X]X$ with bidentate and tridentate N-ligands; $[Pd(PPh_3)_2X_2]$ and $[Pd(P\frown P)X_2]$ featuring mono- and bidentate P-ligands. Synthesis reactions never exceed two hours of mill, and they proceed with high to quantitative yields and excellent product purity. These favorable outcomes are supported by positive green chemistry metrics.

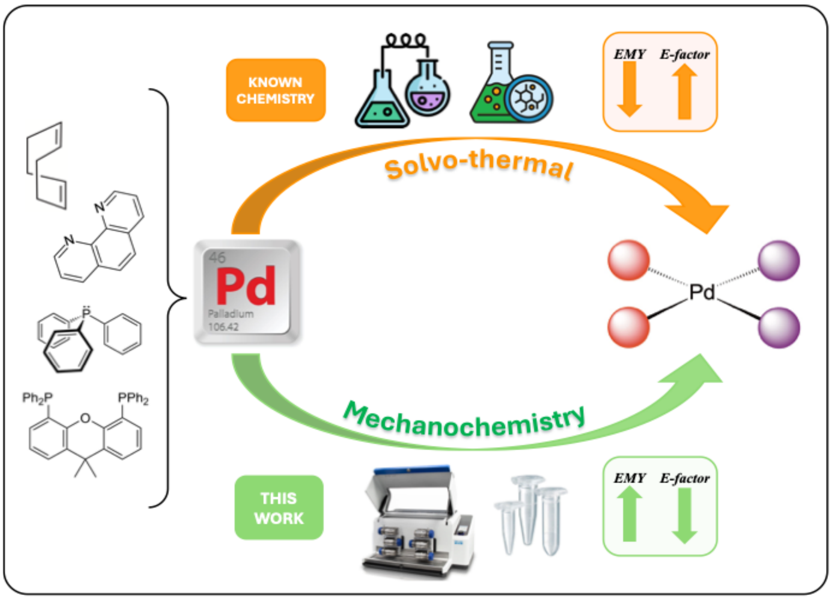

Figure 1. Graphical abstract of the work.

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Poster 20-FP

Combined Spectroscopic Approach for Studying Protein Recognition by *trans*-Pd(II)-based Complexes

Claudia Ghelarducci,[a*] Ester Giorgi,[a] Francesca Binacchi,[a] Michele Mannelli,[b] Andrea Cesari,[a]
Tania Gamberi,[b] Chiara Gabbiani,[a] Alessandro Pratesi[a]

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Despite their widespread clinical use, Pt(II)-based anticancer drugs suffer from several limitations, including severe side effects, resistance phenomena, and the need for intravenous administration.[1] A promising strategy to overcome these drawbacks involves the development of metal-based complexes incorporating alternatives to platinum. In this context, Pd(II) compounds have gained increasing attention as potential anticancer agents due to their structural similarity to Pt(II) analogues and improved water solubility.[2] Although the mechanisms underlying their biological activity are not yet fully elucidated, several *trans*-Pd(II) complexes have demonstrated cytotoxicity comparable to or exceeding that of cisplatin against various cancer cell lines.[3] However, their higher kinetic lability and reduced thermodynamic stability often result in rapid ligand exchange reactions, potentially hindering effective cellular targeting.[4] To tackle this challenge, we established a reproducible methodology to investigate square-planar *trans*-Pd(II) complexes, aiming to lay the groundwork for broader mechanistic studies of metal-based therapeutics.[5] A series of compounds with the general formula *trans*-PdL_2X_2 (where L = pyridine or piperidine, X = Cl, Br, I) was synthesized and characterized (Figure 1). This rational combination of monodentate labile and spectator ligands was designed to enhance the stability of the final molecules during circulation inside the body. The interactions of these complexes with model proteins were explored by a combined UV-Vis/NMR approach, and the *in vitro* activity was evaluated against selected cancer cell lines.

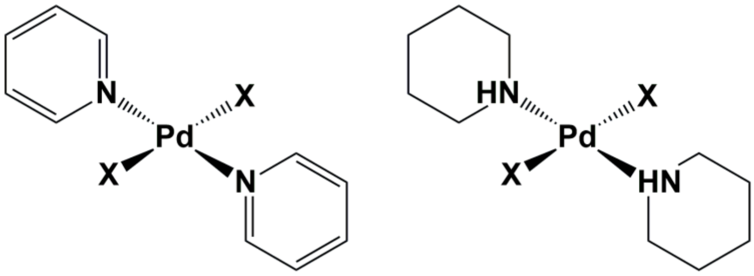

Figure 1

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Poster 21

Pendant-base complexes for CO_2 hydrogenation to CH_3OH

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The hydrogenation of CO_2 and CO_2-derivatives using a homogeneous, molecularly defined catalyst has been widely explored in recent years, but most examples are limited to low TONs, which limit their applicability compared to heterogeneous catalysts for the same reaction. This is mostly due to slow steps in the catalysis, one of the most relevant being the H_2 splitting. In this project, this slow step is tackled using metal-ligand cooperation. [Cp*Ir(bipy)] complexes have been widely studied for CO_2 or formic acid hydrogenation and they present advantageous easy synthesis and air-stability. In this project, these catalysts are further optimized by synthesizing Ir- and Co-based homogeneous catalysts bearing a pendant base in the ligand backbone were synthesized, using the commercially available and air-stable terpyridine ligand, but affording a dynamic bidentate coordination. The dynamicity of the coordination allows for a proton shuttle behavior that can aid H-H splitting by metal-ligand cooperation, which allows for facile hydride formation and therefore a faster catalytic cycle. These catalysts also show pH-responsive activity and present unprecedented selectivity towards methanol and formic acid formation.

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Poster 22

Old Chemistry, New Insights: Alkyl(trimethylsilyl)amido Group 14 Complexes

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Hydrocarbyl(trimethylsilyl)amido ligands, such as Dipp(TMS)N^- (Dipp = 2,6-di-*iso*-propylphenyl), have been widely utilized throughout inorganic chemistry for the stabilization of low-valent metals and main-group elements.[1] The hydrocarbyl-fragment provides a platform for variation of the steric and electronic properties of the ligand, however, group 14 congeners beyond Dipp(TMS)N^- are scarce in the literature.[2, 3] Alkyl(trimethylsilyl)amido complexes of Sn(II) have been reported to undergo C–H activation and disproportionation at low temperature (Figure 1A).[4] Here, we report a combined experimental and DFT study into the mechanism of this decomposition reaction, and explore the reduction and photolysis of the alkyl(trimethylsilyl)amido group 14 complexes.

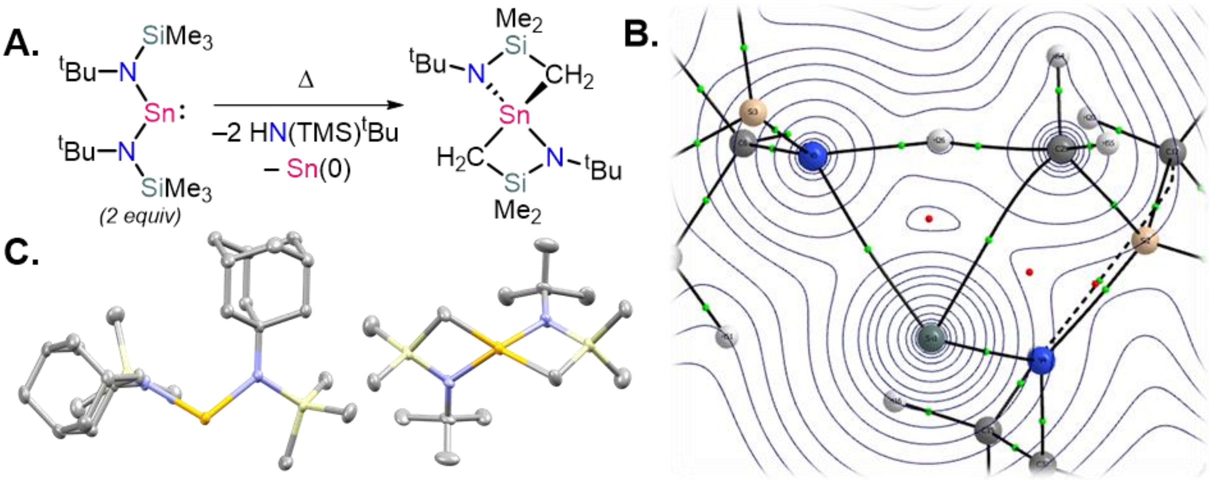

Figure 1: A. Disproportionation of [{^{t}Bu(TMS)N}$_2$Sn] to form [{κ^2-^{t}Bu(SiMe$_2$CH$_2$)N}$_2$Sn(IV)], ^{t}Bu(TMS)NH and elemental tin. **B.** QTAIM contour plot of the initial transition C–H activation transition state. **C.** Solid-state structures of [{Ad(TMS)N}$_2$Sn] (left) and [{κ^2-^{t}Bu(SiMe$_2$CH$_2$)N}$_2$Sn] (right).

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Poster 23

Ligand improvement for the preparation of [Zinc(II)(Pyridine-Containing Ligand)] complexes as efficient catalyst for the cycloaddition of CO_2 to epoxides

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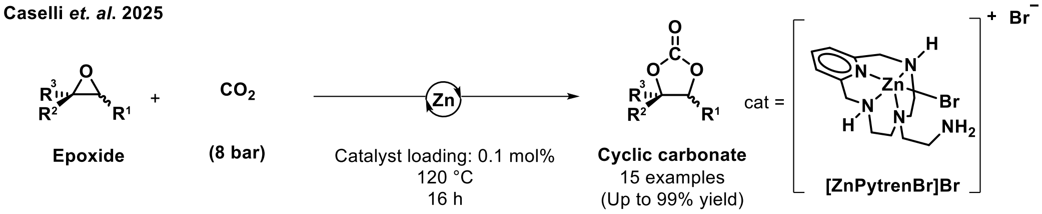
Carbon dioxide is the principal greenhouse gas, largely recognized as responsible for global warming and related climate changes. Driven by the inherent synthetic potential of CO_2 as an abundant, inexpensive and renewable C1 source, the recent years have witnessed renewed interest in devising catalytic CO_2 fixations into organic matter. [1] For decades chemists have been challenged to design novel technologies for converting CO_2 into fine chemicals. [2] Based on our ongoing research interests devoted to the development of innovative catalysts that align with green chemistry principles, [3] we became interested to investigate a too little explored area of homogeneous catalysis: the use of zinc(II) polyazamacrocyclic complexes for the cycloaddition of CO_2 to epoxides.

Herein, we describe the development of a novel approach for the synthesis of cyclic carbonates using carbon dioxide and epoxides employing as catalyst zinc(II) complexes of pyridine containing macrocyclic ligands (Figure 1). Remarkably, the catalytic activity of the catalyst has been improved through a structural modification of its ligand which has allowed full conversions of terminal epoxides to cyclic carbonates under solvent-free and mild reaction conditions. The development of this process and its scope and limitations will be discussed.



- **Fixation of carbon dioxide**
- **Non-noble catalyst**
- **Good yields with a simple protocol**
- **Mild reaction conditions**
- **Solvent-free**
- **High selectivity**

Figure 1

We thank the CARIPLO Foundation: project 2022-0781 “CO_2 Valorization by A Low Economic impact biorefinery, CO_2VALE”, for financial support.

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Poster 24-FP

[Au(I)]-Catalyzed Functionalization of Bicyclo[1.1.0]butanes with Allenes

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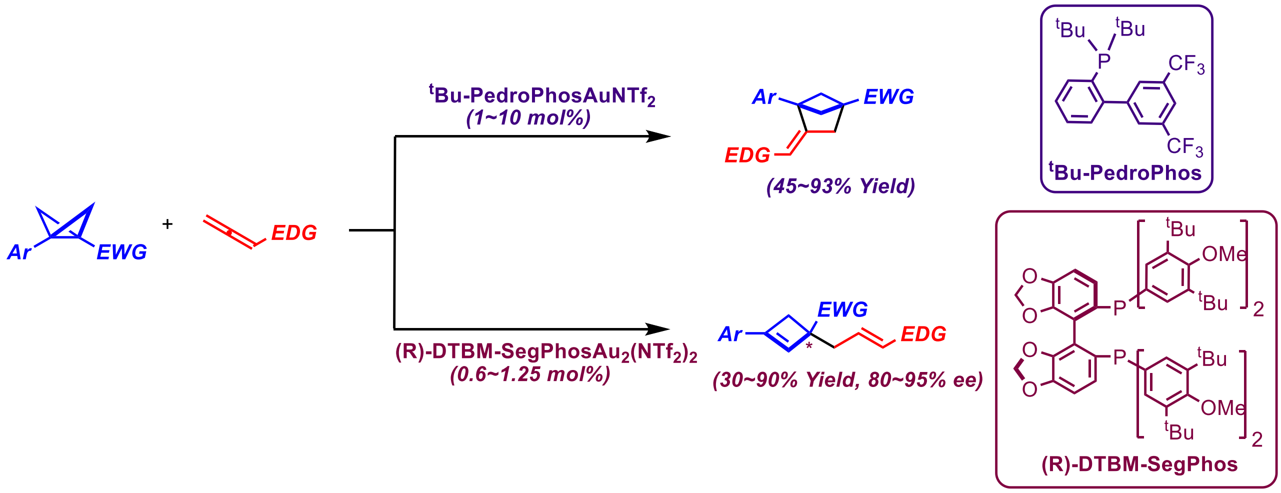
Bicyclo[1.1.0]butanes (BCBs) have recently attracted particular attention, due to their unique reactivity of the strained bridgehead Cα-Cγ bond from the 'butterfly' like double cyclopropane ring structures.[1] In continuation to our interest in homogenous Au(I) catalysis,[2] we developed a novel dual catalytic strategy for the electrophilic activation BCB species. In particular, the use of [Au(PedroPhos)NTf_2] enable to unlock an unprecedented [2σ+2π]-cycloaddition with electron-rich allenes. Here, a large series of bicyclo[2.1.1]hexanes was generated in high yield with excellent regio- and stereoselectivity.[3] Furthermore, when the chiral gold complex [((*R*)-DTBM-SegPhos)$Au_2(NTf_2)_2$] was utilized, the cycloaddition process was interrupted in favor of a second proto-elimination step, to lead chiral 1,3-disubstituted cyclobutanes. Here high enantiomeric excesses were also gained in the final compounds.[4]



Scheme 1

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Poster 25-FP

Valorization of Ambient Pressure CO_2 *via* Sustainable Catalytic Strategies

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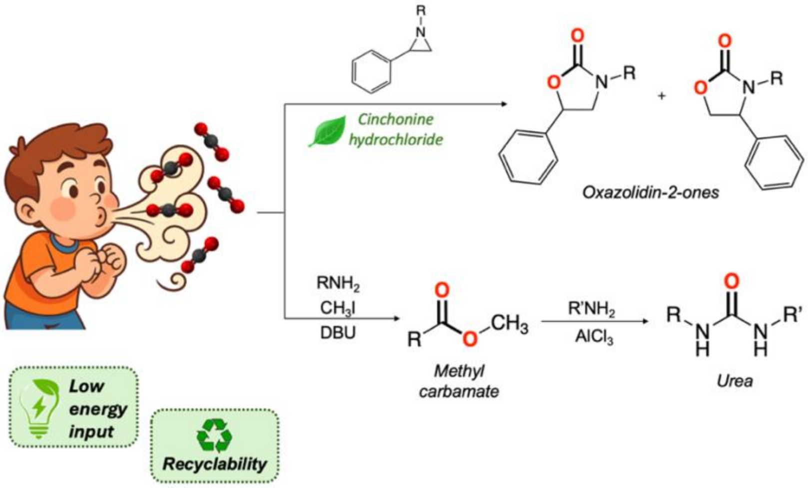
As one of the most abundant greenhouse gases, carbon dioxide (CO_2) poses a major environmental challenge but also offers a unique opportunity. Its direct conversion into valuable products offers a sustainable route to emission reduction and a circular carbon economy. CO_2 valorization can proceed through both non-reductive and reductive pathways. In both cases, truly sustainable processes require careful control of reaction conditions, since the need for high CO_2 pressures impacts energy consumption and overall costs.

In this work, we present two catalytic systems for the non-reductive valorization of CO_2 at ambient pressure. First, the biocompatible cinchonine hydrochloride was found to be able to catalyze the cycloaddition of CO_2 to aziridines, enabling the 100% atom-economical synthesis of oxazolidin-2-ones, key pharmaceutical intermediates and organic synthons.[1] The excellent regioselectivity and catalyst stability enhanced the high synthetic value of this approach.[2] On the other side, we developed a mild, two step protocol for the synthesis of organic ureas using ambient pressure CO_2. Initially, the reaction of this gas with amines and CH_3I in the presence of DBU (1,8-diazabiciclo(5.4.0)undec-7-ene) allowed the formation of methyl carbamates.[3] Subsequently, these carbamates reacted with a second amine molecule in the presence of $AlCl_3$ to yield the desired ureas. Optimization of both steps led to a process characterized by direct CO_2 fixation, low energy input and amine recoverability, offering a green and practical route to valuable ureas from waste CO_2. Together, these methodologies demonstrate the potential of ambient pressure CO_2 valorization as a viable and sustainable strategy for the synthesis of fine chemicals.



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Poster 26-FP

Monosaccharide-based Ru(II) pincer complexes as catalysts for the Guerbet reaction

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The formation of new carbon-carbon bonds is central in organic synthesis for the production of high-value-added chemicals.[1] A recent approach that avoids radical or organometallic pathways involves the direct coupling of primary and secondary alcohols via the Guerbet reaction. This β-alkylation process, based on a "hydrogen-borrowing" strategy, enables the use of alcohols as mild alkylating agents, under sustainable conditions and with water as the sole byproduct.[2]

Over the years, different catalytic systems have been developed, with pincer-based metal complexes showing high activity.[3] Tridentate pincer ligands play a pivotal role in homogeneous catalysis due to their ability to provide thermal stability and structural robustness to metal complexes, while allowing the possibility of finely tuning their electronic and steric properties.[4]

On this basis, Ru(II) octahedral complexes bearing (*N,N,N*)-pincer ligands, functionalized with monosaccharide units *N*-linked at the C1 position (Figure 1, left), were synthesized, characterized, and evaluated as a catalyst in the Guerbet reaction of 1-phenylethanol with benzylic alcohol (Figure 1, right).

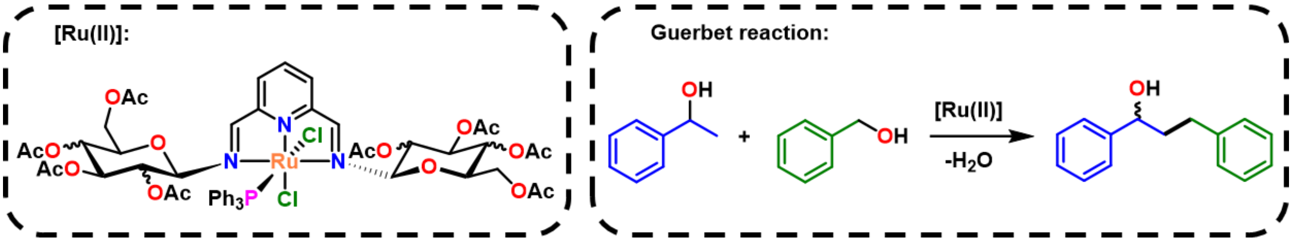

Figure 1 – Structure of the pincer Ru(II) complexes (left) and Guerbet reaction (right) studied in this work.

The aim of the work was to optimize the catalytic conditions, exploring alternative energy sources such as microwave irradiation, and to investigate the influence of chiral sugar moieties on reactivity and potential enantioselectivity.

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Poster 27-FP

Ruthenium-Catalyzed Valorization of HMF: Synthesizing 2,5-Diformylfuran and its Polyimine Derivatives

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The drive for sustainable energy and chemicals highlights the importance of biomass-derived 5-hydroxymethylfurfural (HMF).[1] Its versatile derivative, 2,5-diformylfuran (DFF), is crucial for producing furan-functionalized chemicals and advanced materials like fluorescent agents and biopolymers. This study details the homogeneous ruthenium-catalyzed synthesis of DFF, tackling critical selectivity issues such as over-oxidation and cross-polymerization. We evaluated various organometallic ruthenium complexes, including Shvo's dimer, using quinones as hydrogen acceptors and Co-salen as an electron transfer mediator. Optimal reaction conditions were identified through comprehensive parametric studies. Subsequently, DFF served as a key monomer for polyimine synthesis via polycondensation with ethylenediamine and p-phenylenediamine (Figure 1).[2] Characterization confirmed the formation of imine bonds and oligomeric chains, though with modest thermal properties compared to traditional polyimines. The varying catalytic performance informed an efficient biomimetic catalytic cycle. Future work will focus on optimizing polymerization to enhance the mechanical properties of these promising furanic polyimines.

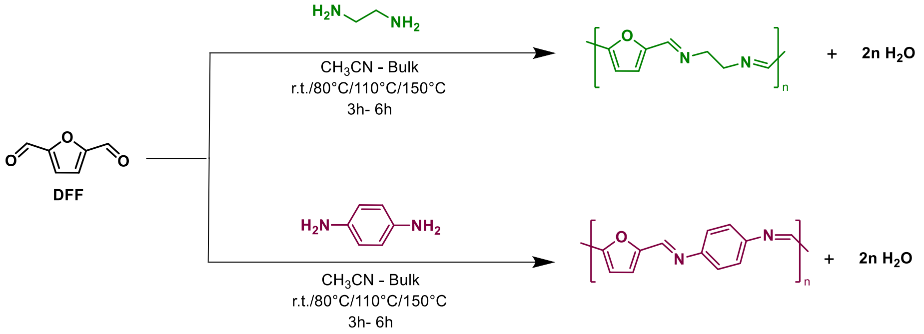

Figure 1: Synthesis of the polyimines obtained by reacting DFF with ethylenediamine (in green) and with p-phenylenediamine (in magenta)

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Within the Ecosister project, funded by Mission 04 Component 2 Investment 1.5 – NextGenerationEU, Spoke 1 focuses on "Materials for Sustainability and Ecological Transition," (CUP J33C22001240001).

Poster 28

Towards Novel Radiopharmaceuticals: Synthesis and Characterization of Rhenium(I) Complexes with Bis(N-heterocyclic carbene) Ligands

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Technetium-99m, with its ideal physicochemical properties and availability, is the most used radionuclide in SPECT imaging, while rhenium-188 has emerged as an attractive candidate for endoradiotherapy.[1] The biodistributive equivalence of stable technetium and rhenium complexes with identical coordination spheres underscores the importance of studying their coordination chemistry to develop matching theranostic pairs for diagnosis and therapy.

N-heterocyclic carbenes (NHCs), known for their strong σ-donor properties, form robust bonds with various metal ions and have been extensively studied in catalysis, luminescence, and pharmaceutical chemistry. However, the chemistry of Tc and Re with NHCs has been primarily explored in oxidation state I, with limited studies in states III and V.[2-4]

This work presents the synthesis and the crystal structures of novel Re(I) complexes with chelating bis(NHCs) ligands. By varying the bis(NHC) ligand the formation of different *exo* and *endo* isomers was observed (fig. 1). We are currently investigating the factors influencing the formation of these isomers also via DFT calculations. These studies not only elucidate the structural diversity of these complexes, but also offer valuable information for the rational design of new radiopharmaceuticals.

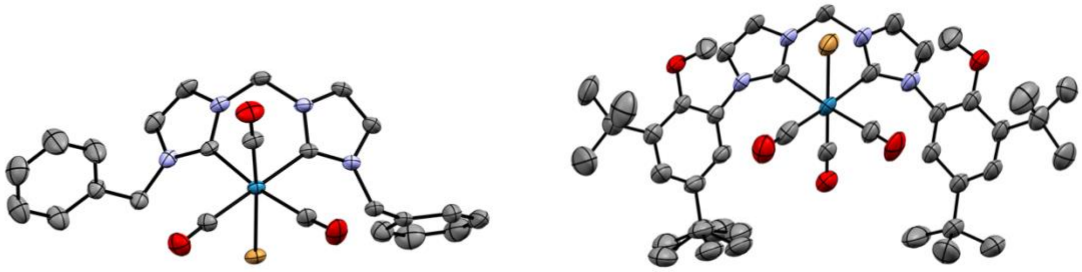

Figure 1

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Poster 29

Coordination compounds with substituted azoles displaying unexpected photophysical properties

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Azoles are a class of ligands that can stabilize a wide variety of transition metals, including those of group 11th. Among them, imidazolyl NHC carbenes or pyrazoles are particularly prominent because their stereo-electronic properties can be easily modulated by modifying the azoles' ring with diversely functionalized organic groups.[1] For example, carbazole scaffolds are widely known for their optoelectronic features, mostly consisting of high triplet energies and hole-transporting capabilities.[2] These properties make them suitable chromophores in the design of host materials for organic light-emitting diodes (OLEDs).[2] For this reason, the functionalization of azoles with carbazole moieties represents a reasonable strategy to obtain efficient blue-emitting materials based on coordination compounds. Noteworthy, even if the emission behavior seems to be dominated by IL transitions attributed to the carbazole scaffold, their incorporation in NHC ligands, furtherly coordinated to gold(I), affects their intrinsic emissive properties, by blue-shifting the emission band positions[3] and/or by enhancing the emission quantum yields compared to the bare carbazole scaffold.[4] In this communication, we present the photophysical characterization of a series of coordination compounds obtained with azoles functionalized with photoactive substituents. For example, mono and bis(NHC carbazole)gold(I)halide-based complexes have been investigated; the mono NHC gold(I) carbene complex, *1-(1,4-phenylene-1yl)-4-carbazolyl-9yl)-3-benzyl-2-imidazolyl-2yl-gold(I)chloride* shifts the blue emission of the ligand toward the violet canceling the green components upon irradiation at 360 nm, while there is no evidence of the typical ^{3}MC phosphorescence.[5]

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Poster 30

Activation of hydrogen peroxide catalyzed by manganese(II) complexes derived from chelidamic acid for oxidation of chromophores

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Hydrogen peroxide can be used as a bleaching agent in laundry detergent to remove stains by oxidizing the double bond or the other moieties in the chromophores. Since the reactivity of this oxidant is not kinetically favoured, the development of transition metal complexes as bleaching catalysts for the activation of hydrogen peroxide continues to be an ongoing area of research. [1]

Manganese complexes are widely used as oxidation catalysts thanks to their rich redox chemistry.[2] The first manganese complex reported on the oxidation activity was a μ-oxo-bridged Mn(IV) dinuclear compound, inspired by the catalytic site of manganese catalase enzymes, with Me_3tacn (1,4,7-trimethyl-1,4,7-triazacyclononane) as ligand.[3]

Over the years, several manganese complexes containing different ligands, such as Schiff bases, macrocyclic, and terpyridine ligands, were patented as bleaching catalysts.[4]

Given these general premises, our study aims to the synthesis of manganese(II) complexes containing ligands derived from chelidamic acid for the activation of hydrogen peroxide as bleaching agents (Figure 1).

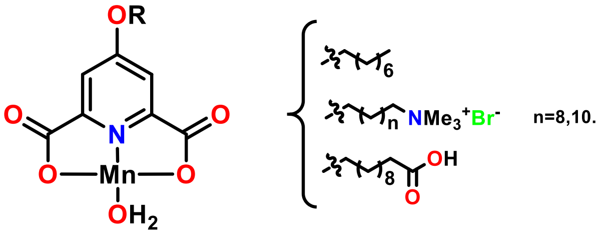

Figure 1- Manganese(II) complexes derived from chelidamic acid used in this study.

Different chromophores were chosen as bleaching model stains. The catalysts, which showed a good activity, were tested in alkaline (pH 8) aqueous media, and in the presence of SDS as surfactant to miming the laundry condition. These promising results obtained open the door for future investigation focused on optimizing the catalysts.

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Poster 31

Hydrogenation Reactions of Carbonyl Compounds Catalyzed by New Ruthenium Diphosphine Complexes in Water

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Transfer hydrogenation (TH) and hydrogenation (HY) of carbonyl compounds by ruthenium(II) catalysts are currently the most appealing routes for the synthesis of alcohols. In particular, complexes bearing phosphorus and nitrogen donor ligands, typically prepared from the precursor $[RuCl_2(PPh_3)_3]$, have been deeply investigated.[1,2] Thus, extensive studies have demonstrated the high efficiency of diphosphine ruthenium(II) complexes, combined with amino-pyridine based ligands, in HY reactions.[3,4] Herein, we present the synthesis and catalytic evaluation of a novel series of ruthenium(II) complexes, $[Ru(X)_2(NN)(DPPBTS)]$ (NN = ampy, en; X = COD, CO, OAc, Cl), which incorporate the water-soluble sulfonated diphosphine dppb (DPPBTS) (Figure 1).[5] These complexes were specifically designed for homogeneous hydrogenation of carbonyl compounds under mild conditions (5 atm H_2, T = 80 °C), providing a more sustainable method for conducting reduction reactions in water.

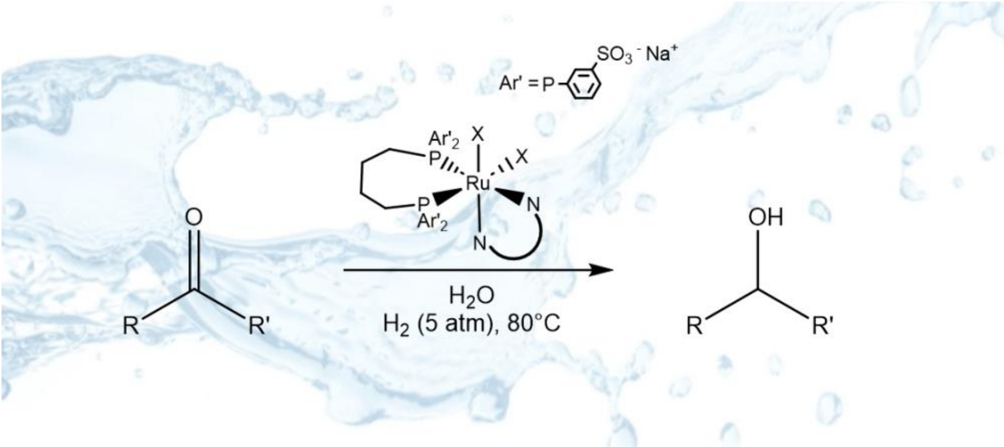

Figure 1

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Poster 32

Organolithium-Mediated Conversion of Aryl Azides to Aryltriazenes in Deep Eutectic Solvents

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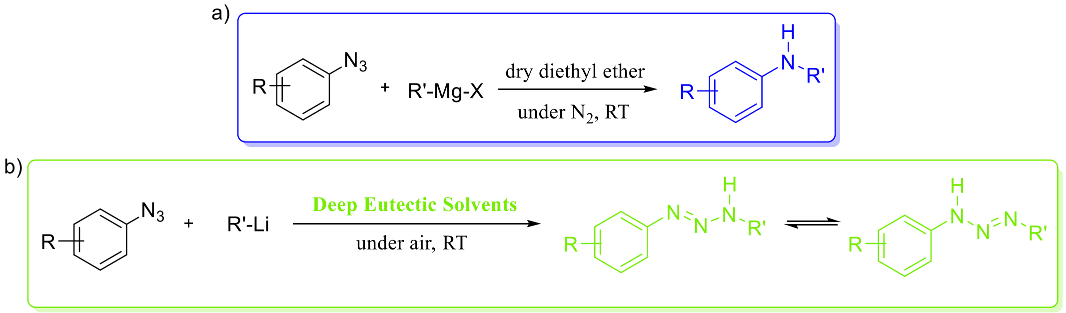
Typically, the reaction between aryl azides and Grignard reagents in diethyl ether at room temperature leads to the formation of *N*-alkylanilines[1] (Figure 1a). When the temperature is lowered to 0 °C, the use of either Grignard or organolithium reagents shifts the reactivity toward the formation of aryltriazenes[2] –valuable intermediates in organic synthesis. Notably, Gandelman and co-workers have employed diaryltriazenes in innovative "triazenolysis" protocols for the generation of amines from alkenes[3]. In addition, these species are versatile precursors for the synthesis of benzotriazoles.[4] Our group has long been engaged in the study of polar organometallic reactivity in bio-inspired solvents such as water and Deep Eutectic Solvents (DESs).[5] Building on this expertise, we investigated the potential of DESs as green reaction media for the alkylation of aryl azides with organolithium reagents (Figure 1b).

Interestingly, this new protocol also proved efficient for the synthesis of both dialkyl- and monoalkyltriazenes – species that are typically difficult to access via classic diazonium coupling, due to their tendency to undergo overreaction with diazonium ions to give undesired penta-azadienes. Given the intrinsic challenges in purifying triazenes, we're further exploring their utility as intermediates in one-pot benzotriazoles synthesis conducted in DESs.



R' = aryl or alkyl organometallic compounds

Figure 1 a) Synthesis of *N*-alkylanilines via the reaction of aryl azides with Grignard reagents in conventional solvents. b) Reaction of aryl azides with organolithium reagents in DESs.

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Poster 33-FP

Synthesis of Mugineic Acid Family Phytosiderophore Analogues as Low-Cost and Sustainable Fertilizers for Agriculture in Poor Soil

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Plants, like all living organisms, require a wide range of essential nutrients to support fundamental physiological processes that are vital for their growth, development, and defense against environmental stress. When these nutrients are deficient or unavailable in the soil, plants become vulnerable to a variety of adverse effects that can undermine their health and productivity. One common and damaging nutrient deficiency is iron chlorosis, which frequently occurs in plants grown in calcareous soils. This condition manifests as yellowing of the leaves, a significant reduction in crop yield, and, in severe cases, the death of individual plant parts or the entire plant. The primary solution for combating iron chlorosis is the application of iron chelates as fertilizers. However, the production methods for most commercial chelating agents -developed in the 1970s- are unsustainable, contribute to pollution, and are costly. As such, there is an urgent need to explore more innovative and sustainable methods for producing these fertilizers, ensuring both cost-effectiveness and environmental responsibility.

One promising approach comes from the work of Professor Namba's research group, which demonstrated that soil application of synthetic 2′-deoxymugineic acid (DMA)—a natural phytosiderophore derived from the *Poaceae* family—can alleviate iron deficiency in plants grown in calcareous soils.[1] Unfortunately, the high cost and poor stability of synthetic DMA hinder its practical agricultural use. In this study, we present a solution by developing proline-derived analogues of DMA (PDMA) that are both more stable and cost-effective. Through practical synthesis, density functional theory (DFT) calculations, and biological testing, we demonstrate that these PDMA analogues can form stable complexes with Fe(III) and offer a viable alternative to synthetic DMA for addressing iron deficiency in plants.

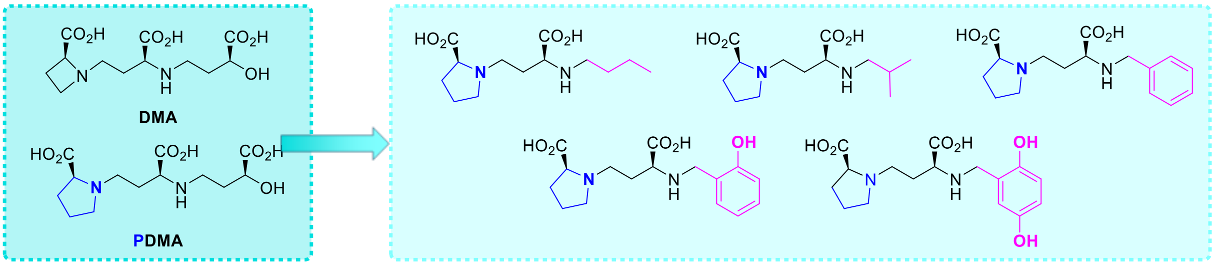

Figure 1: Previous results (left) and new differently substituted synthetic analogues of PDMA (right).

This publication is part of the project PNRR-NGEU which has received funding from the MUR – DM352/2022

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Poster 34-FP

Synthesis and characterization of new water-soluble Iridium (III) complexes

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Research on iridium complexes has been experiencing exponential growth due to their outstanding chemical and physical properties[1]. In particular, the ability to synthesize iridium complexes that are water-soluble without the need for additional organic solvents, combined with their excellent luminescent behavior and high stability, presents significant potential for their application in the biological field[2]. These applications include, but are not limited to, bioimaging, sensing, catalysis, and theranostics[2].

To explore this potential, a series of heteroleptic bis-cyclometallated complexes derived from functionalized phenylpyridine was synthesized, with the aim of evaluating how different functional groups influence solubility. Following synthesis, a comprehensive photophysical and morphological characterization was carried out, and a solubility scale was subsequently developed. Additionally, in vitro assays were conducted to assess the biocompatibility of the synthesized complexes, further supporting their potential use in biomedical applications.

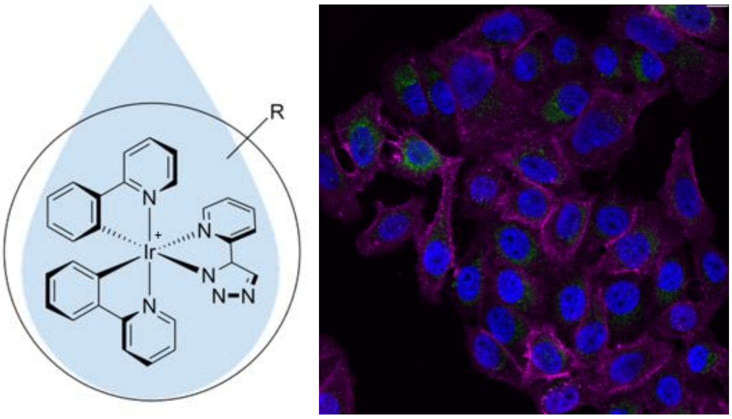

Figure 1

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Poster 35-FP

Design and Synthesis of conjugated organic Spacers for Two-Dimensional Perovskite Solar Panels

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Perovskite solar cells (PSCs) represent the most promising photovoltaic technology, given the high efficiencies achieved in a short period of time. The main issue with these devices is that perovskite crystals undergo degradation when exposed to humidity, lowering the photovoltaic performance. To address this problem, a new technology based on two-dimensional (2D) perovskites has emerged in recent years, offering significant improvements in terms of stability.[1] 2D perovskites are obtained by replacing methylammonium cations with larger organic cations in the perovskite formulation. Such large organic cations can't incorporate into the perovskite structure, instead they act as "spacers" between perovskite crystals, generating a "layered" structure that gives the perovskite greater stability against humidity due to the presence of hydrophobic organic molecules. Unfortunately, the layer of organic molecules also has low dielectric constant hampering the flow of electrons and lowering the photovoltaic performances.

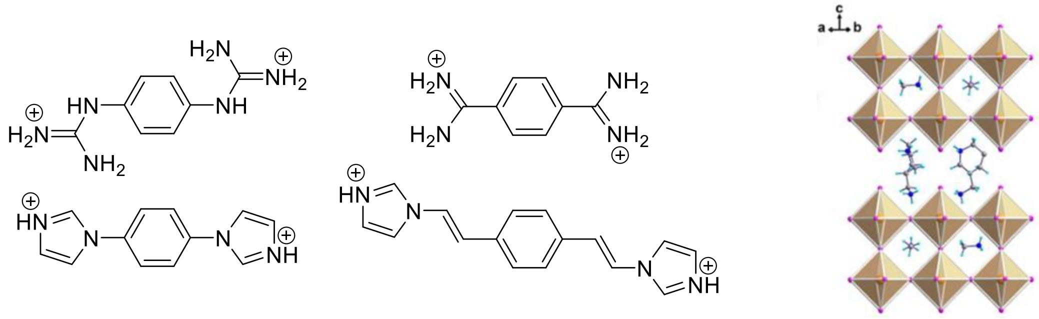

Figure 1: Structures of the organic conjugated spacers and representation of the 2D perovskite in DJ phase.

In this work, we designed and synthesized organic spacers with a double positive chare capable of linking two 2D-perovskite layers in a Dion-Jacobson (DJ) phase.[2] In order to favour charge transport between inorganic layers, conjugation was preserved along the cations using aromatic scaffolds and replacing the ammonium function (generally used to interact with the perovskite) with unsaturated guanidinium, fomamidinium or imidazolium ones. Finally, given the need for economic and scalable process, low-cost commercially available aromatic cores and short synthetic routes were preferred. The developed conjugated cations were structurally characterized and their exploitation in 2D-PSC is currently ongoing.

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Poster 36-FP

Harnessing Mechanical Energy: Synthesis of Metal Bipyridine Complexes Via Mechanochemistry

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Polypyridyl metal complexes have been extensively investigated in the fields of coordination chemistry and catalysis. 2,2'-Bipyridine is one of the most common and widely explored chelating ligands and has been studied for decades in areas such as medicine,[1] catalysis,[2] batteries, and solar cells.[3] Although metal-bipyridine compounds are widely synthesised in laboratories and industries, green and sustainable approaches to this class of compounds remain unexplored. Mechanochemistry challenges these traditional synthesis routes, promising an environmentally friendly, efficient and rapid approach to the synthesis of organometallic compounds.

This work[4] describes the mechanosynthesis of several metal-bipyridine complexes based on Ru, Fe, Co, Pd, Pt and Ir, without the need for intense, harsh conditions, complex procedures or bulk solvents. This approach was found to be highly productive compared to conventional solution-based methodologies, as measured by Effective Mass Yield (EMY), E-factor and reaction time. For most of our reactions, we observed optimal EMY and E-factor values, and the reactions were completed in 30 minutes to 1 hour without purification steps. These results highlight the significance of mechanochemistry as a selective and complementary approach to the rapid and environmentally friendly synthesis of organometallics.

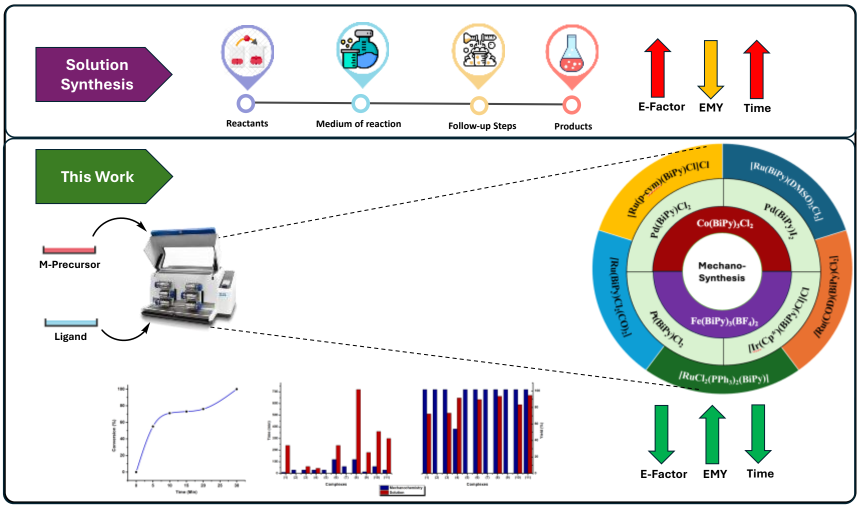

Figure 1

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Poster 37

Development of Colorless Cobalt and Manganese Complexes for high transparent Dye-Sensitized Solar Cells

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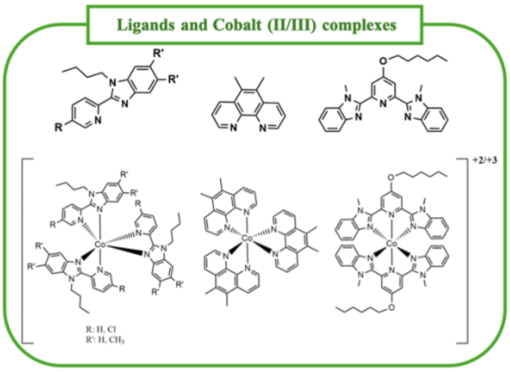
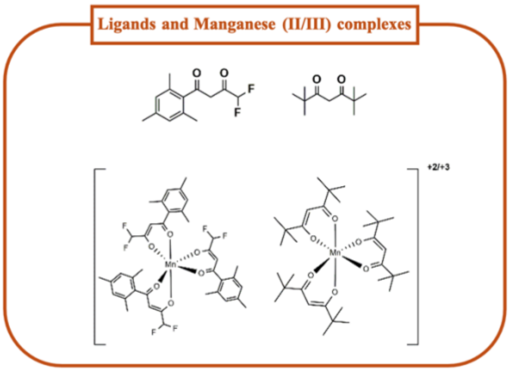
The advancement of photovoltaic (PV) technology is fundamental for sustainable energy production, with silicon-based solar cells being the most prevalent due to their efficiency and cost-effectiveness. Integrating photovoltaic panels into private and public buildings can be challenging due to dark coloration of silicon-based photovoltaic devices. In order to address this issue, some researchers are focusing on the development of alternative photovoltaic devices, such as dye-sensitized solar cells (DSSCs)[1].[1] DSSCs typically consist of a photoanode composed by titanium dioxide (TiO_2) coated with a light-sensitive dye. When sunlight strikes the dye, a photoexcitation process occurs, causing electrons to be injected into the conduction band (CB) of the TiO_2, which then flow through an external circuit, generating an electric current. The oxidized dye molecules are regenerated by a redox mediator in the electrolyte, usually iodide/triiodide, which transfers electrons back to the dye. For better integration of DSSCs into buildings, the use of colorless materials is essential. For this reason dyes that absorb in the near-infrared and transparent redox mediators to visible light are being studied.[2] [2] In this work, we present new pyridinyl benzo[d]imidazole ligands designed to coordinate cobalt ion (green box) and ligands designed to coordinate manganese ion (orange box), forming colorless octahedral metal complexes. These ligands (except for the last on the orange box) were synthesized and characterized, then used to prepare their respective ones complexes, future substitutes for the common redox mediators previously mentioned.





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Acknowledgment: We thank the Ministry of Environment and Energy Security (POR H_2, A.d.P. MASE/ENEA-CNR-RSE, CUP B93C22000630006 and "IEMAP" project, A.d.P. MASE/ENEA-CNR-IIT-RSE, CUP B82C21001820001) and project "nuovi Concetti, mAteriali e tecnologie per l'iNtegrazione del fotoVoltAico negli edifici in uno scenario di generazione diffuSa" ("CANVAS"), funded by the Italian Ministry of the Environment and the Energy Security, through the Research Fund for the Italian Electrical System (type-A call, published on G.U.R.I. n. 192 on 18-08-2022) for funding.

Poster 38-FP

Metal-Oxide Catalysts with Tuned Activity for the Selective Depolymerization of Polyurethanes

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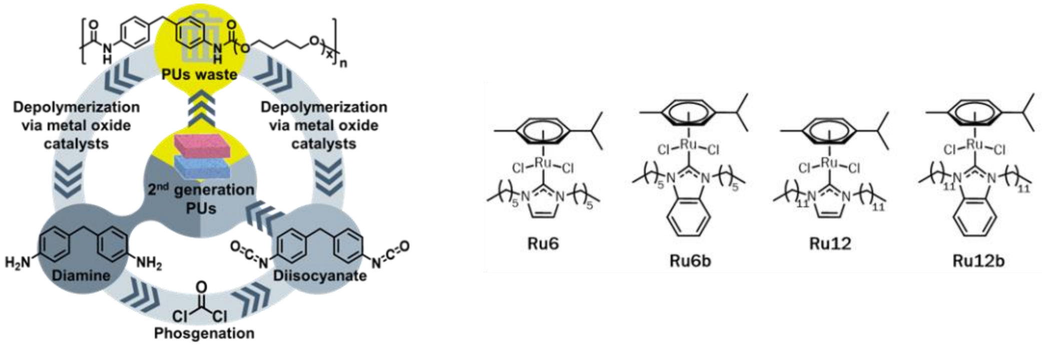
The growing accumulation of plastic waste is an increasingly urgent environmental challenge. Polyurethanes (PUs) are highly versatile, durable plastics produced by the polymerization of diisocyanates, derived from the phosgenation of the corresponding diamines, and polyols. Chemical recycling of PUs has indeed gained significant importance, yet the catalytic depolymerisation of PUs remains underexplored.[1] In this work, we employ common metal oxides and less-investigated, easily-tuneable metal oxide perovskites as catalysts to selectively depolymerise different model urethanes and real PU waste into their key components: polyols, diamines, and diisocyanates (Figure 1, (a)).[2] The fine-tuning of the catalysts' composition and the optimization of the reaction conditions is being investigated through a broad screening procedure that includes strategies like immobilization of ruthenium species from synthesised organometallic precursors (Figure 1, (b)) on the metal-oxides surface, targeted doping of cations, and enhancement of oxygen vacancies.



(a) (b)

Figure 1

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Poster 39-FP

Scalable Ruthenium-Catalyzed Guerbet Reaction for Upgrading Bioethanol to Higher Alcohols: A Sustainable Route to Next-Generation Biofuel Production

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In 2022, global bioethanol production exceeded 100 billion litres, with 80% originating from the USA and Brazil. Besides being used as a biofuel, it can be utilized as a renewable commodity to obtain several valuable chemicals. One of the possible transformations is the homologation of ethanol to form butanol and longer chain alcohols by means of the Guerbet reaction. This process consists of three key steps: initially, ethanol is converted into acetaldehyde then following an aldol condensation mechanism, crotonaldehyde is generated. Lastly, crotonaldehyde is transformed into butanol via hydrogenation.[1] To accomplish the dehydrogenation/hydrogenation steps, a redox catalyst is required. At prof. Mazzoni's lab we synthetised and tested a ruthenium homogenous catalyst (Ru-NHC) obtaining good results on this transformation in terms of ethanol conversion and butanol selectivity.[2] Adding benzoquinone as a co-catalyst (1.5 mol %) alongside the ruthenium catalyst significantly boosted selectivity for longer chain alcohols (+18%).[3] This catalytic pair was also tested on some upscaling experiments finding that by decreasing the headspace volume in the reactor a better carbon balance is observed.[4] This led to scale-up studies with drastic efficiency gains: 0.02 mol% Ru-NHC and 5 mol% base yielded up to 2400 TON.

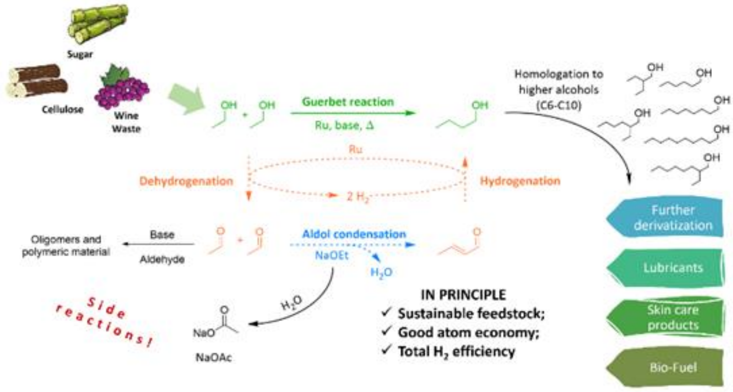

Figure 1

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Acknowledgements: Authors wish to acknowledge PRIN 2022 "Biomass-derived alcohols and polyols valorization and use by dehydrogenation/hydrogenation reactions promoted by bifunctional, proton-responsive homogeneous catalysts (ALCOVAL)" CUP J53D23008500006 for financial support. Within the Ecosister project, funded by Mission 04 Component 2 Investment 1.5 – NextGenerationEU, Spoke 1 focuses on "Materials for Sustainability and Ecological Transition," (CUP J33C22001240001).

Poster 40-FP

Phosphorescent Ir(III) Metallapolymers for Solar Light Harvesting

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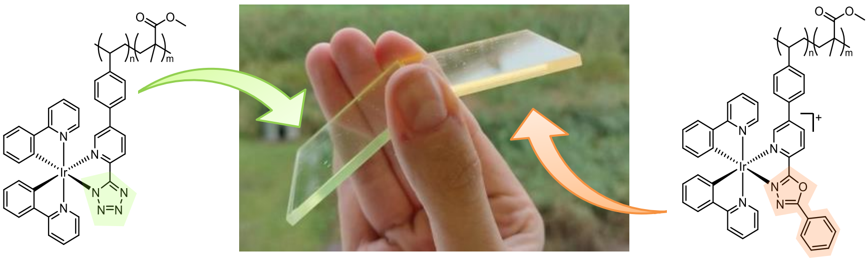
With the growing global demand for sustainable energy solutions, the development of new materials for efficient solar light harvesting is of crucial importance. To overcome the limited efficiency of traditional Si-based solar cells towards the UV part of the solar radiation, Luminescent Solar Concentrators (LSCs) have been developed. These devices embed chromophores within polymeric waveguides, down-converting high-energy to lower-energy photons.[1] UV-absorbing luminophores enable transparent or semi-transparent LSCs ideally suited for building integrated photovoltaics (BIPV).[2] In this context, we proposed a first example of colourless LSCs obtained by physical dispersion of Ir(III) phosphors into different acrylic matrices.[3] Then, to anchor the emissive species to the polymer network, a set of "polymerizable ligands" – *i.e.* capable of coordinating the metal centre and to copolymerize with methacrylic monomers – was designed and prepared. The corresponding metallapolymers were obtained either by complexation with Ir(III) fragments of a pre-formed MMA-L copolymer, or by copolymerization of the mononuclear Ir(III) complexes with MMA. The new hybrid materials displayed intense phosphorescence in the solid state, with high PLQY and Ir(III)-centred emission colours spanning from green to red, and were therefore assessed for their application in the LSCs technology (Figure 1).



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Poster 41-FP

Sustainable Conversion of Fatty Esters and Natural Oils to High Value Fatty Alcohols under Homogeneous Catalytic Conditions

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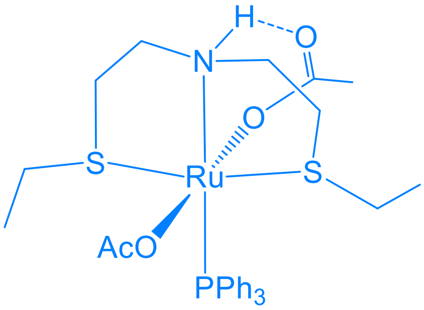
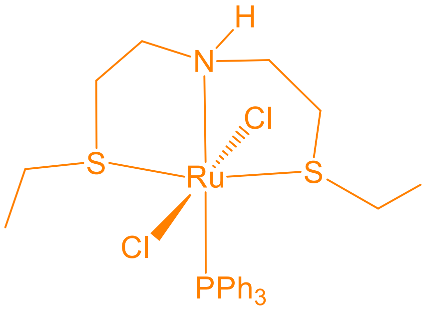
This project focuses on the enhancement of Gusev™ Catalysts for the conversion of fatty esters and natural oils into high-value fatty alcohols, targeting a production capacity of **3 million tons/year** for biodegradable detergents and personal care products. We developed novel **ruthenium acetate catalysts** that operate under mild conditions, optimizing efficiency and minimizing environmental impact.

Key advancements include optimized hydrogenation conditions using **27 atm of H_2** and **NaOEt (50 mol%)** at **40 °C** for **16 hours**, achieving a substrate-to-catalyst (S/C) ratio of up to **100,000**. This research demonstrates the potential of the resulting fatty alcohols for various biodegradable applications, contributing to sustainable chemical processes.



C1-751 Ru-SNS acetate



C1-750 Ru-SNS chloride

Figure 1

[1] Gusev et al. Angew. Chem. Int. Ed. 2012, 51, 2772.
[2] Grainger et al. Chim. Oggi, 2019, 37, 8.

Poster 42

Synthesis, characterization, and application of gold(I) complexes bearing thiol and thioacetate-functionalized NHC

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In the last few decades, N-heterocyclic carbene ligands (NHCs) have been widely used in organometallic chemistry for the synthesis of late transition metal complexes. This success is due to their strong donating capabilities, which allow to stabilize metal complexes, and to the possibility of modifying their electronic and steric properties by changing the backbone and nitrogen substituents.[1] Moreover, it is possible to develop bidentate ligands by adding another donating atom to the nitrogen-substituent (tipically N, P, O).[2] Also the sulfur atom has been evaluated as second coordinating moiety in NHC pendant substituents. Indeed, thanks to its weak σ-donor capabilities, it can establish an hemilabile equilibrium as chelating agent. This property is really useful both in homogeneous catalysis and in biological activity. Actually, gold(I) and gold(III) complexes bearing NHC-thioether ligands have been synthesized and studied as anticancer agents.[3] In this contribution, we discuss the synthesis of gold(I) complexes bearing alkyl chains of different Ienghts with terminal thioacetate or thiol moiety. These new ligands, unlike those with the thioether pendant group, allow to move to other chemical areas, for example the coordination of gold complexes on gold surface and the possibility to favour the oxidative addition to gold(I) centers. Anyway, some preliminary results in homogeneous catalysis and biological environment will be reported.

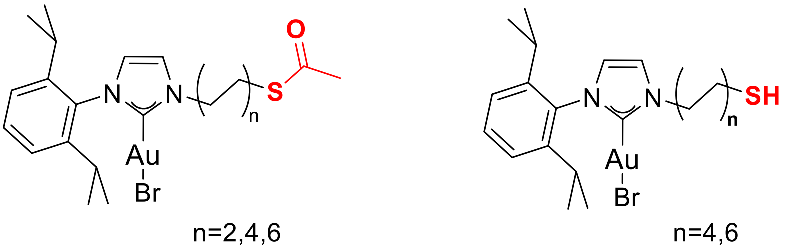

Figure 1. Gold(I) complexes with NHC ligand bearing an alkyl chain and a sulfur-based terminal group.

[1] Benhamou, L.; Chardon, E.; Lavigne, G.; Bellemin-Laponnaz, S.; César, V. Chem. Rev, **2011**, 111(4), 2705-2733

[2] Peris, E. Chem. Rev, **2018**, 118(19), 9988-10031

[3] De Marco, R.; Dal Grande, M.; Baron, M.; Orian, L.; Graiff, C.; Achard, T.; Bellemin-Laponnaz, S.; Pöthig, A.; Tubaro C. Eur. J. Inorg. Chem, **2021**, 40, 4196-4206

Poster 43

Central and axial chirality in NIR-CPL/CD active Yb(III) complexes

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NIR emitting Ln(III) complexes are particularly interesting because of their potential use in the biological and medical field.[1] Moreover, if CPL (Circularly Polarized Luminescence) active, they are promising materials for optical fibers[2] or laser systems.[3]

New NIR-CPL/CD active Yb(III) complexes (Figure 1) were synthesized by combining two ligands involving different types of chirality: central and axial chirality.[4]

CPL analysis showed how the axial chirality dominates, in this case, determining the sign of the spectra (Figure 1). Central stereochemistry seems instead to contribute to the sign of NIR-CD. DFT calculations confirmed the experimental data.

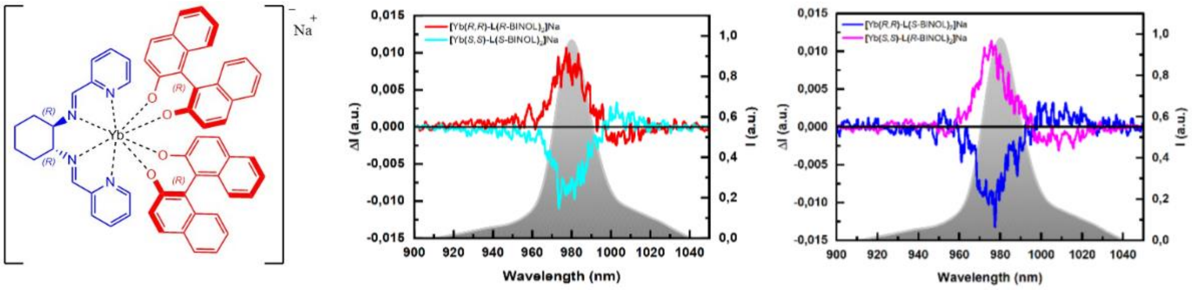

Figure 1. Yb(III) complexes synthesised (the [Yb(*R*,*R*)-L(*R*-BINOL)$_2$]Na has been chosen as representative) (left); NIR-CPL spectra of the two enantiomeric couples of the investigated Yb(III) complexes (centre and right).

[1] Cavalli, E.; Nardon, C; Willis, O. G.; Zinna, F.; Di Bari, L.; Mizzoni, S.; Ruggieri, S.; Gaglio, S. C.; Perduca, M.; Zaccone, C.; Romeo, A.; Piccinelli, F. *Chem. Eur. J.* **2022**, *28*, e202200574.
[2] Willis, O. G.; Zinna, F.; Di Bari, L. *Angew. Chem. Int. Ed.* **2023**, *135*, e202302358.
[3] Willis, O. G.; Pucci, A.; Cavalli, E.; Zinna, F.; Di Bari. *J. Mater. Chem. C.* **2023**, *11*, 5290.
[4] Ruggieri, S.; Willis, O. G.; Mizzoni, S.; Cavalli, E.; Sanadar, M.; Melchior, A.; Zinna, F.; Di Bari, L.; Bisag, G. D.; Fochi, M.; Bernardi, L.; Piccinelli, F. *Inorg. Chem.* **2025**, *64*, 5505.

Poster 44

Ternary Metallic Systems for CO_2 Hydrogenation to Methanol: A Step Toward the Design of Bifunctional Catalysts for Hydrocarbons Production

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Marcello Crucianelli,[a,b] Nicola Vecchini,[c] Alfredo Aloise[a,b]

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The catalytic hydrogenation of CO_2 to methanol represents a crucial first step in its valorization into more complex hydrocarbons such as light olefins[1]. This work investigates the performance of metals and metal oxide systems, supported on ZrO_2, as potential catalysts for CO_2 activation and partial hydrogenation under high-pressure conditions[2]. A schematic representation of the catalytic process is show in Figure 1.

Among the tested systems, $Cu/ZnO/ZrO_2$ demonstrated the highest alcohol yield at 300 °C and 50 bar, with high selectivity toward methanol. This window of temperature and pressure has been identified as the optimal one for balancing both CO_2 conversion and alcohol selectivity. In contrast, systems based on Indium and Gallium, respectively, as Copper substitute in the ternary system, showed near-zero CO_2 conversion and complete selectivity toward CO, indicating that Copper plays a crucial role in driving H_2 dissociation and stabilizing formate intermediates[3].

These results then highlight the activity of Cu-based systems in stabilizing partially-reduced CO_2 species and promoting their conversion into methanol, under industrially relevant conditions. Future work will explore the effect of binary systems (e.g., Zn/ZrO_2) and other transition-metal ternary combinations to further elucidate the correlation between catalyst structure and activity, with the ultimate goal of developing bifunctional catalysts for methanol *in-situ* upgrading.

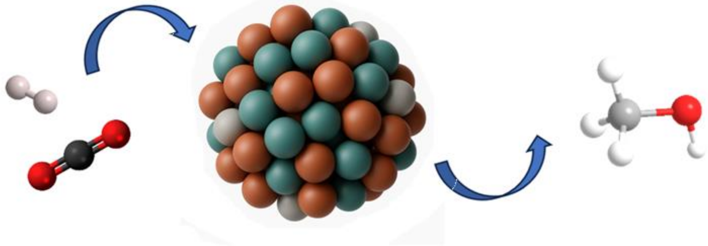

Figure 1. Representation of CO_2 hydrogenation over mixed metal based-catalyst.

[1] Pacchioni G., *ACS Catalysis* **2024**, *14*(4), 2730-2745.
[2] Etim, U. J., Zhang, C., & Zhong, Z., *Nanomaterials* **2021**, *11*(12), 3265.
[3] Ren, Menghao, et al, *Catalysts* **2022***, 12*(4): 403.

Poster 45-FP

Synthesis and Characterization of Manganese- and Iridium-Pincer Complexes

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Manganese and iridium *NNN*-pincer based non-innocent complexes were designed and developed. These complexes are synthesized and characterized by NMR, FT-IR and XRD-crystallography (Figure 1). The Mn- and Ir-complexes show metal-ligand cooperation (MLC) as they consist the non-innocent ligand backbone which could undergo aromatization-dearomatization during the catalysis. Similar manganese and iridium complexes are generally employed in various catalysis such as hydrogenation, dehydrogenation, C–H activation, CO_2 insertions reactions etc.[1] We have previously reported the ruthenium complexes using the same *NNN*-ligand and utilized for the dehydrogenative coupling reactions.[2] The activity of current Mn- and Ir-based pincer complexes are currently been explored in various catalysis.

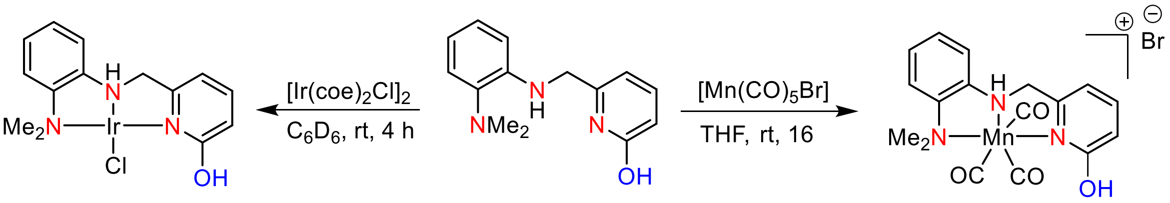

Figure 1. Synthesis of Mn- and Ir-*NNN* pincer complexes.

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[1] a) Bisarya, A., Jasra, R. V., & Kumar, A. *Organometallics*, **2023**, *42*, 1818–1831; b) Bisarya, A., Dhole, S., & Kumar, A. *Dalton Transactions*, **2024**, *53*, 12698–12709; c) Völker, M.; Schreyer, M.; Burger, P. *Chemistry* **2024**, *6*, 1230-1245.

[2] Garg, N. K., Goriya, Y., Manojveer, S., Wendt, O. F., & Johnson, M. T. *ChemCatChem*, **2024**, *16*, e202301601.

Poster 46

Light-Assisted Hydrogen Transfer Reactions Using Ruthenium Complexes with PN Ligands

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Transfer hydrogenation (TH) involves the reduction of unsaturated organic compounds via hydrogen transfer from donor molecules such as isopropanol or formic acid, eliminating the need for molecular hydrogen (H_2). While conventional TH reactions often require harsh conditions and significant energy input, photoinduced transfer hydrogenation has emerged as a promising alternative, aligning with the principles of green and industrially sustainable chemistry. Complexes **1–3** were obtained by reacting $[Ru(\eta^2\text{-}OAc)_2(PPh_3)_2]$ with phosphine–pyridine (PN) ligands in methanol. These ruthenium species catalyze the light-driven transfer hydrogenation of ketones, employing isopropanol as the hydrogen source and NaOiPr as the base at 30 °C. A variety of ketone substrates were evaluated, all of which underwent complete conversion to the corresponding alcohols. Catalysts **2** and **3** demonstrated similar photoreactivity, showing limited activity in the dark but significantly enhanced rates under light irradiation. Interestingly, complex **1** was completely inactive in the absence of light, revealing a strict dependence on photoactivation for catalytic function.

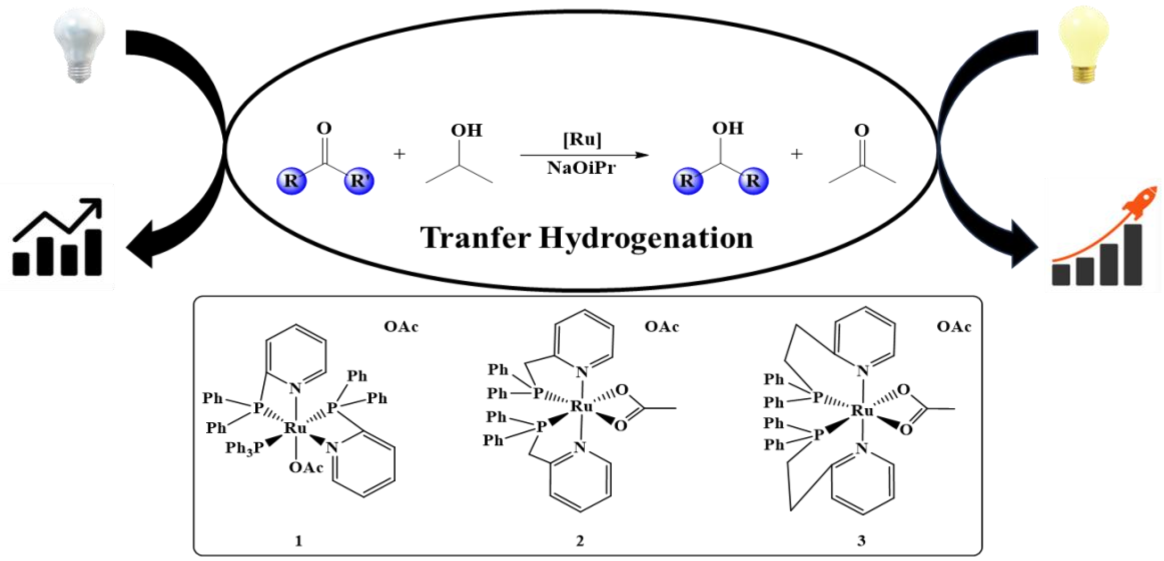

Figure 1: Transfer hydrogenation catalyzed by **1**, **2**, and **3**.

[1] Ballico, M., Alessi, D., Jandl, C., Lovison, D., Baratta, W., *Chem. Eur. J.* **2022,** *28*, 65.

[2] Masson, G. H. C., Ballico, M., Goi, B. E., Carvalho-Jr, V. P. Baratta, W. *Mol. Catal.*, **2022,** *564*, 11433.

Poster 47

Hydrogen Spillover on Waste-Based Carbon Supports: Metal Deposition Strategies for Catalytic Applications

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The development of an efficient hydrogen storage system is one of the key challenges to be addressed to enable a hydrogen-based economy. One of the most promising solutions involves hydrogen adsorption on porous materials with a high specific surface area, such as activated carbons (ACs)[1]. The aim of this study is to develop low-cost hydrogen storage material capable of improving adsorption capacity. For this purpose, a commercial activated carbon derived from coconut shells and produced via physical activation was investigated. The surface of the material was then functionalized with cobalt (Co) and copper (Cu) metal nanoparticles to promote the hydrogen spillover mechanism[2,3]. The resulting material can be used not only for hydrogen storage but also as a heterogeneous catalyst [4]. This approach focuses on cost-effectiveness, in line with the principles of the circular economy and green economy.

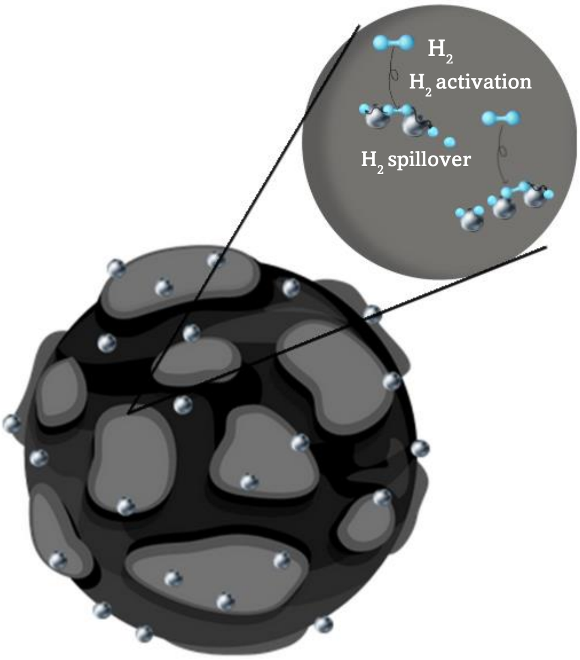

Figure 1. Schematic representation of the spillover process.

[1] N. Bader, A. Ouederni / Journal of Energy Storage 13 (2017) 268–276.
[2] H. Shen et al. / Green Energy & Environment 7 (2022) 1161–1198.
[3] Darryl S. Pyle et al. / International Journal Of Hydrogen Energy 41 (2016) 19098-19113.
[4] Somayeh Taghavi et. al / Carbon Trends 13 (2023) 100316.

Poster 48

New Rh-phosphine carbonyl clusters: synthesis, characterization, and catalytic activity

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Rhodium is a transition metal known for its versatility in catalysing a range of reactions, and the addition of phosphine ligands can further enhance its reactivity and selectivity.[1] The phosphine-substituted $Rh_4(CO)_{12-x}L_x$ and $Rh_6(CO)_{16-x}L_x$ clusters have demonstrated catalytic abilities in various reactions, such as hydrogenation, hydroformylation, and carbonylation, owing to the synergistic effects of the ligands and the metal core.[2] This work investigated the reactivity of $Rh_4(CO)_{12}$ as a precursor in the presence of different bidentate phosphines, performing the reactions under a nitrogen atmosphere. New species of phosphine-substituted rhodium clusters have been characterized by IR, $^{31}P\{^1H\}$ NMR, and SC-XRD (Figure 1), and isolated with good selectivity and yield. To compare the catalytic activity of these clusters with those known in the literature,[2-3] the new species $Rh_4(CO)_{10}$(dppe) was investigated as a catalyst for the homogeneous hydroformylation of model substrates (*i.e.*, 1-octene). Under the same conditions, the cluster $Rh_4(CO)_{10}$(dppe) has shown better selectivity in the aldehyde products than $Rh_4(CO)_{12}$.

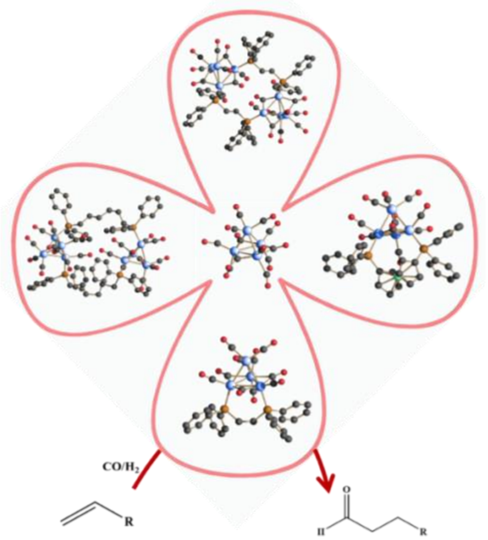

Figure 1. SC-XRD molecular structures of new phosphine-substituted rhodium carbonyl clusters.

[1] Cesari C.; Shon J.H; Zacchini S.; Berben L.A., *Chem. Soc. Rev.*, **2021**, *50*, 9503-9539.
[2] Tunik S. P.; Koshevoy I. O.; Poë A. J.; Farrar D. H.; Nordlander E.; Haukka M.; Pakkanen T. A., *J. Chem. Soc. Dalton Trans.* **2003**, 2457-2467.
[3] Dey S.; Dettling L.; Gàl D.; Bruhn C.; Kelemen Z.; Muller C.; Pietschnig R., *Journal of Catalysis*, **2025**, *442*, 115871.

Poster 49-FP

Mechanochemical activation for sustainable oxidation of benzylic alcohols

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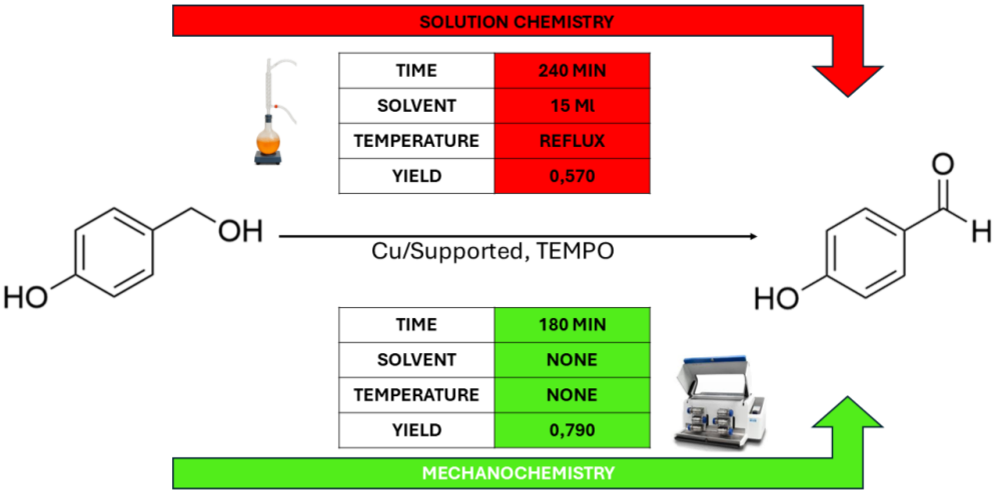
This study focuses on developing a new sustainable synthesis method for oxidizing alcohols into carbonyl compounds using a mechanochemical protocol. Oxidation reactions are widely employed in the chemical industry; however, they generate large amounts of waste and score poorly on green chemistry metrics.[1] As reported in the literature, mechanochemistry has proven to be a valuable tool for chemists to achieve more sustainable reactions[2] and to activate catalytic processes.[3] Preliminary studies in this work have shown that the use of copper-supported catalysts in combination with TEMPO can effectively oxidize *p*-hydroxybenzyl alcohol into its corresponding carbonyl compound. After three hours of reaction a conversion about 80% is achieved (Figure 1). The solid reagents are placed in the mixing vial and then subjected to ball milling.

The green assessment[4,5,6] indicates that this method presents greener parameters compared to the equivalent solution synthesis. Additionally, it is less energy and time intensive and offer better selectivity.



TIME	240 MIN
SOLVENT	15 Ml
TEMPERATURE	REFLUX
YIELD	0,570

TIME	180 MIN
SOLVENT	NONE
TEMPERATURE	NONE
YIELD	0,790

Figure 1: comparison of the conventional solution and the mechanochemical process

[1] Sheldon, R.A. *Chem. Soc. Rev.* **2012**, *41,* 1437-1451.
[2] Robertson, J.C., Coote, M. L., Bissember, A. C. *Nat. Rev. Chem*. **2019**, *3(5),* 290-304.
[3] Piermattei, A., Karthikeyan, S., Sijbesma, P. *Nat. Chem*. **2009**, *1*, 133-137.
[4] McElroy, C.R., Constantinou, A., Jones, L.C., Summerton, L., Clark, J.H. *Green Chem*, **2015**, *17*(5), 3111-3121.
[5] Andraos J., Sayed, M. J. *Chem. Educ*. **2007**, *84(6),* 1004.
[6] Aneggi E., Campagnolo F., Segato J., Zuccaccia D., Baratta W., Llorca J., Trovarelli A., *Molecular Catalysis*, **2023**, *540,* 113049.

Poster 50

Micronized Wool Enables Pickering-Type Emulsions for Efficient Metal-Catalyzed Reactions in Water

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Water is a very attractive medium for organic synthesis thanks to its unique structure, supramolecular organization, together with its suitable properties (i.e. nonflammability and nontoxicity) aligning with the principles of green chemistry. Micellar catalysis has recently been successfully applied by Novartis and other pharmaceutical companies in the industrial preparation of different Active Pharmaceutical Ingredients (API) and can be considered as a sustainable approach for the future green chemical production in water.[1] Nevertheless, the synthesis of surfactants frequently requires not properly ecofriendly reactions conditions in term of solvents and reagents and still present some biodegradability issues.

Wool is known for its ability to coordinate metals as well as for the emulsifying properties of hydrolysed keratin.[2] Today, around 95% of wool is unsuitable for textiles and ends up in landfill at considerable cost to breeders and with a negative environmental impact.[3]

The application of waste micronized wool as an emulsifier to perform metal catalyzed transformations (i.e. hydroformylation, Suzuki, and Heck cross couplings) in water is here reported. Micronized wool demonstrated to be able to form Pickering-type emulsions positively impacting in the reaction outcome. The evaluation of the environmental impact of the developed protocols by Life Cycle Assessment (LCA) demonstrates that the procedures are fully sustainable with respect to other alternatives in water and/or organic solvents.

[1] J. L. Tyler, F. Katzenburg, F. Glorius *Chem. Sci.* **2023**, *14*, 7408.
[2] D. R. Perinelli, A. Cambriani, M. Cespi, A. Tombesi, L. Pecchielan, B. Sabbatini, G. Bonacucina, G. F. Palmieri, *ACS Omega* **2025**, *10*, 12224.
[3] M. I. Khan, L. Wang, R. R. Padhye *Resour. Conserv. Recycl. Adv.* **2023**, *18*, 200154.

Poster 51-FP

Rh(I)-Catalysed Decarboxylative-Sulfonylation Reaction Unlocking Thiazete Dioxide Scaffold

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* virgil.pierron@cea.fr

Wilkinson's rhodium (I) catalyst, [(PPh$_3$)$_3$RhCl], was first described in 1967.[1] Since then, the commercially available complex is extensively described for the hydrogenation of olefins.[2] The group of Ohe demonstrated that Wilkinson's complex in stoichiometric amounts can also insert into the weak N–O bond of oxime derivatives, leading to well-defined rhodacycles (Figure 1a).[3] A reactivity, his group used to develop pyrrole's synthesis from isoxazolidinones.[4] Recognizing that rhodium(I) complexes can coordinate a SO$_2$ molecule (Figure 1b),[5-6] we aimed at merging these two reactivities.

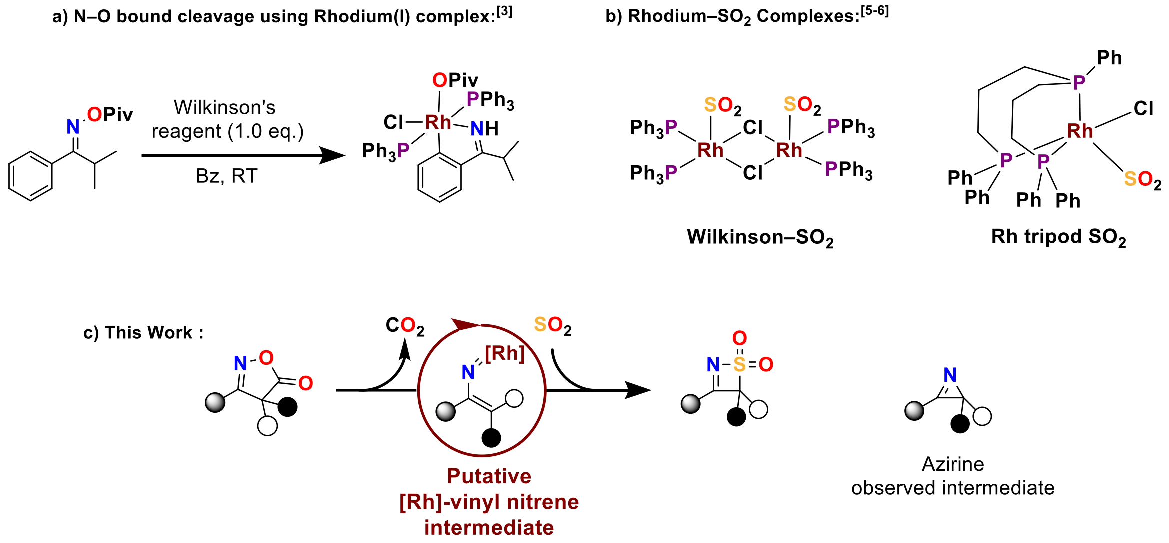

Figure 1

In this project, we have thus developed a rhodium–(I) catalyzed decarboxylative-sulfonative reaction, starting with easily accessible isoxazolidinones, where a CO$_2$ molecule is formally replaced with SO$_2$, leading to an unusual thiazete dioxide scaffold (Figure 1c). The structure of the product was confirmed through XRD analysis. Preliminary investigations on the catalytic system revealed that the catalyst's preparation is necessary to avoid rapid oxidation of the ligand by the SO$_2$ atmosphere. The reaction first goes through the *in situ* formation of azirine, which probably results from a [Rh]-vinyl nitrene.[3]

[1]: J. A. Osborn, G. Wilkinson; *Inorg. Synth.,* **1967**, *10*, 67–71.
[2]: B. Richter, A. L. Spek, G. van Koten, B.-J. Deelman; *J. Am. Chem. Soc.*, **2000**, *122*, 3945–3951
[3]: T. Shimbayashi, K. Okamoto, K. Ohe; *Organometallics,* **2016**, *35*, 2026−2031.
[4]: T. Shimbayashi, G. Matsushita, A. Nanya, A. Eguchi, K. Okamoto, K. Ohe; *ACS Catal.* **2018**, 8 (*9*) 7773–7780.
[5]: G.J. Kubas, R.R. Ryan; *Crystal. Struct. Commun.*, **1977**, 6, 295.
[6]: P. Gary Eller, R. R. Ryan; *Inorg. Chem.*, **1980**, *19*(1) 142–147.

Poster 52

Synthesis of azastibocine dithiocarbamates as potential nanomaterials precursors

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Bismuth sulphide nanoparticles have previously been synthesized in a straightforward manner from organobismuth(III) dithiocarbamates,[1] thereby highlighting the potential for the preparation of analogous antimony-containing compounds.

The coordination chemistry of organoantimony(III) dithiocarbamates remains undeveloped, with only a limited number of examples reported in literature.[2-4] In this study, we report the synthesis and characterisation of a novel series of organoantimony(III) complexes incorporating a *CNC*-pincer ligand, *i.e.* ^{i}PrN(CH$_2$C$_6$H$_4$)$_2$, and a dithiocarbamato moiety. Employing a slightly modified synthetic methodology (Figure 1),[3] complexes bearing dimethyl- (**2**), diethyl- (**3**), and pyrrolidinyldithiocarbamates (**4**) ligands were obtained in good yields. All compounds were characterized by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy. Single-crystal X-ray diffraction analysis provided the solid-state structure of compounds **2** and **4**. The obtained azastibocine dithiocarbamates exhibit both air- and moisture-stability, underscoring their potential utility for the synthesis of nanomaterials. Furthermore, thermogravimetric analysis of compounds **2** and **3** was conducted under both inert and oxidative conditions to assess their thermal behaviour.

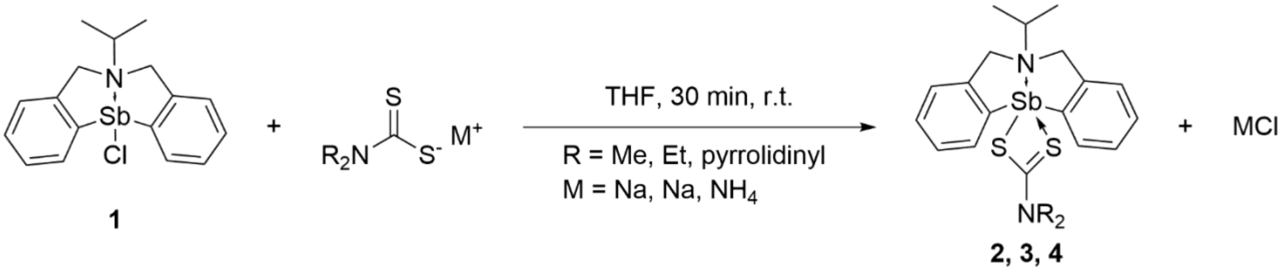

Figure 1 – Synthetic pathway for the synthesis of azastibocine dithiocarbamates

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Poster 53-FP

Exploring Structure and Emission in Manganese(I) Complexes with Bis(imidazo[1,5-*a*]pyridine)methane

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Imidazo[1,5-a]pyridines constitute a prominent class of heterocyclic compounds, widely acknowledged in scientific literature for their remarkable photophysical and biological properties.[1] When suitably functionalized, these molecules serve as effective ligands in the coordination of transition metals,[2] often leading to complexes with noteworthy luminescent behavior.

Despite the growing interest in this class of compounds, bis(imidazo[1,5-*a*]pyridine)methane derivatives, featuring a methylene bridge linking the two heterocyclic units, have received limited attention. To date, only a handful of studies have investigated this subclass,[3] and none have explored their fluorescence properties.

Bis(imidazo[1,5-*a*]pyridine)methane can be readily functionalized through deprotonation of the methylene bridge, followed by alkylation with appropriate alkyl or benzyl halides.[4] The corresponding manganese(I) complexes can be efficiently synthesized in high yields via reaction with $Mn(CO)_5Br$ (Figure 1).

Single-crystal X-ray diffraction analysis reveals that coordination to the manganese(I) center induces a slight bending of the ligand, resulting in loss of symmetry. The photophysical properties and reactivity of these manganese(I) complexes are discussed herein.

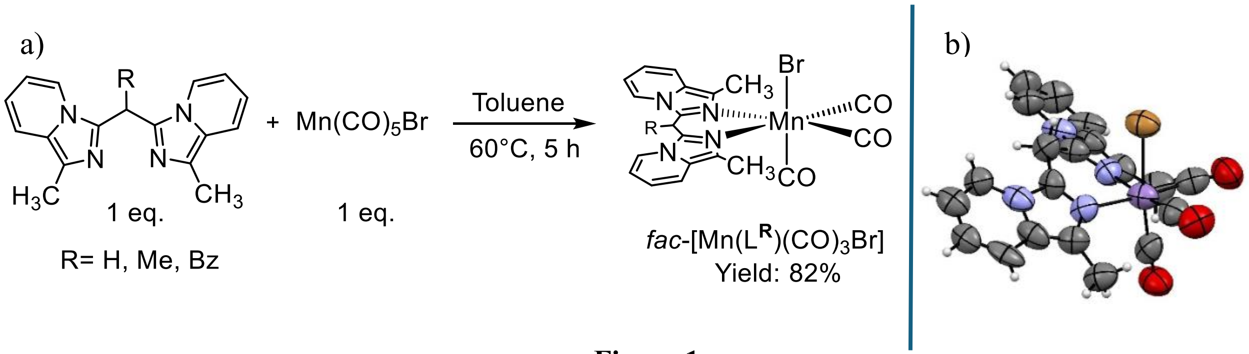

Figure 1

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Poster 54

Novel Anticancer Iron-Iridium Conjugates

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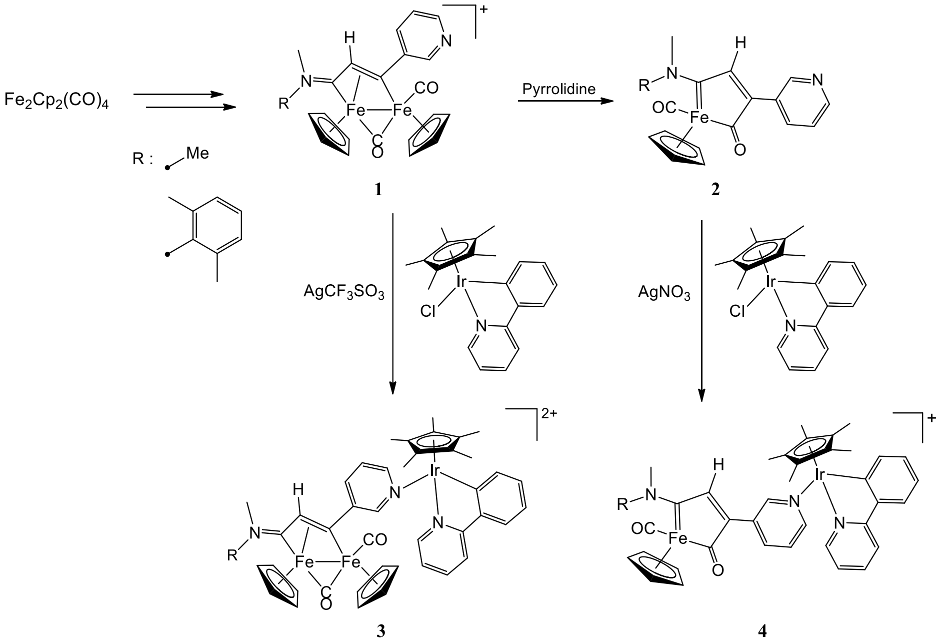
Iron-based metallodrugs show promise as anticancer agents due to iron's non-toxicity, abundance, and potentially reduced side effects.[1] This study explores the synthesis of diiron complexes, specifically $Fe_2Cp_2(CO)_4$ derivatives with bridging vinyliminium ligands (**1**, *Scheme 1*), as versatile scaffolds for novel anticancer therapeutics.[2] These diiron complexes undergo a base-promoted clean fragmentation to form ferracycles (**2**).[3] By incorporating pyridyl-decorated vinyliminium moieties into either the diiron complexes or their monoiron fragmentation products, novel heteronuclear complexes featuring the anticancer iridium scaffold [IrCp*(Phpy)Cl] were synthetized. These new iron-iridium complexes (**3**,**4**), characterized extensively, exhibit strong and selective cytotoxicity against various cancer cell lines (A2780, A549, U87), often surpassing cisplatin's efficacy. Their enhanced anticancer activity is linked to increased iridium uptake in cancer cells, suppressed oxygen consumption, and elevated ROS production. This research establishes a new, straightforward method for developing synergistic heteronuclear anticancer complexes and highlights the potential of diiron vinyliminium complexes as platforms for metallodrug design.



Scheme 1

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Poster 55

Novel Half-Sandwich Ru(II) Complexes with Curcumin and Bisdemethoxycurcumin Conjugates: Synthesis and Evaluation of Antitumor Activity

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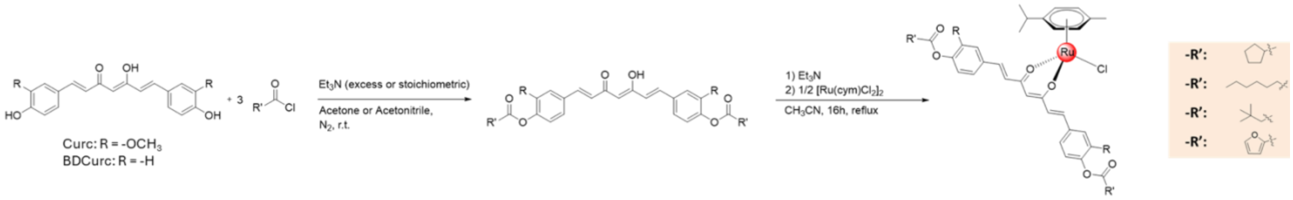
Although curcumin is widely recognized as the main bioactive compound in turmeric, the therapeutic potential of its less-studied analogue, bisdemethoxycurcumin, may have been underestimated and deserves further investigation. In this work, the synthesis of a series of conjugated curcumin and bisdemethoxycurcumin ligands - each featuring a different acyl fragment replacing the hydroxyl groups – along with their corresponding Ru(II)-cymene complexes, is reported (Scheme 1). All compounds were fully characterized in solution and solid state. The in vitro anticancer activity of Ru(II)-cymene complexes was evaluated on a panel of human cancer cell lines (HepG2, Caco-2, MCF-7), including non-tumorigenic models. The complexes exhibited good selectivity and cell-type-specific cytotoxicity compared to the free ligands, particularly against Caco-2 cells, on which they showed even higher efficacy and specificity than cisplatin. Mechanistically, their anticancer activity appears to arise from a multitargeted mode of action: primarily through proteotoxic stress via proteasome inhibition and p62 accumulation, and secondarily through HMG-CoA reductase–mediated downregulation of PCNA expression, ultimately leading to cancer cell death. Overall, the multitarget profile and promising cytotoxic activity of these complexes highlight their potential as candidates for the development of novel metal-based anticancer agents.[1]



Scheme 1: *Synthetic procedure for ligands and complexes*

[1] Pagliaricci, S., Pagliaricci, N., Tombesi, A., Pettinari, C., Cuccioloni, M., Juricic, H., Galindo, A., Fadaei-Tirani, F., Pettinari, R., Marchetti, F. "Ruthenium (II)-bisdemethoxycurcumin conjugate complexes as potent antitumour agents through simultaneous inhibition of 20S proteasome and HMG-CoA reductase." *Dalton Transactions, **2025**.*

Poster 56

Unveiling the Solution-Phase Mechanism of Thiophosphate Formation for Solid-State Electrolytes

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Sulfide-based materials have become central to the design of advanced solid electrolytes for next-generation solid-state batteries. However, their electrochemical performance is highly dependent on the synthesis approach, as different methods can result in distinct structural and compositional features. Among these, wet-chemical strategies are attracting growing attention, despite limited mechanistic insight into the reactions involved. Only a few studies have begun to illuminate the intermediate species and pathways characteristic of these solution-based processes.[1-3]

In this work, we explore the solution chemistry of thiophosphates by examining the reaction between P_4S_{10} and Li_2S. Employing advanced NMR techniques—including T_1 relaxation, pulsed-field gradient diffusion (PGSE), and two-dimensional correlation spectroscopy—we identified and characterized several key intermediates and side products. Our findings indicate that P_4S_{10}, when dissolved in carbon disulfide or toluene, exists as a monomer consistent with its crystal structure. In acetonitrile, its interaction with Li_2S through electrostatic dissolution leads to an adduct that gives rise to a unique intermediate, $P_4S_{11}^{2-}$, confirmed via NMR and single-crystal X-ray diffraction. This species subsequently evolves into a range of thiophosphate compounds, including polymeric $(PS_3^{-})_n$ and smaller anions like $P_2S_6^{2-}$ and $P_2S_8^{2-}$ (Figure 1).[4]

Combining all spectroscopic and structural results, a detailed reaction pathway for the transformation of P_4S_{10} into complex thiophosphate salts emerges, which might serve as a guide for optimizing the synthesis of higher performing sulfide-based materials.

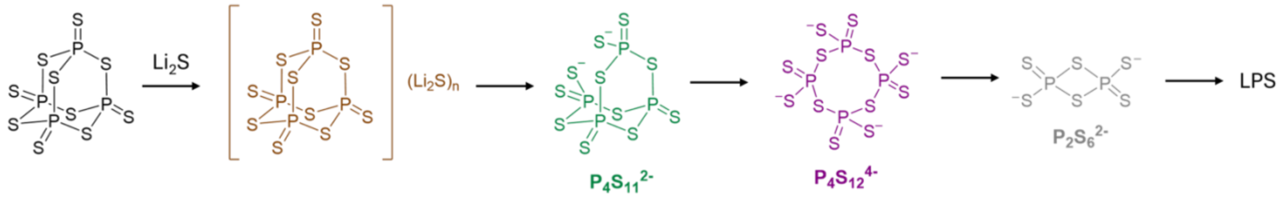

Figure 1

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Poster 57

Advancing C–N Coupling Reactions Through Green Hydrogen Borrowing in Deep Eutectic Media

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The advancement of sustainable catalytic methodologies stands as a central goal in modern green chemistry. Among these, the hydrogen borrowing strategy has gained significant attention for enabling the use of alcohols as alkylating agents through a catalytic sequence involving oxidation, condensation, and reduction steps, typically mediated by a suitable metal catalyst (Figure 1)[1,2]. Despite their synthetic value, these transformations often rely on scarce and costly transition metals and require harsh reaction conditions, which limit their environmental compatibility and industrial applicability. Deep eutectic solvents (DESs), composed of biodegradable and renewable components, are increasingly recognized as green and tunable media for both catalytic and stoichiometric processes. Their versatile physicochemical properties make them well-suited for promoting and modulating catalytic reactions[3].

This project aims to apply hydrogen borrowing methodologies for C–N bond formation, using alcohols and amines as in situ hydrogen donors, within DES-based systems. By employing selected DESs this research seeks to overcome the drawbacks of traditional approaches, improving substrate scope, reaction efficiency, and selectivity under milder, more sustainable conditions. Beyond minimizing environmental impact, this strategy offers the potential to unlock new chemical reactivity, paving the way for a more innovative and eco-conscious future in synthetic chemistry.

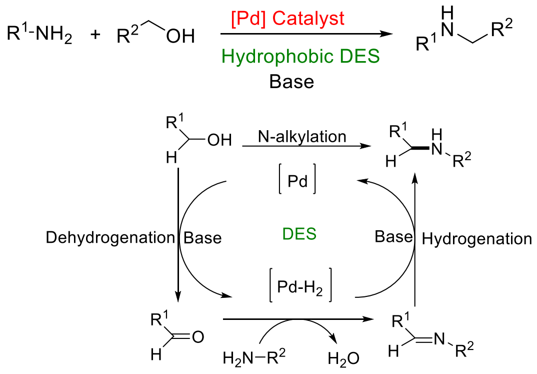

Figure 1. A generalized transition-metal-catalyzed borrowing hydrogen reaction in DES.

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Poster 58

Novel Water-Soluble Half-Sandwich Ruthenium And Osmium Complexes Containing Hydrazinocurcuminoid-Like Ligands

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Curcumin and bisdemethoxycurcumin are natural products found in the rhizome of *Curcuma longa* and studies have demonstrated their therapeutic potential in the fields of chemoprevention and cancer treatment. However, the clinical application of curcuminoids is limited by their low water solubility, resulting in poor oral bioavailability and low chemical stability. In particular, keto-enolic tautomerism in solution was found to be responsible for the rapid degradation of curcumin and modification at this site may lead to superior anticancer activity. Furthermore, extending the conjugated system of azo compounds increases the chemical and thermal stability, and solubility.[1] Based on these considerations, we strategically modified the curcumin scaffold and synthesized a series of half-sandwich Ru(II) and Os(II) complexes incorporating hydrazinocurcuminoid like ligands (Scheme 1). The ligands coordinate the metal centers as neutral *N*,*N*-donors, forming five-membered chelating rings and yielding ionic complexes, as confirmed by X-ray studies in the solid state. The innovative nature of these complexes is highlighted by the asymmetrical nature of their ligands, which differ from the conventional curcuminoid O,O-donors. Notably, the complexes exhibit good solubility and stability in polar solvents, including water. In addition, One ruthenium derivative also exhibited favorable cytotoxicity against A2780 and A2780cis cells, effectively overcoming cisplatin resistance, while showing considerably less activity toward the two non-tumorigenic cell lines tested.

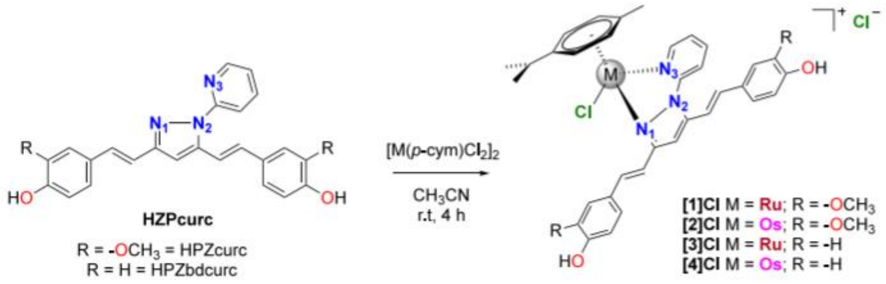

Figure 1. Synthesis of Ru and Os compounds [1]Cl-[4]Cl

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Acknowledgements: *CALL PRIN 2022 PNRR D.D. 1409 666 −(P20222TPZS) CUP N.J53D23014660001 and European Union - NextGenerationEU, Mission 4, Component 2, - VITALITY - CUP J13C22000430001*

Poster 59

MASTER-H2: Development of Advanced Bipyrazole-based MOFs for Hydrogen Storage and CO_2 reduction

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The MASTER-H2 project focuses on the development of advanced Metal-Organic Frameworks (MOFs) for hydrogen storage, a clean and versatile energy carrier[1]. Hydrogen storage presents significant challenges, such as its flammability and low volumetric density, and the MASTER-H2 project aims to overcome these limitations through the use of MOFs. These porous crystalline materials offer high surface areas and tunable pore structures, which are crucial for hydrogen absorption[2]. The MOFs developed in the MASTER-H2 project are based on bipyrazole with various structural modifications. Some specific examples include:

MOFs with the general formula M(BPZ), where M can be: Cd, Co, Cu, Ni, Zn, Pd, Hg, Ag. MOFs derived from H_2Me_2BPZ, H_2Me_4BPZ. MOFs containing functional groups such as NO_2 ($M(BPZNO_2)$) and NH_2 ($M(BPZNH_2)$)[3]. MOFs with ligands such as $H_23,5NH_2BPZ$ and $H_23,3'NH_2BPZ$. MOFs derived from H_2Me_4BDP, H_2Me_4BDPB, H_3BTPP, H_4ttps, and H_2BTZPX. Among these, the MOFs M(BPZNO2) (M = Co, Cu, Zn) have been studied for their dipole-quadrupole interactions with hydrogen, with $Zn(BPZNO_2)$ showing the highest specific surface area (778 m^2/g). Furthermore, mixed-metal Cu/Ni MOFs based on bis(amino)-tagged bipyrazolate have been developed, which have shown potential in the electrochemical reduction of CO_2. These materials demonstrate the formation of metallic CuO nanoparticles during electroreduction. Data indicate that mixed MOFs with a Cu/Ni ratio of approximately 0.05 show the best results in CO_2 reduction.

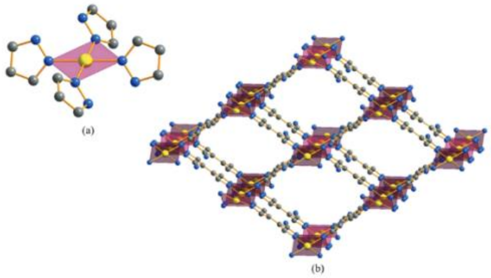

Figure 1. Crystal structure of $Cu(BPZNH_2)$

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