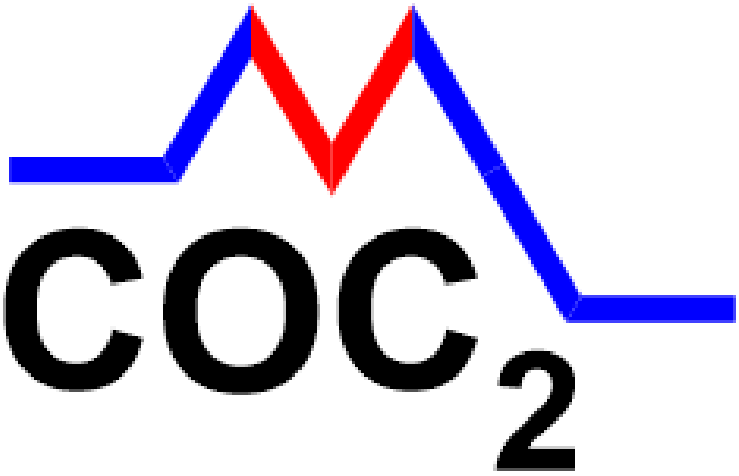


33rd Colloquy on Organometallic Chemistry for Catalysis

September 21 – September 23, 2026

Bayreuth- Germany

UNIVERSITÄT BAYREUTH

Program

General information: Keynote Lecture (KN) 40min + 5 min discussion, Invited Lecture (IL) 30 min + 5 min discussion, Oral Contribution (OC) 20 min + 5 min discussion

Day 1 (21.09.2026) morning session: 9.00 am - 12.15 am

Session chair: Shoubik Das

Opening: 9.00- 9.05 am	**Rhett Kempe**
KN1 9.05 -9.50 am	**Matthias Beller:** *"How to live more sustainably in the future (or Why do we love eating chocolate)?"*
KN2 9.50-10.35 am	**Qiang Liu:** *"Empowering catalytic hydrogenation via anionic metal hydrides"*

Coffee break 10.35 - 11.05 am

IL1 11.05-11.40 am	**Robert Wolf:** *"Cobalt-catalyzed quinoline hydrogenation controlled by carbene ligands"*
IL2 11.40-12.15 am	**Evgeny Pidko:** *"The condition-dependent dance of homogeneous catalytic ensembles: The curious case of RuSNS ester hydrogenation catalysis"*

Break including lunch and social interaction (Options: hiking, sightseeing, golf, please sign in for planning) 12.15 am - 3.20 pm

Day 1 (21.09.2026) afternoon session: 3.20 pm - 6.25 pm

Session chair: Qiang Liu

KN3 3.20-4.05 pm	**Xin-Yuan Liu:** *"Cu/chiral anionic ligand-catalyzed enantioselective radical reactions"*
IL3 4.05-4.40 pm	**Weiping Liu:** *"Fe- and Mn-catalyzed asymmetric borrowing hydrogen reactions"*
IL4 4.40-5.15 pm	**Kathrin Junge:** *"Redox catalysis with molecular-defined manganese catalysts"*
IL5 5.15-5.50 pm	**Biplab Maji:** *"Manganese-catalyzed hydrogen-transfer reactions: From ligand and reaction design to waste valorization"*
IL6 5.50-6.25 pm	**Saravanakumar Elangovan:** *"My research journey in manganese catalysis"*

Poster session, Franconian "Brotzeit" and beer and drinks: 6.30 pm – 10.00 pm maximum

Day 2 (22.09.2026) morning session: 9.00 am - 12.25 am

Session chair: Axel Jacobi von Wangelin

KN4 9.00-9.45 am	**Shoubhik Das:** *"One atom at a time: 3d transition metal photocatalysts for sustainable chemistry"*
IL7 9.45-10.20 am	**Xiaoming Zeng:** *"Hydroborylation and hydroborylsilylation of carboxylic esters enabled by low-valent chromium catalysis"*
IL8 10.20-10.55 am	**Grzegorz Hreczycho:** *"Sustainable and effective methodologies for the synthesis of organometalloidal compounds"*

Coffee break 10.55 - 11.25 am

IL9 11.25-12.00 am	**Piotr Pawluc:** *"Cobalt(II) Schiff base complexes as efficient (pre)catalysts for hydrometallation and cross-coupling reactions"*
OC 12.00-12.25 am	**Aritra Nath:** *"Visible-light-mediated difunctionalization of nonactivated alkenes"*

Break including lunch and social interaction (Options: hiking, sightseeing, golf, please sign in for planning) 12.25 am - 3.30 pm

Day 2 (22.09.2026) afternoon session: 3.30 pm – 6.15 pm

Session chair: Xin-Yuan Liu

KN5 3.30-4.15 pm	**Zhan Lu:** *"CUT Ligands for Iron and Cobalt Catalysis"*
IL10 4.15-4.50 pm	**Guoyin Yin:** *"Nickel chain-walking catalysis"*
IL11 4.50-5.15 pm	**Marko Hapke:** *"3d metal catalysis for the construction and coupling of molecules"*
IL12 5.15-5.40 pm	**Guoying Zhang:** *"High-value transformation of coal-based chemicals and its application in aqueous organic flow battery energy storage"*
IL13 5.40-6.15 pm	**Tao Tu:** *"Fabrication of solid molecular catalysts and valorization of platform molecules"*

Poster session, dinner and beer and drinks: 6.15 pm – 10.00 pm maximum

Day 3 (23.09.2026) morning session: 9.00 am - 12.25 am

Session chair: Zhan Lu

KN6 9.00-9.45 am	**Axel Jacobi von Wangelin:** *"Explorations into 3d-metal catalysis in dark and light"*
IL14 9.45-10.05 am	**Stefan Weber:** *"Iron in a macrocyclic PNPN environment – electronic structure and catalysis"*
IL15 10.05-10.40 am	**Dragos-Adrian Rosca:** *"Compressing the spin ladder: Understanding electronic structure for reactivity control in earth-abundant transition metal catalysis"*

Coffee break 10.40 - 11.10 am

IL16 11.10-11.45 am	**Jarl Ivar van der Vlugt:** *"Coordination chemistry-based strategies for C(sp^3)-H amination catalysis"*
IL17 11.45-12.20 am	**Robert Langer:** *"Metal–ligand cooperation and catalysis driven by carbodiphosphoranes: Harnessing earth-abundant aluminum for metal–metal-cooperative bond activation"*
"Goodbye" 12.20-12.25 am	**Rhett Kempe**

Keynote Lectures

KN 1 **"How to live more sustainably in the future (or Why do we love eating chocolate)?"**
Matthias Beller

KN 2 **"Empowering catalytic hydrogenation via anionic metal hydrides"**
Qiang Liu

KN 3 **"Cu/chiral anionic ligand-catalyzed enantioselective radical reactions"**
Xin-Yuan Liu

KN 4 **"One atom at a time: 3d transition metal photocatalysts for sustainable chemistry"**
Shoubik Das

KN 5 **"CUT Ligands for Iron and Cobalt Catalysis"**
Zhan Lu

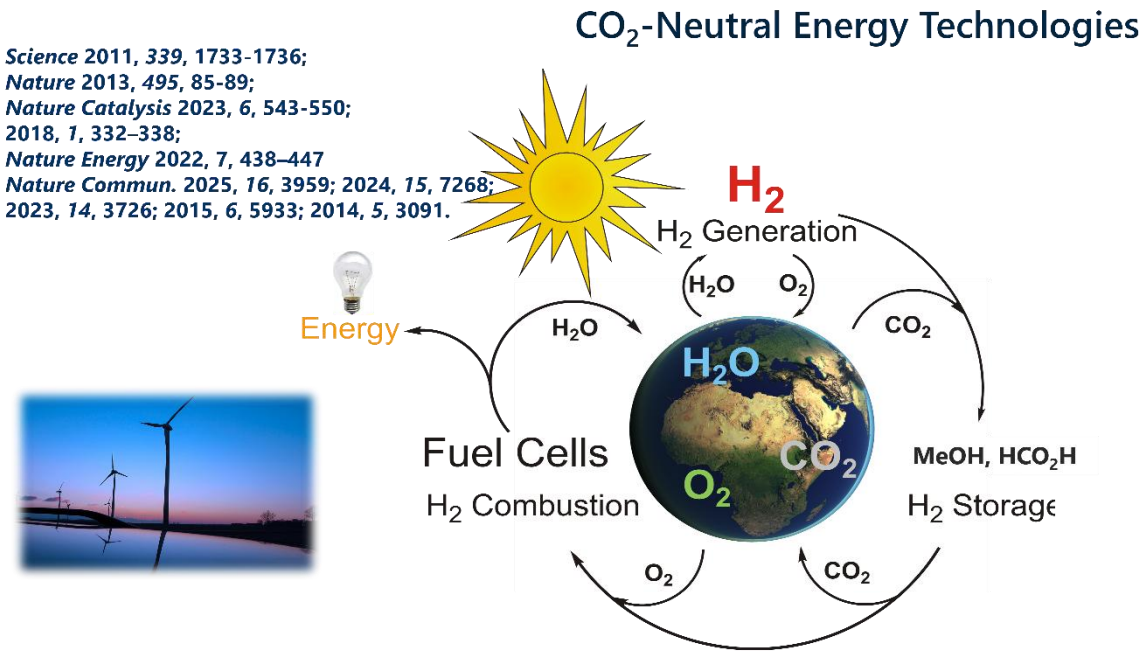
KN 6 **"Explorations into 3d-metal catalysis in dark and light"**
Axel Jacobi von Wangelin

Lectures

How to Live More Sustainably in the Future (or Why Do We Love Eating Chocolate)?

Matthias Beller

Leibniz-Institute for Catalysis, University of Rostock, Albert-Einstein-Str. 29a, 18059 Rostock, Germany
Email: matthias.beller@catalysis.de



CO_2 to C_{2+}: *Angew. Chem. Int. Ed.* 2022; DOI: 10.1002/anie.202200723; CO_2 to MeOH: *Chem. Soc. Rev.* 2021, *50*, 4259-4298.

Ensuring a reliable and sustainable supply of food, energy, and consumer goods for 10 billion people is the central challenge we will face in the future. In the coming years and decades, it will be crucial to develop new, much more efficient processes and technologies to meet this demand. In this presentation, I will share two examples of our current scientific research how to contribute to the development of green energy technologies and carbon neutrality in the chemical industry.

Empowering Catalytic Hydrogenation via Anionic Metal Hydrides

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Catalytic hydrogenation stands as a foundational and indispensable transformation in synthetic chemistry. However, conventional catalytic systems suffer from a chronic overreliance on neutral metal hydride intermediates as the active species [1]. Constrained by their inherently limited hydricity, these systems often fail to efficiently convert inert substrates such as esters and amides[2]. Consequently, the fine chemical industry remains shackled to stoichiometric metal hydride reductants, which are plagued by low atom economy, severe environmental penalties, and an intractable inability to control stereoselectivity.

To address these long-standing challenges, we pioneer a new strategy to establish a "novel anionic metal hydride catalytic system [1-5]." By engineering transition metal hydride intermediates supported by multidentate anionic ligands and harnessing the synergistic interplay of counter-cations, we successfully construct the highly reactive anionic metal hydride species. This architectural blueprint preserves formidable hydride-reducing power while enabling a robust catalytic cycle utilizing H_2 as the terminal reductant. By revolutionizing the catalytic paradigm at the fundamental level of the intermediate's charge state, we overcome the traditional perception of anionic metal hydride complexes solely as stoichiometric reagents, and fundamentally expand the capability boundaries of catalytic hydrogenation reactions.

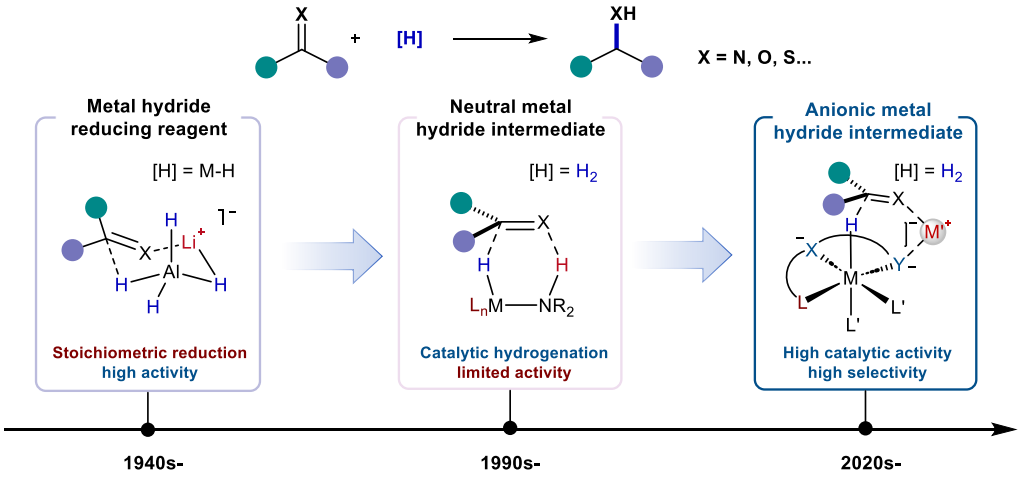


Fig.1. Anionic Metal Hydrides: From Stoichiometric Reagents to Highly Reactive Catalysts

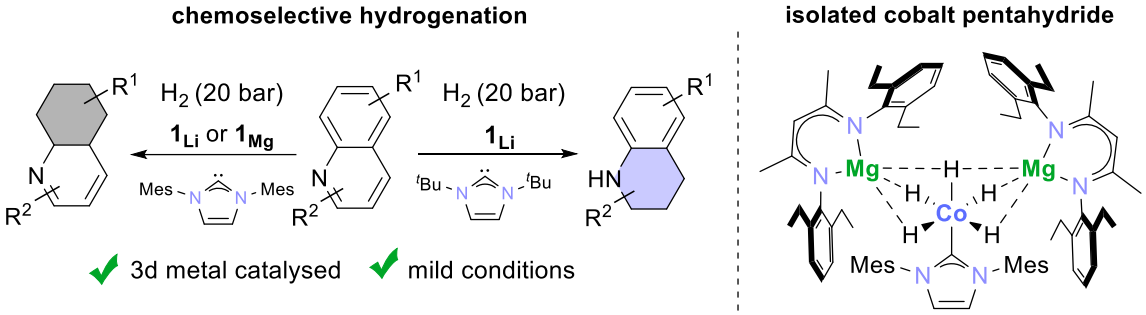
Literature:

[1] Y. Wang, S. Liu, H. Yang, H. Li, Y. Lan, Q. Liu, *Nat. Chem*. **2022**, *14*, 1233-1241.
[2] H. Yang, S. Liu, H. Dong, H. Huang, Y. Wang, W. Hao, Y. Lan, Q. Liu, *J. Am. Chem. Soc*. **2025**, *147*, 13491–13501.
[3] M. Wang, S. Liu, H. Liu, Y. Wang, Y. Lan, Q. Liu, *Nature* **2024**, *631*, 556–562.
[4] C. Liu, X. Liu, Q. Liu, *Chem*. **2023**, *9*, 2585-2600.
[5] C. Liu, M. Wang, Y. Xu, Y. Li, Q. Liu, *Angew. Chem. Int. Ed.* **2022**, *61*, e202202814.

Cobalt-Catalyzed Quinoline Hydrogenation Controlled by Carbene Ligands

Robert Wolf, Franziska Gilch, Tobias Villing

University of Regensburg, 93040 Regensburg, Germany



Quinoline hydrogenation serves as a benchmark for developing highly selective, sustainable 3d-metal catalysts capable of preparing essential heterocyclic building blocks.[1] Until now, carbocycle-selective quinoline hydrogenation has mainly relied on precious-metal precatalysts. Here, we introduce the carbocycle-selective hydrogenation of (iso)quinolines using 3d transition metal catalysts. By combining cobaltates $[M(THF)_x\{Co(COD)_2\}]$ (where M = Li, Mg, and COD = 1,5-cyclooctadiene)[2,3] with *N*-heterocyclic carbenes, we achieve ligand-controlled chemoselectivity. Using the aryl-substituted carbene IMes (1,3-bis-(2,4,6-trimethylphenyl)imidazol-2-ylidene), selective hydrogenation of the carbocyclic ring occurs under mild conditions (30 °C, 20 bar H_2). In contrast, the alkyl-substituted I*t*Bu (1,3-di-tert-butylimidazol-2-ylidene) directs reduction toward the *N*-heterocycle. Catalyst poisoning experiments indicate different catalytic pathways: IMes favors a homotopic route, likely involving hydridocobalt intermediates, whereas I*t*Bu likely leads to a heterotopic cobalt catalyst.[4],[5] The isolation of a quinoline cobalt complex and a magnesium-capped cobalt(III) pentahydride complex $[(^{Dep}BDI)Mg]_2[(IMes)Co(H)_5]$ offers insights into potential catalytic intermediates. This research presents a base-metal approach for the chemoselective hydrogenation of fused heteroarenes and emphasizes the mechanistic importance of NHC ligands.

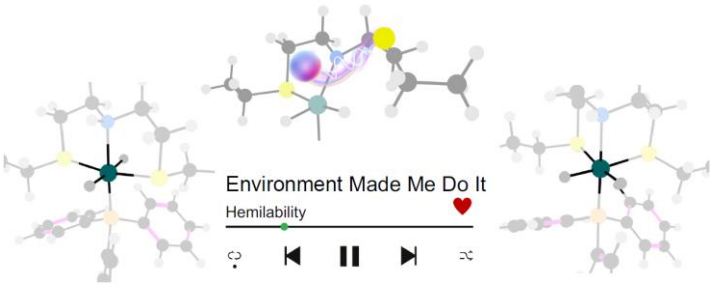
Literature:

[1] M. P. Wiesenfeldt, Z. Nairoukh, T. Dalton, F. Glorius, *Angew. Chem. Int. Ed.* **2019**, *58*, 10460.
[2] a) K. Jonas (Studiengesellschaft Kohle mbH), US4169845 A, **1977**; b) K. Jonas, R. Mynott, C. Krüger, J. C. Sekutowski, Y.-H. Tsay, *Angew. Chem.* **1976**, *88*, 808.
[3] M. Gawron, F. Gilch, D. Schmidhuber, J. A. Kelly, T. M. Horsley Downie, A. Jacobi von Wangelin, J. Rehbein, R. Wolf, *Angew. Chem. Int. Ed.* **2024**, *63*, e202315381.
[4] P. Büschelberger, E. Reyes-Rodriguez, C. Schöttle, J. Treptow, C. Feldmann, A. J. von Wangelin, R. Wolf, *Catal. Sci. Technol.* **2018**, *8*, 2648–2653.
[5] R. H. Crabtree, *Chem. Rev.* **2012**, *112*, 1536–1554.

The Condition-Dependent Dance of Homogeneous Catalytic Ensembles: The Curious Case of RuSNS Ester Hydrogenation Catalysis

Sumeia Yassiri, Alexander Kolganov, Rick Louwersheimer, Martino Saita, Evgeny Uslamin, Evgeny Pidko

Department of Chemical Engineering, Delft University of Technology, The Netherlands



Rational design of homogeneous catalysts commonly begins with a single, fixed molecular structure. Under catalytic conditions, however, activation, ligand rearrangement, substrate and product binding, ion pairing, inhibition, and deactivation generate ensembles of interconverting species whose populations evolve throughout the reaction.[1] In our high-throughput in silico survey of Ir(III), Ru(II), and Mn(I) complexes, configurational diversity was found across all three metals, while up to 70% of Ru and Mn complexes give multiple thermodynamically accessible stereoisomers.[2] Identifying the species formed under the reaction conditions and responsible for catalytic turnover is therefore a general challenge in homogeneous catalysis. Our recent studies on RuSNS pincer ester hydrogenation catalyst provide a well-defined case that reveals the complex relationship between catalyst speciation, reaction conditions, and performance.

RuSNS pincer complexes are among the most active catalysts for ester hydrogenation.[3,4] Their optimization pushed TONs above 30,000 in the hydrogenative depolymerization of post-consumer PET,[5] illustrating that metal abundance, catalyst loading, lifetime, and process efficiency should be considered together when assessing sustainability. Time-resolved kinetic studies, dynamic and CEST NMR spectroscopy, kinetic modelling, and DFT calculations show that the activated catalyst forms an interconverting ensemble of meridional and facial RuSNS dihydrides.[6] The mer-isomer carries catalytic turnover, whereas the fac-form is essentially inactive, while the interconversion between these two forms is highly condition-dependent. In particular, the presence of the alkoxide base promotor controls their speciation through a cation-assisted pathway involving reversible dissociation of a sulfur donor arm. These findings call for a departure from fixed-structure representations toward a holistic, condition-dependent ensemble description of the catalyst system.

Literature:

[1] W. Yang, G. A. Filonenko, E. A. Pidko, *Chem. Commun.* **2023**, *59*, 1757–1768.
[2] A. V. Kalikadien, N. J. van der Lem, C. Valsecchi, L. Lefort, E. A. Pidko, *Digital Discovery* **2025**, *4*, 2033–2044.
[3] D. Spasyuk, S. Smith, D. G. Gusev, *Angew. Chem. Int. Ed.* **2013**, *52*, 2538–2542.
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[6] S. Yassiri, E. Huang, M. Saita, A.A. Kolganov, E. A. Uslamin, E. A. Pidko, submitted.

Cu/Chiral Anionic Ligand-Catalyzed Enantioselective Radical Reactions

Xin-Yuan Liu

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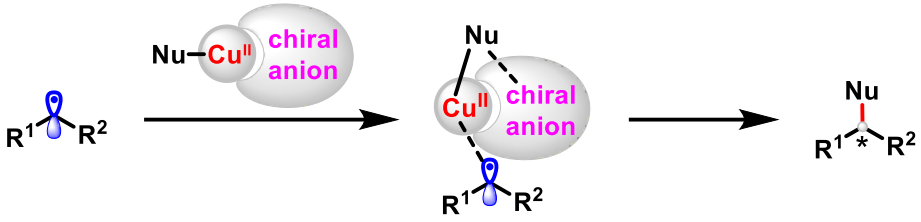

Radical reactions have emerged as one of the most powerful and efficient tools for the construction of carbon–carbon and carbon–heteroatom bonds in organic synthesis. However, the development of catalytic asymmetric radical reactions to realize the stereochemical control of open-shell intermediates still remains a formidable challenge owing to the high reactivity of such free radical species. To solve this problem, our group has developed copper(I)/chiral anionic ligand catalyst to achieve a number of enantioselective radical transformations: such as the C–H functionalization, alkene difunctionalization and cross-coupling of alkyl halides, etc. The role of chiral anionic ligand is dual: it not only tunes the reducing capability of copper for the reaction initiation but also provides excellent stereocontrol induction of the reactive radical species through multiple models.

Literature:

[1] Zhang, Y.-F.; Wang, B.; Chen, Z.; Liu, J.-R.; Yang, N.-Y.; Xiang, J.-M.; Liu, J.; Gu, Q.-S.; Hong, X.; Liu, X.-Y. *Science* **2025**, *388*, 283.

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[3] Tian, Y.; Li, X.-T.; Liu, J.-R.; Cheng, J.; Gao, A.; Yang, N.-Y.; Li, Z.; Guo, K.-X.; Zhang, W.; Wen, H.-T.; Li, Z.-L.; Gu, Q.-S.; Hong, X.; Liu, X.-Y. *Nat. Chem.* **2024**, *16*, 466-475.

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[5] Wang, F.-L.; Yang, C.-J.; Liu, J.-R.; Yang, N.-Y.; Dong, X.-Y.; Chang, X.-Y.; Li, Z.-L.; Xu, G.-X.; Yuan, D.-L.; Zhang, Y.-S.; Gu, Q.-S.; Hong, X.; and Liu, X.-Y. *Nat. Chem.* **2022**, *14*, 949-957.

[6] Dong, X.-Y.; Zhang, Y.-F.; Ma, C.-L.; Gu, Q.-S.; Wang, F.-L.; Li, Z.-L.; Jiang, S.-P.; Liu, X.-Y. *Nat. Chem.* **2019**, *11*, 1158-1166.

Fe and Mn-catalyzed asymmetric borrowing hydrogen reactions

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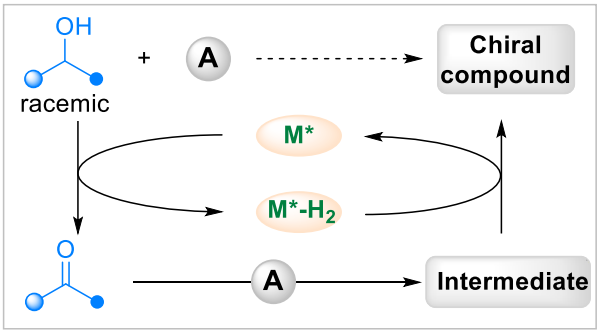

Alcohols are benign and sustainable resources, which are abundantly available from a large number of biomass materials.[1] However, the high stability of the C-O and *β*-C-H bonds in alcohols presents significant synthetic challenges, often necessitating the use of stoichiometric halogenating agents or oxidants to convert alcohols into alkyl halides or carbonyl compounds. These traditional approaches typically generate stoichiometric byproducts or waste, requiring tedious multi-step operations and intermediate purifications. Transition metal-catalyzed borrowing hydrogen (BH) reactions could reduce the need for intermediate isolation, external oxidants and reductants, has demonstrated as an atom- and step-economical platform in organic synthesis.[2]

In recent years, our group focused on the development of earth-abundant metal-catalyzed BH reactions.[3] Specifically, our major discoveries on asymmetric BH transformations include: a) Iron-catalyzed asymmetric amination of secondary alcohols;[4] b) Manganese-catalyzed asymmetric hydrophosphination of allylic alcohols to construct remote *C,P*-dual-chiral hydroxyphosphine compounds;[5] c) Manganese-catalyzed asymmetric transformations to access chiral tetrahydroquinolines.[6]

Literature:

[1] a) K. Barta, P. C. Ford, *Acc. Chem. Res.* **2014**, *47*, 1503-1512; b) T. P. Vispute, H. Zhang, A. Sanna, R. Xiao, G. W. Huber, *Science* **2010**, *330*, 1222-1227.
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Redox Catalysis with Molecular-Defined Manganese Catalysts

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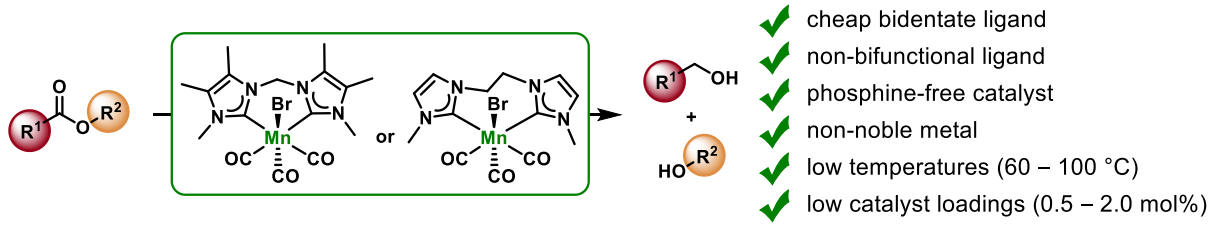
The cost-effective and waste-free synthesis of materials, life science goods and all kinds of organic products require efficient chemical transformations. In this regard, development of more active and selective catalysts constitutes a key factor for achieving improved processes and providing the basis for a sustainable chemical industry. Despite continuous advancements in all areas of catalysis, organic syntheses as well as the industrial production of most chemicals can be improved significantly in terms of sustainability and efficiency.

In this contribution, it will be shown how new and improved homogeneous non-noble metal-based catalysts can be developed. Specifically, the phenomenon of cooperative catalysis will be addressed in the context of non-noble metal-pincer and bidentate catalysts for the reduction of carboxylic acid esters.[1] In detail, it will be demonstrated that recently developed pincer manganese catalysts enable catalytic hydrogenation processes with high yields and unprecedented selectivity. Especially, the influence of different substitution patterns at the phosphorous binding site as well as at the metal site on the catalytic performance of these complexes is presented.[2]



In addition, the principle of cooperative catalysis will be shown in the context of modern phosphorous-free and or ligand free Mn catalysts for hydrogenation reactions.[3,4] By rational design novel ligands and complexes have been synthesized, which allow for unprecedented efficiency in such transformations.[5]

Literature:

[1] S. Elangovan, C. Topf, S. Fischer, H. Jiao, A. Spannenberg, W. Baumann, R. Ludwig, K. Junge, M. Beller, *J. Am. Chem. Soc.* **2016**, *138,* 8809−8814.
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[3] V. Papa, Y Cao, A. Spannenberg, K. Junge, M. Beller, *Nat. Catal.* **2020**, *3*, 135.
[4] N. Both, J. Fessler, A. Vincenzi, K. Andres, K. Junge, M. Beller, *ChemCatChem* **2024**, *9*, e202301562.
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Manganese-Catalyzed Hydrogen-Transfer Reactions: From Ligand and Reaction Design to Waste Valorization

Biplab Maji

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The global emphasis on sustainable chemistry has motivated chemists to develop catalysts based on Earth's abundant first-row-transition metals as an alternative to the precious noble metals. In recent years, significant progress has been made using iron, cobalt, nickel, and copper as non-noble transition metal catalysts. In this regard, manganese, the third most abundant transition metal in the Earth's crust (after iron and titanium), is an attractive metal of choice. In the recent years, a considerable development using low-valent manganese complexes in hydrogenation, dehydrogenation, and their cascade reactions have been made.[1] Our research focuses on developing a robust manganese catalyst based on cheap and readily available starting materials. Applications of such recently developed manganese catalysts for alkylation and olefination reactions will be discussed in this short presentation.[2-7] The reactions are highly environmentally benign, producing only water (and hydrogen gas) as a by-product. We will showcase that a phosphine-free manganese catalyst can be used as the catalyst for the olefination of methyl-substituted heteroarenes with primary alcohols.[2] We will demonstrate the importance of ligand structure for the development of the C-alkylation reaction of nitriles compared to the ketones.[3] We will also display a novel bench-stable manganese catalyst that served as an efficient catalyst for the stereoselective synthesis of carbocyclic compounds.[4] Multi-substituted alicyclic compounds are omnipresent as the core structure in a wide range of pharmaceutical agents, natural products, and materials. Despite the substantial importance of these multifaceted structural motifs, their modular synthetic routes are limited. Large availability and bench stability of the starting precursors would ideally make our process attractive and will allow the uniform synthesis of different families of cycloalkanes. The same catalyst can be applied for the chemodivergent hydrogenation of nitriles,[5] anti-Markovnikov hydroamination reactions,[6] and the valorization of vicinal glycols.[7] The importance of the bifunctional ligand design and hemilability in the sulfur-arm is the key design principle for such catalysis.[8,9] Finally, the applications of these chemistry will be shown for the upcycling of plastic waste to valuable chemicals.[10]

Literature:

[1] B. Maji, M. K. Barman, *Synthesis* **2017**, *49*, 3377.
[2] M. K. Barman, S. Waiba, B. Maji, *Angew. Chem. Int. Ed.* **2018**, *57,* 9126.
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[10] S. Das Adhikary, S. K. Jana, B. Maji, *Angew. Chem. Int. Ed.* **2025**, *64*, e202513145.

My Research Journey in Manganese Catalysis

Saravanakumar Elangovan

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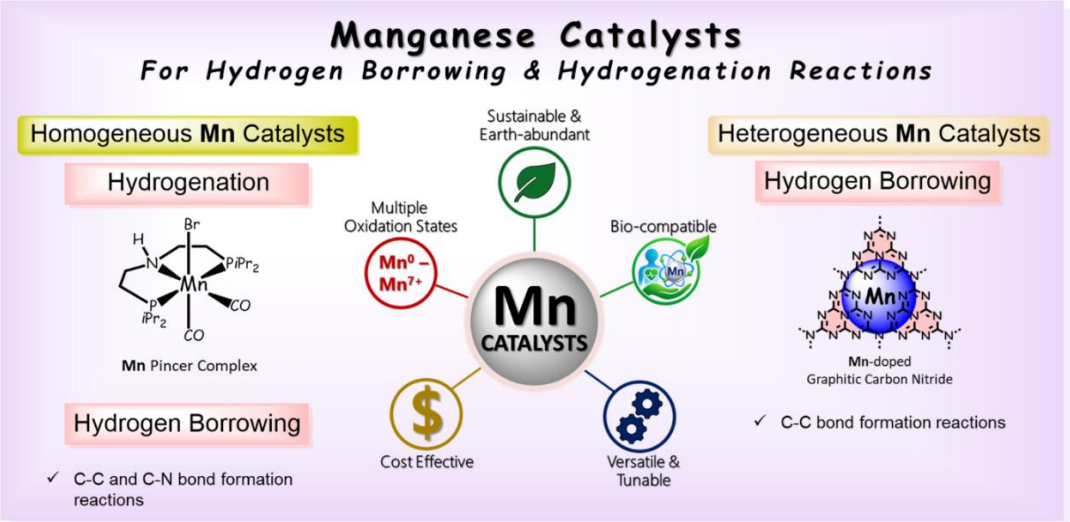

Replacing precious metals with inexpensive and abundant transition metals is a hot area of research, given sustainability and economic considerations. Especially, the use of manganese is interesting due to its abundance (3rd most abundant transition metal), bio-relevant and inexpensive. Since 2016, manganese-based homogeneous catalysts have been extensively explored for hydrogenation and hydrogen-borrowing reactions.[1,2] However, manganese heterogeneous catalysis is comparatively underexplored.

In this talk, I present my research journey with manganese catalysts, including homogeneous and heterogeneous catalysts, and their application in hydrogenation and hydrogen-borrowing reactions.[3] In the first part, I discuss the development of homogeneous pincer manganese catalysts for hydrogenation and hydrogen-borrowing reactions. In the second part, I discuss our recent development of a recyclable graphitic carbon nitride (gCN)-supported manganese-based heterogeneous catalyst for C–C bond formation reaction via hydrogen borrowing pathway, for the direct β-alkylation of secondary alcohols with primary alcohols[4] as well as the selective Csp^3-monoalkylation of fluorenes with a wide range of alcohols.[5]

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One Atom at a Time: 3d Transition Metal Photocatalysts for Sustainable Chemistry

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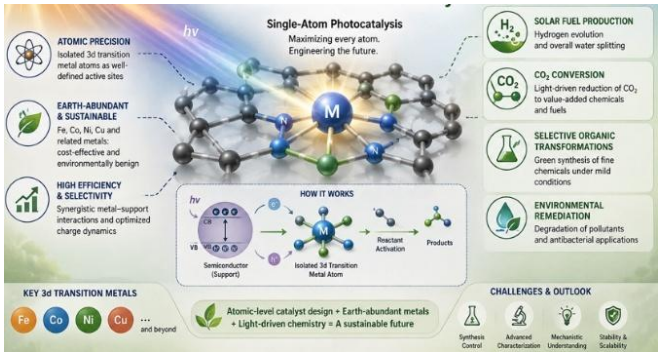
The transition toward sustainable chemical processes requires catalytic technologies that combine high efficiency and selectivity with reduced dependence on scarce and expensive materials. Single-atom photocatalysis has emerged as a promising strategy in this direction, bridging the advantages of homogeneous molecular catalysts and heterogeneous photocatalytic materials. By dispersing catalytically active metals as isolated atoms on suitable supports, single-atom photocatalysts can maximize metal utilization while creating well-defined and tunable active sites for light-driven chemical transformations. This presentation will provide an overview of the growing role of earth-abundant 3d transition metals, including Fe, Co, Ni, Cu, and related elements, in single-atom photocatalysis. Particular attention will be given to how the local coordination environment, electronic structure, metal–support interactions, and photoinduced charge-transfer processes determine catalytic activity, selectivity, and stability. The unique ability of isolated metal centers to facilitate charge separation and activate challenging chemical bonds offers opportunities to design photocatalytic systems with improved performance under mild reaction conditions.



Representative applications in sustainable chemistry will be discussed, including solar fuel production, CO_2 conversion, hydrogen evolution, selective organic transformations, and environmental remediation**.** The presentation will also highlight current challenges in the synthesis, characterization, mechanistic understanding, and long-term stability of single-atom photocatalysts. Overall, the emerging combination of atomic-level catalyst design, earth-abundant 3d transition metals, and light-driven chemistry provides a compelling platform for developing more resource-efficient and sustainable catalytic processes. Understanding these systems at the atomic and electronic levels will be essential for translating their fundamental advantages into practical technologies for a more sustainable chemical future.

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Hydroborylation and Hydroborylsilylation of Carboxylic Esters Enabled by Low-Valent Chromium Catalysis

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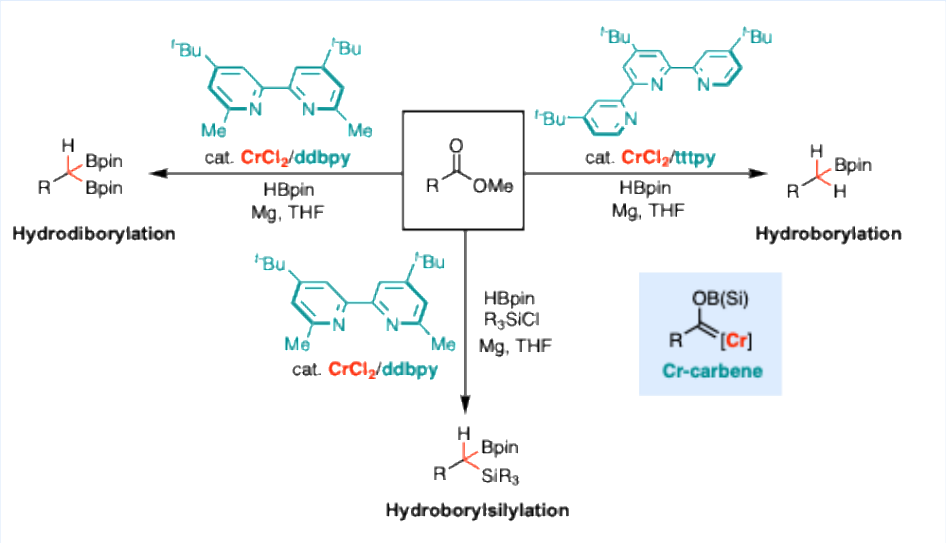

Fischer carbene complex is an archetype of organometallics bearing a carbon-metal double bond, and its discovery in the 1960s marked a paradigm shift in organometallic chemistry, and expanded the toolbox of organic synthesis.[1] However, these reactive intermediates are usually derived from high-energy starting materials such as activated diazo compounds and moisture-sensitive alkyllithium reagents.[2] Safety concerns and the complexity of these experimental procedures have stimulated the search for simpler and milder alternatives using naturally abundant and thermodynamically stable precursors. We report here a complementary strategy for the catalytic generation of boryloxy- or silyloxycarbene–chromium complexes from simple aryl esters, enabled by a combination of pinacolborane/chlorosilane, magnesium metal, and a chromium catalyst. The reaction converts the ester to mono-, bis(boryl)alkanes or borylsilylalkanes—valuable intermediates for synthetic diversification—depending on the choice of bipyridine or terpyridine ligand. Multiple lines of evidence, including cyclopropanation, deuterium quenching, and DFT analysis, support a low-energy pathway involving chromium–carbene intermediates by the cleavage of unactivated acyl C–O bonds.[4] The ligand-controlled bifurcation arises from subtle energy differences between quintet and triplet pathways for hydroborylation, elucidated by the DFT calculations.

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Sustainable and effective methodologies for the synthesis of organometalloidal compounds

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Modern chemical synthesis places a strong emphasis on sustainability by minimizing the use and generation of hazardous substances. This objective can be achieved through the application of catalysts that provide access to alternative reaction pathways, improve process selectivity, and enable the use of less reactive substrates [1].

First-row transition-metal complexes represent an important and extensively studied class of homogeneous catalysts. These systems are often characterized by relatively straightforward synthesis, high stability, and excellent activity and selectivity in reactions such as hydrogenation, hydroboration, hydrosilylation, and various bond-forming processes [2–4]. An important advantage of these catalysts is their tunable reactivity and selectivity, which can be controlled by modifying the reaction conditions or the ligand structure.

In this communication, I will present selected methods for the synthesis of organosilicon and organoboron compounds catalyzed by first-row transition-metal complexes. The developed methodologies enable ligand-controlled transformations that follow the principles of sustainable chemistry and provide access to valuable classes of functional compounds [5–7].

Acknowledgments: This work was supported by a National Science Centre Grant: UMO-2024/53/B/ST4/03116.

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Cobalt(II) Schiff Base Complexes as Efficient (Pre)catalysts for Hydrometallation and Cross-Coupling Reactions

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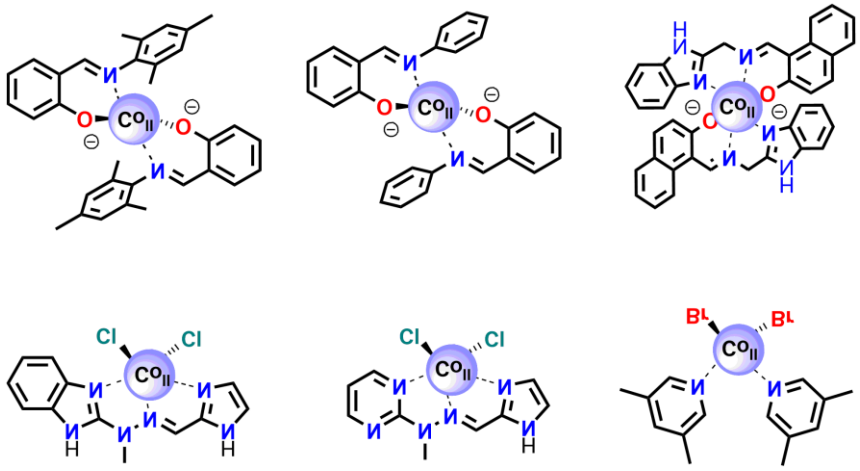
Hydrometallation and cross-coupling reactions are key catalytic transformations widely applied in the synthesis of functionalized organic and organometallic compounds. Traditionally, these processes have relied on noble-metal catalysts, particularly palladium, platinum, and rhodium. However, their high cost and limited sustainability have driven the development of more economical and environmentally benign alternatives based on Earth-abundant first-row transition metals (*3d* elements), such as iron, cobalt, and nickel.

In this context, we have developed efficient and selective catalytic systems for the hydrosilylation and hydroboration of functionalized alkenes and alkynes.[1-5] These systems employ cobalt(II) complexes bearing *N,N,N*-, *N,O*- or *N,N,O*-donor Schiff-base ligands, combined with alkali-metal trialkylborohydrides or HMDS as co-catalysts. Building on this work, simple cobalt(II) pyridine and phenoxyiminato complexes were also explored as catalyst precursors for Suzuki-Miyaura and Negishi cross-coupling reactions.[6]

An important aspect of the research involves the optimization of catalytic procedures to improve the efficiency and selectivity of the investigated systems, as well as efforts to elucidate the mechanisms of the catalytic transformations. Particular attention will be devoted to understanding how the ligand structure influences the activity and selectivity of cobalt-based (pre)catalysts.



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Visible-Light-Mediated Difunctionalization of Nonactivated Alkenes

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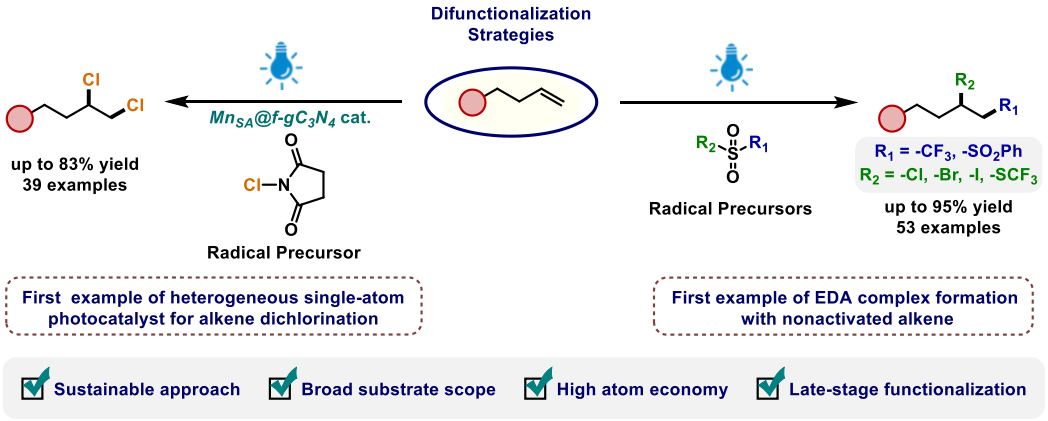
Visible-light-mediated difunctionalization of nonactivated alkenes offers a sustainable and efficient strategy for constructing diverse molecular frameworks relevant to medicinal chemistry, polymer science, and synthesis of fine chemicals, yet the low reactivity of nonactivated C–C double bonds remains a significant challenge.[1] Our group has developed a visible light driven Mn single-atom photocatalytic platform for the vicinal dichlorination of nonactivated alkenes using N-chlorosuccinimide as a mild chlorinating reagent. The catalyst features atomic dispersion of Mn on aryl-amino-substituted graphitic carbon nitride (f-gC_3N_4), enabling efficient C–Cl bond formation across a broad range of terminal, internal, cyclic, and functionalized alkenes, providing access to vicinal dichlorides under mild conditions.[2] Building on this approach to visible-light activation of nonactivated alkenes, we subsequently explored direct radical pathways enabled by electron donor-acceptor (EDA) complex formation with sulfonyl-based precursors.[3] This led to a catalyst-free difunctionalization strategy that circumvents the need for specially designed substrates commonly required in EDA-based approaches.[4] These expands the applicability of this strategy to a broad range of nonactivated alkenes. Using photons as traceless reagents, reactive radical intermediates undergo addition to nonactivated alkenes, affording diverse difunctionalized products, including chlorotrifluoromethylated, iodosulfonylated, bromotrifluoromethylated, iodotrifluoromethylated, and thiotrifluoromethyl-sulfonylated products, with excellent functional-group tolerance and applicability to the late-stage functionalization of bioactive and drug molecules, as well as gram-scale synthesis. Computational studies further guided radical selection and provided mechanistic and regioselectivity insights.[3] Together, these studies demonstrate that visible light can provide complementary pathways, from metal-centered photocatalysis to catalyst-free radical activation, for overcoming the intrinsic challenges of nonactivated alkene difunctionalization and enabling versatile molecular diversification.



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CUT Ligands for Iron and Cobalt Catalysis

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In the past several decades, many efficient reactions have been developed by using precious metals catalysis such as palladium, rhodium, iridium, and gold. These methods provide new materials as a solid foundation for numerous technological innovations. Compared with precious metals, the earth-abundant transition metals iron and cobalt widely exist in nature and are prone to change valence and spin states as well as coordination modes, which provides the possibility for diversified reactions. However, because there is no mature law of ligand design, its high selective catalysis has great challenges, such as few reaction types, low efficiency and selectivity.

Based on the characteristics of redox active ligands, the applicant proposed, designed and constructed a series of new **C**hiral **U**nsymmetric *NNN*-**T**ridentate (**CUT**) neutral or anionic ligands and their iron and cobalt complexes, realized the efficient and selective asymmetric hydroelementation of olefins, and also proposed combined catalysis, ligand relay catalysis, and other strategies to realize the asymmetric sequential reaction of alkynes. These results provide some new catalysts, new catalytic systems, and new ideas for solving the scientific problems such as catalytic efficiency and selectivity-control in the field of earth-abundant transition metal catalysis.

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Nickel Chain-Walking Catalysis

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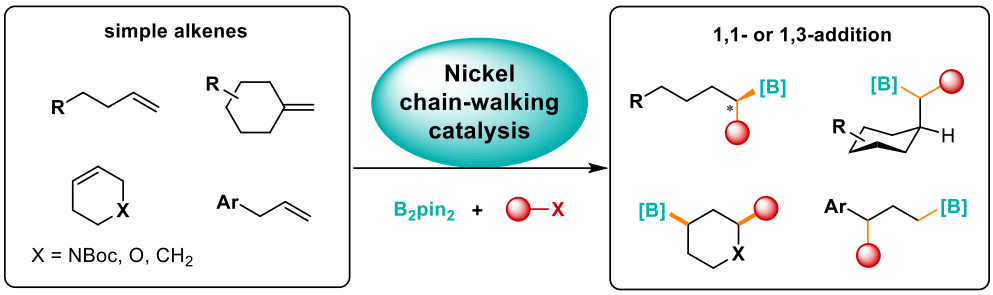

Chain-walking offers extensive opportunities for innovating synthetic methods that involve constructing chemical bonds at unconventional sites[1]. This approach provides previously inaccessible retrosynthetic disconnections in organic synthesis. Through chain-walking, transition metal-catalyzed alkene difunctionalization reactions can take place in a 1, n-addition (n≠2) mode. Unlike classical 1,2-regioselective difunctionalization reactions, there remains a scarcity of reports regarding migratory patterns. Moreover, the range of olefins utilized in these studies is quite limited. The Yin group focuses on developing valuable migratory difunctionalization reactions of alkenes through chain-walking[2-5]. Our focus was on carboboration of alkenes utilizing nickel catalysis. The incorporation of a versatile boron group introduces a wealth of possibilities for subsequent diversifications, significantly enhancing the value of the resulting products and allowing for the creation of a broader range of valuable derivatives and applications.

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3d Metal Catalysis for the Construction and Coupling of Molecules

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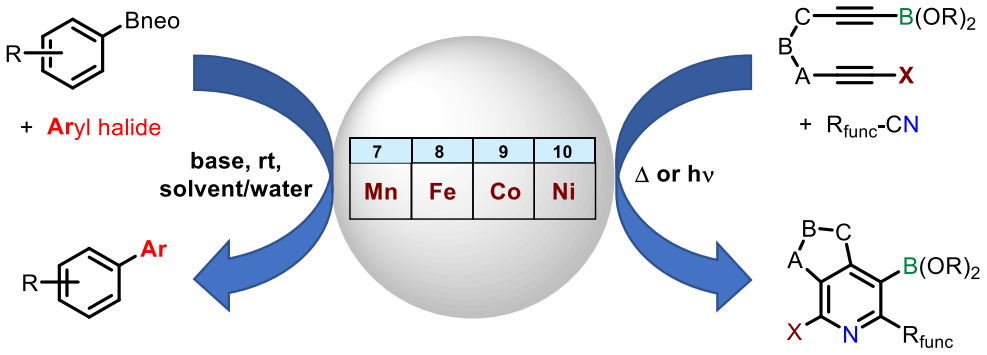

Regioselective synthesis represents a fundamental strategy in modern organic chemistry, facilitating the targeted formation of distinct regioisomers from identical classes of starting materials. In the functionalization of carbocyclic and heterocyclic frameworks, the degree of substitution is frequently linked to the number of synthetic steps and the overall effort required to achieve a desired substitution pattern. The concept of constructing novel and structurally complex molecules from readily accessible, simpler building blocks has garnered significant interest over the past two decades. In this context, [2+2+2] cycloaddition reactions have proven to be exceptionally valuable, developing into a highly versatile synthetic methodology compatible with a broad range of transition metal catalysts. In addition, the introduction of energy to conduct such reactions has included photo- and electrocatalytic approaches, allowing reactions to proceed under particularly mild conditions and opening up novel reaction pathways. We will present the development of catalytic systems as well as application in the synthesis of functional molecules.[1]

More recently, nickel-catalyzed cross-coupling reactions, in particular Suzuki coupling, have emerged as a powerful complementary approach for the efficient decoration of carbo- and heterocyclic scaffolds under sometimes remarkably mild conditions. The utilization of earth-abundant 3d transition metals such as nickel offers distinct advantages over their noble metal counterparts like palladium, including lower cost, reduced toxicity, and enhanced sustainability, while simultaneously enabling unique reactivity pathways that are often inaccessible with precious metal catalysts. Examples for the use of nickel catalysts in the interplay with appropriate substrates will also be presented.

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High-Value Transformation of Coal-Based Chemicals and Its Application in Aqueous Organic Flow Battery Energy Storage

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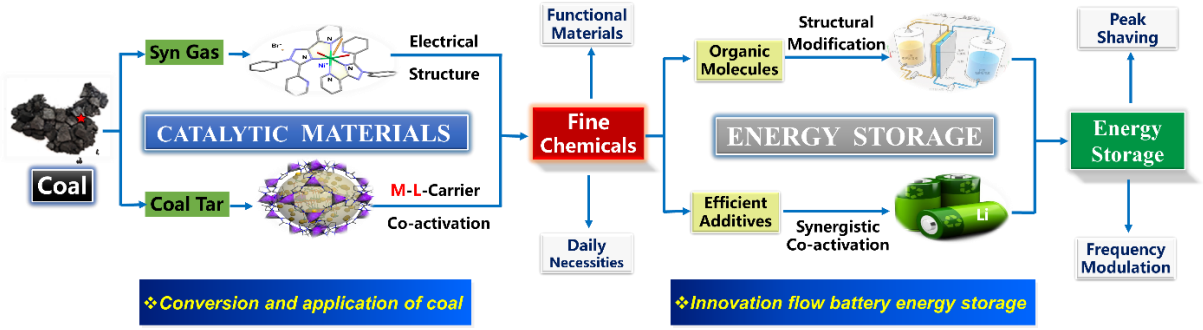
Aligned with “dual carbon” strategy, this work addresses two fundamental bottlenecks hindering the practical deployment of aqueous organic flow batteries (AOFBs): (i) the limited operational stability of multi-electron redox-active organic molecules, and (ii) the absence of scalable, value-adding pathways for coal-derived feedstocks. To bridge these gaps, we establish an integrated research paradigm: “coal-based precursors → rationally designed electrolytes → homologous interfacial engineering”, spanning molecular synthesis, electrolyte formulation, and electrode, electrolyte interface optimization. Leveraging transition metal-catalyzed regioselective functionalization of coal-derived polycyclic aromatic hydrocarbons, we construct a structurally diverse, functionally tunable library of coal-sourced organic electrolytes. Through deliberate integration of multi-electron redox activity, kinetic stabilization, and intrinsic compatibility with neutral aqueous media, we identify and validate high-capacity, long-cycle-life active species. Furthermore, using in situ spectroscopic and computational analyses, we elucidate how conserved aromatic backbones enable preferential π–π stacking and interfacial charge redistribution at the electrode surface, thereby enabling the development of a predictive “homologous interface performance model” for fully coal-integrated AOFBs. This work provides not only a materials-to-system design blueprint but also a conceptual framework for sustainable, resource-aligned electrochemical energy storage.



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Fabrication of Solid Molecular Catalysts and Valorization of Platform Molecules

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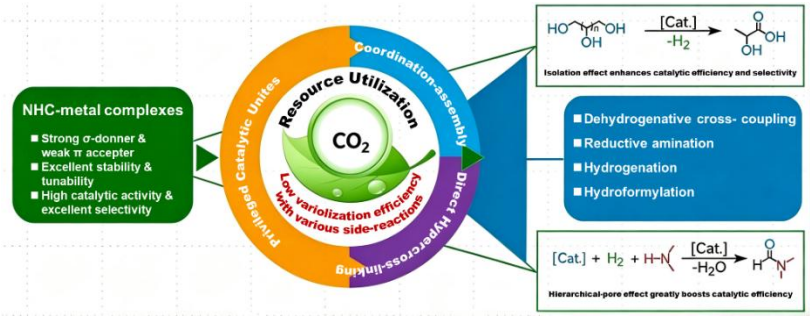

A series of robust, efficient, atom-dispersed porous solid molecular catalysts have been efficiently constructed via coordination assembly or direct hypercross-linking strategies based on privileged N-heterocyclic carbene-metal and pincer complexes. These porous solid molecular catalysts enable highly efficient and selective catalysis for amine hydroformylation of carbon dioxide, as well as hydrogenation, dehydrogenation, and reductive amination of diverse biomass-derived platform molecules under extremely low catalyst loadings. Featuring stability, the catalysts can be readily recycled by simple filtration without extra activation, and retain catalytic performance over more than dozens cycles with negligible decay in activity and selectivity. Notably, kilogram-scale production of target products has been achieved with low (ppm) catalyst loadings in representative reactions including lactic-acid synthesis from biopolys and DMF preparation from CO_2, demonstrating promising prospects for industrial implementation. Control experiments combined with theoretical calculations reveal that coordination assembly and hypercross-linking effectively suppress catalyst deactivation originating from the aggregation of homogeneous N-heterocyclic carbene-metal catalysts. As a result, the solid molecular catalysts exhibit superior activity and selectivity relative to their homogeneous counterparts, delivering state-of-the-art turnover numbers in various high-value-added transformations. The prominent catalytic activity, excellent selectivity, facile recyclability and broad substrate scope of porous solid molecular catalysts highlight their great potential in variolization of biomass and CO_2 toward industrial applications, and lay a research foundation for the advancement of carbon-neutral transformation.

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Explorations into 3d-Metal Catalysis in dark and light

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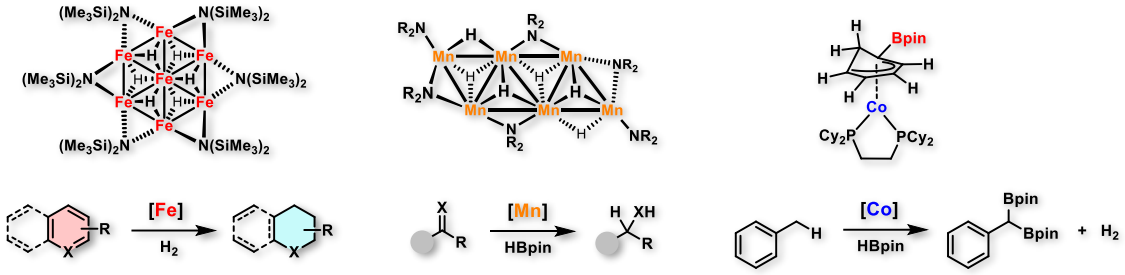

This talk discusses on various applications of Fe, Mn, Co, and Ni complexes to the synthesis of novel metal complexes, unusual cluster architectures, and in the context of catalytic reactions. Recent examples from our laboratories include:

i) Discrete metal clusters (Mn, Fe, Co) constitute snapshots of larger cluster growth mechanisms that are especially rare owing to rapid aggregation or decomposition pathways. We have developed a synthetic strategy that enables the rapid and high-yielding access to 3d metal nanoclusters with amido, hydrido, and hydrocarbyl ligands.[1]

ii) Amine-bearing iron hydride species were demonstrated to act as highly active catalysts in alkene and alkyne functionalizations, including effective hydrogenations of deactivated arenes.[2]

iii) A rapid access to versatile cobalt(I) complexes has been developed that exhibit high activity in hydrofunctionalizations, hydrogenations, CH activation, and cross-coupling reactions.[3]

iv) Combinations of photocatalysis and Ni catalysis have enabled new cross-coupling reactions of C1-building blocks.[4]

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[1] a) P. Ghosh, R. Schoch, M. Bauer, A. Jacobi von Wangelin, *Angew. Chem. Int. Ed.* **2022**, *61*, e202110821; b) A. Jacobi von Wangelin, P. Ghosh, *Angew. Chem. Int. Ed.* **2021**, *60*, 16035; c) A. Jacobi von Wangelin, U. Chakraborty, S. Demeshko, F. Meyer, *Angew. Chem. Int. Ed.* **2019**, *58*, 3466; d) U. Chakraborty, E. Reyes-Rodriguez, S. Demeshko, F. Meyer, A. Jacobi von Wangelin, *Angew. Chem. Int. Ed.* **2018**, *57*, 4970; e) T. N. Gieshoff, U. Chakraborty, M. Villa, A. Jacobi von Wangelin, *Angew. Chem. Int. Ed.* **2017**, *56*, 3585.

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Iron in a Macrocyclic PNPN Environment – Electronic Structure and Catalysis

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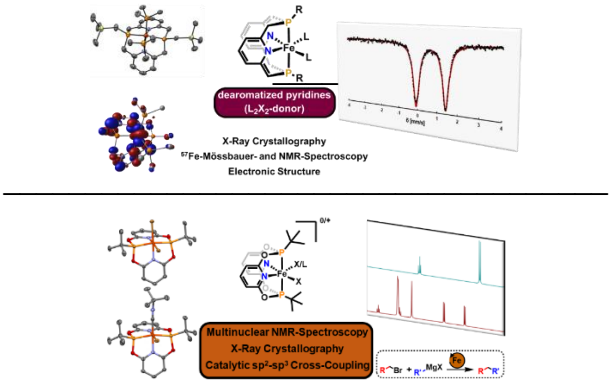
The activation of weakly (or non-) polarized bonds represents a challenging task in the field of modern organometallic chemistry. In order to facilitate such transformations, the metal center can be supported by ligands containing an acidic site which can be reversibly (de)protonated in order to achieve metal-ligand cooperativity. This process may lead to a dearomatized system which is capable of activating strong bonds. Such mono dearomatized systems were intensively studied over the last decades. However, reports of double dearomatized systems are thus limited to manganese[1] and ruthenium[2] supported by NSNS ligands.



Scheme 1. Iron Complex Based upon Dianionic (top) and Neutral (bottom) PNPN Ligand.

This contribution will focus on iron(II) complexes supported by two seesaw PNPN ligands. One ligand framework contains two acidic sites. Deprotonation leads to double dearomatization in conjunction with uptake of π-acidic ligands (Scheme 1). Notably, the double dearomatized system could be stabilized upon coordination of norbornadiene. Iron(II) alkene complexes are rare and a diene complex has thus far not been reported. The (electronic) structure of these systems was elucidated by e.g., multinuclear NMR- ^{57}Fe-Mößauer spectroscopy, single crystal analysis and computationally modeled. The reactivity of these complexes with small molecules e.g., CO and ligand substitution reactions will be presented.[3]

Furthermore, investigations of a topologically related PNPN seesaw ligand, which cannot undergo dearomatization will be discussed. Similarities and divergences in coordination chemistry and implications for catalytic transformations (e.g., cross-coupling reactions) of iron complexes supported by these two similar but distinct PNPN ligands will be lined out.[4]

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Compressing the spin ladder: Understanding electronic structure for reactivity control in earth-abundant transition metal catalysis

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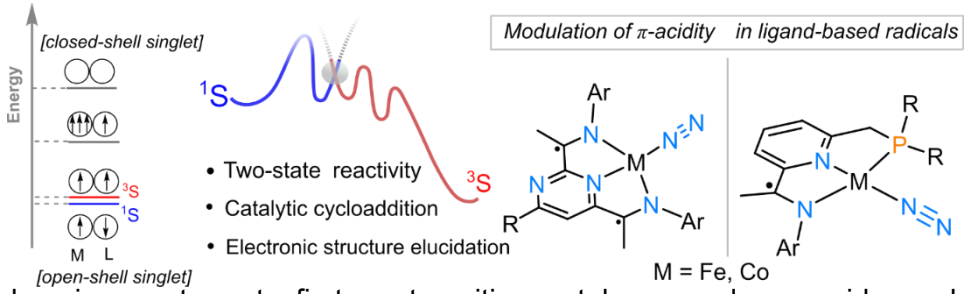

Unlike their heavier counterparts, first-row transition metals can undergo rapid, coupled changes in oxidation state, spin state, and coordination geometry. This flexibility complicates the prediction and control of catalytic pathways, often resulting in reduced selectivity and competing deactivation under turnover conditions. Redox-active ligands provide a powerful way to tune these systems: by engaging directly in electron-transfer steps and by placing otherwise inaccessible excited states within thermal reach, they add additional handles for directing mechanisms and selectivity.

Our work focuses on iron and cobalt complexes that operate *via* two-state reactivity,[1] where key steps can proceed on a spin surface different from the ground state. Crossing between spin manifolds can reshape activation barriers and product distributions, giving rise to electronic structures that, albeit potentially challenging to describe, enable reactivity patterns that are orthogonal to those typically associated with noble-metal catalysis.[2]

Our strategy relies on an integrated approach combining ligand design, spectroscopy, and computational approaches (including the modelling of spectroscopic observables) to connect electronic structure with reaction mechanisms and, ultimately, catalyst performance. We have developed iron- and cobalt-based catalysts for hydroelementation and cycloaddition that operate at loadings below 0.5 mol%.[3] Applications to the synthesis of building blocks relevant to material science and medicinal chemistry will also be highlighted.[4]

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[2] For examples, see: a) P. He, S. F. Zhu, *Chem. Eur. J.* **2024**, *30*, e202403437; b) H. H. Cramer, C. Duchemin, C. B. Kovel, J. Kim, M. V. Pecoraro, P. J. Chirik, *J. Am. Chem. Soc*. **2024**, *146*, 9947; c) S. A. Lutz, A. K. Hickey, Y. Gao, C. H. Chen, J. M. Smith, *J. Am. Chem. Soc.* **2020**, *142,* 15527; d) D. Kim, G. Pillon, D. J. DiPrimio; P. L. Holland, *J. Am. Chem Soc*. **2021**, *143*, 3070.

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Coordination chemistry-based strategies for C(sp^3)-H amination catalysis

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The direct functionalization of C(sp^3)−H bonds is a powerful and atom-efficient methodology to generate new carbon−nitrogen (C−N) bonds. Although challenging, due to the thermodynamic and kinetic stability of typical C(sp^3)−H bonds, intra- and intermolecular C(sp^3)−H amination has seen much progress in the past decade.[1] Synthesis of (chiral) *N*-heterocycles – prevailing building blocks in natural products, pharmaceuticals, and functional materials – via direct C(sp^3)−H amination using aliphatic azide substrates is a particularly appealing strategy in this context.[2] Nitrene insertion into a C(sp^3)−H bond is perhaps the most efficient and best studied approach for C(sp^3)−N bond formation. In situ generation of a metal-bound nitrene (radical) species from readily available aliphatic organoazides could trigger constitute an efficient approach for (asymmetric) catalytic C−H amination.[3]

Our group is exploiting different coordination chemistry-based strategies to develop, understand and improve catalytic systems that can convert organoazides into sought-after *N*-heterocycles. The first line of investigation combines well-defined redox-active ligands with noble metals, which has opened up novel avenues for single-electron-type reactivity with these “redox-inert” elements. Progress from our group on the Pd-mediated C(sp^3)-H amination using organoazides via the previously established Ligand-to-Substrate Single-Electron Transfer mechanism[4] will be discussed, using data from multinuclear NMR spectroscopy, UV-Vis absorption spectroscopy, cyclovoltammetry, EPR and XRD analysis and supported by DFT calculations.

A second avenue that is actively pursued is the development of enantioselective Fe catalysts for this type of transformation. Iron catalysis has made its way to various important classes of organic chemical transformations, including hydroaddition chemistry and recently also C–H activation,[5] but the Fe-mediated functionalization of aliphatic C(sp^3)-H bonds is still a formidable challenge, especially in an asymmetric fashion and in the absence of directing or protecting groups. Herein, we discuss the synthesis, characterization and reactivity of various homo- and heteroleptic high-spin Fe complexes and their catalytic performance in the enantioselective C(sp^3)−H amination, including kinetic and mechanistic investigations.[6]

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Metal–Ligand Cooperation and Catalysis Driven by Carbodiphosphoranes: Harnessing Earth-Abundant Aluminum for Metal–Metal-Cooperative Bond Activation

Robert Langer

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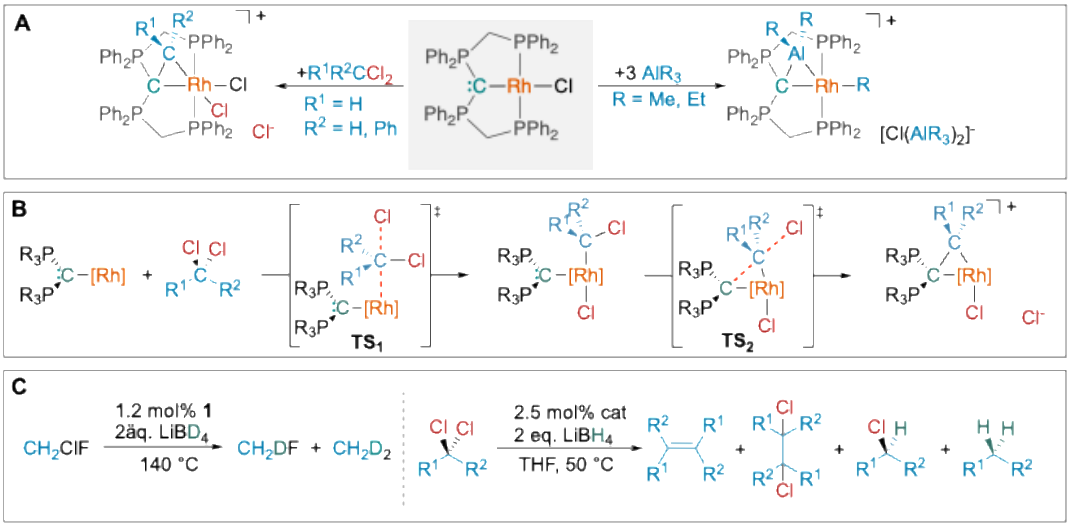

Metal–ligand cooperation (MLC) enables low-energy bond activation, unconventional catalytic pathways, and sustainable chemical transformations, frequently leveraging earth-abundant metals. This presentation explores metal–ligand-cooperative reactivity patterns driven by carbodiphosphoranes (CDPs), which exhibit strongly electron-donating properties and low basicity as ligands, but possess a highly nucleophilic ligating carbon atom (Fig. 1A).[1-3] This unique property facilitates the dual activation of carbon–halogen bonds via consecutive metal-centered oxidative addition and ligand-centered S_N2-type cleavage (Fig. 1B). In the presence of hydride sources, this platform promotes catalytic olefination and hydrodehalogenation reactions (Fig. 1C). More strikingly, the nucleophilic ligand coordinates and activates aluminum compounds (Fig. 1A), yielding a highly reactive metal–metal-cooperative system that efficiently converts carbon dioxide to carbon monoxide and aluminum oxo-species.

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Poster

Propylene Carbonate as a Sustainable CO_2 Surrogate for the Highly Selective Reductive Mono-N-Methylation of Primary Aromatic Amines

Jacqueline Maslack,[a] Katja Andres,[a] Victoria Pfennig,[b] Faral Akhtar,[a] Kathrin Junge,[a] Laurel Schafer,[b] and Matthias Beller[a]

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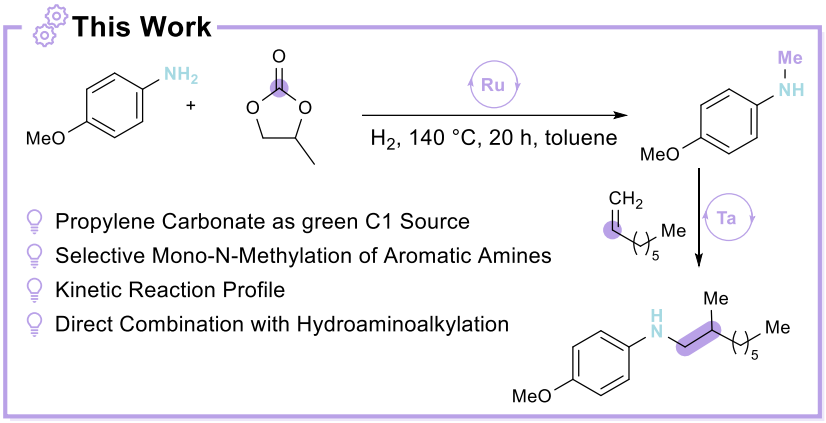

An efficient and sustainable method for the selective mono-N-methylation of primary amines is presented, utilizing a Ru/triphos catalyst and propylene carbonate (PC) as a green C1 source. This approach makes use of PC, a readily available surrogate produced directly from CO_2, in conjunction with molecular hydrogen as the reducing agent, maximizing atom efficiency. The production of PC amounts to multiple kilo tons per year and it is primarily made from propylene oxide and carbon dioxide.[1]

Our novel protocol provides the desired mono-methylated products in high yield and excellent selectivity, effectively minimizing the production of typically unwanted dimethylated byproducts through careful optimization of the reaction conditions. This methodology circumvents the need for toxic methyl halides or protective group strategies often required in traditional methylation processes, offering a greener and more direct synthetic route to valuable methylated amines. Mechanistic investigations clarify the role of the acid additive and the nature of the active species.

The combination of the selective mono-*N*-methylation with the hydroaminoalklylation offers an atom-efficient pathway to access complex aniline derivates without any protection-deprotection strategies.

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Structure-activity relationships in iron mediated [2+2]-cycloaddition of diallylamines

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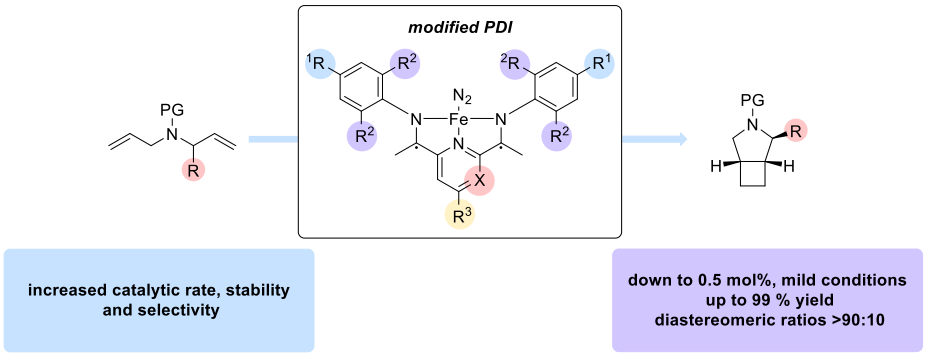
The iron catalyzed thermal [2+2]-cycloaddition of diallylamines has proven itself as a highly efficient method for the synthesis of nitrogen containing bicyclic structures.[1,2] Although the cyclobutane motif is of interest in the development of pharmaceuticals,[3,4] preparative access to the cyclobutane-fused *N*-heterocycles stemming from unactivated olefins had so far been challenging. A significant limitation for previous approaches is the reliance of pre-functionalisation of the olefin starting materials as well as rapid catalyst deactivation.

Herein we report that through tailored ligand design of the iron catalyst, it is possible to suppress catalyst deactivation during the cycloaddition, increase the reaction rate and influence the selectivity of the reaction, achieving in some cases very low catalyst loadings (< 0.5 mol%).[1,5] Structure-activity relationships were explored by steric and electronic modification of the pyrimidine diimine ligand. The most active catalysts were shown to efficiently cyclize substituted diallylamines with high diastereoselectivity. Furthermore, the reaction could be expanded to the formation of six- and seven-membered bicycles and a range of protecting groups was shown to be well tolerated. This methodology therefore allows for the efficient synthesis of novel bicyclic amine building blocks.



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A dimeric, mixed-spin/valent PNN iron hydride complex: Lewis-base tolerant catalytic olefin hydrogenation

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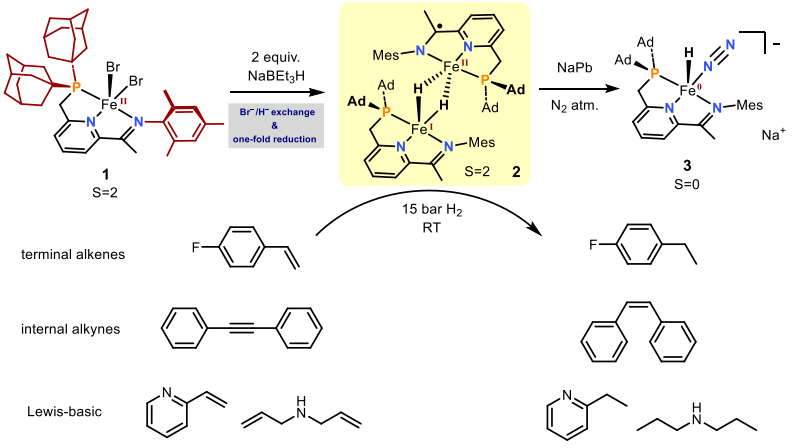
The reduction of iron(II) precursor (^{Ad}PNN^{Mes})FeBr$_2$ (**1**) with two equivalents NaBEt$_3$H afforded the dimeric, *μ*-hydride bridged iron complex **2** *via* a net one-electron reduction and a bromide-hydride metathesis. The formation of such a dimeric hydride complex featuring a redox-active PNN pincer ligand is unprecedented for this class of ligands, and was achieved by fine-tuning the steric demand of both the phosphine and imine side-arms.[1,2]

While a S = 2 ground state was observed for the paramagnetic iron hydride **2** *via* SQUID magnetometry, describing its electronic structure remains challenging due to the presence of four redox-active subunits (two PNN ligands and two iron centers). Mössbauer spectroscopy revealed two distinct iron sites, indicating that the dimeric complex **2** adopts a mixed-valent or mixed-spin state. A subsequent one-fold reduction of **2** with NaPb under a nitrogen atmosphere yields the monomeric, anionic hydride complex **3**.[2]

Interestingly, both the paramagnetic dimeric hydride **2** and the diamagnetic monomeric hydride **3** promote the catalytic hydrogenation of various olefins and internal alkynes under mild conditions (RT, 15 bar H$_2$) at low catalyst loadings (0.2 mol%). Furthermore, these hydrogenation reactions have proven to be notably robust toward Lewis-basic functional groups, such as tertiary and secondary phosphines, as well as secondary amines.[3]



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Investigation of Hydrogen Bonding Interactions in the Secondary Coordination Sphere of an Iron-based Catalyst

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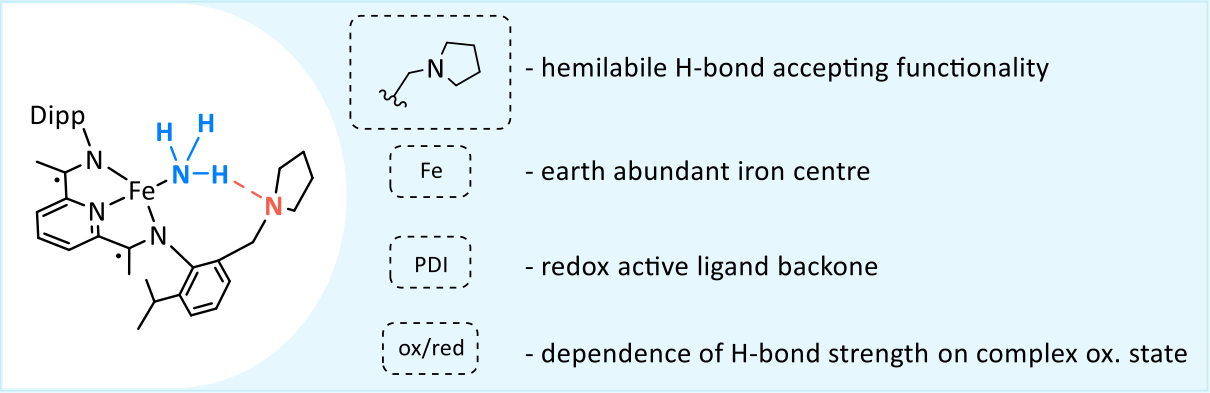

The incorporation of a hydrogen-bond accepting functionality into a redox active ligand scaffold enhances complex stability, as well as reactivity towards substrates bearing protic functionalities. Hydrogen bonds are common in many biological systems (e.g. Enzymes[1]) where they serve as energy currency for many transformations and furthermore have been recently employed in the design of homogeneous catalytic cycles (e.g. for ammonia oxidation[2]).

This works presents an iron based complex with a redox active pyridinediimine (PDI) ligand equipped with a lateral pyrrolidine-arm, that can **a)** block and vacate a coordination site in the primary coordination sphere, by directly coordinating to the iron centre in a hemilabile fashion and **b)** engage in hydrogen-bonding interactions with substrates in the secondary coordination sphere, thereby orienting the substrate and lowering the activation barrier to access subsequent reaction pathways.[3,4]

This concept is illustrated on a (PDI)Fe ammonia complex, which shows hydrogen bonding interactions with the ligand backbone as evidenced by ^{1}H NMR, IR spectroscopy and well as X-ray diffraction studies. The redox activity of the complex was further investigated by cyclic voltammetry which suggests reversibly accessible reduced and oxidised species. In an effort to establish how the hydrogen bonding strength varies with oxidation state, chemical oxidation and reduction studies were further pursued and will be discussed herein. In addition, computational calculations of the rotational barrier of the hydrogen bond were performed to shed additional insights into the relevance of the hydrogen bond in the neutral, oxidised and reduced complex.

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Photocatalytic Steam Reforming of Methyl Formate

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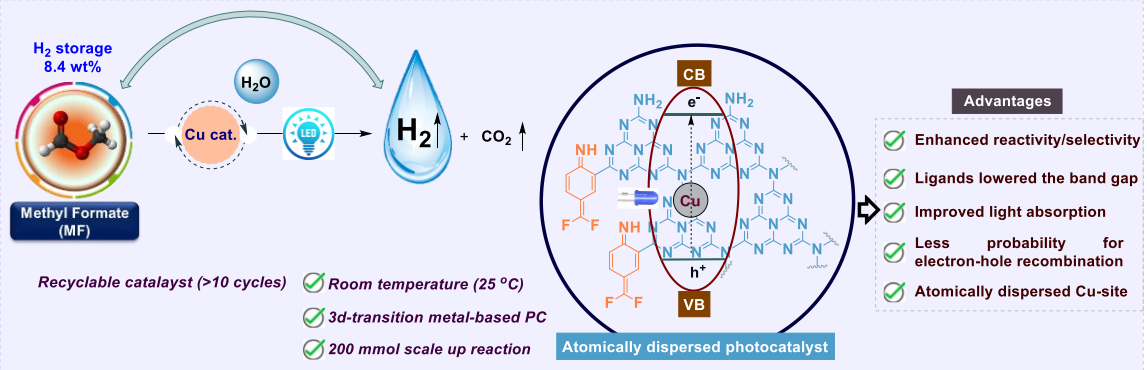

Green hydrogen is critical to establish a sustainable energy future as it offers a clean, renewable, and a versatile alternative for decarbonizing industries, transportation, and power generation.[1-2] However, the limitations of current methods significantly restrict the scope and hinder many of the envisioned applications. This study aims to report on the first example of a 3d-metal-based (Cu) heterogeneous photocatalytic system to produce green hydrogen *via* dehydrogenation of methyl formate (MF), a reaction previously known to require 4d/5d transition metals.[3] Employing a Cu-based atomically dispersed heterogeneous photocatalyst supported on aryl-amino-substituted graphitic carbon nitride (d-gC_3N_4), the protocol offers numerous key advantages, including the recyclability of the photocatalyst for >10 cycles without significant activity loss, sustained hydrogen production (>15 days!) with high hydrogen yield (19.8 mmol g_{cat}^{-1}) and negligible CO emission, following an operationally simple, sustainable, and efficient catalytic pathway. Furthermore, the photocatalyst is characterized (using HAADF-STEM, SS-NMR, XAS, EPR, and XPS), all of which clearly demonstrated the presence of single atomic Cu-site. Additionally, com-prehensive mechanistic investigations together with DFT calculations allow for a thorough mechanistic rationale for this reaction. It is strongly believed that this atomically dispersed heterogeneous photocatalytic approach will open new avenues for establishing liquid organic hydrogen carrier (LOHC) technologies.

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Metal-Free Porous Organic Polymer Photocatalyst for CO_2 Reduction to Formic Acid

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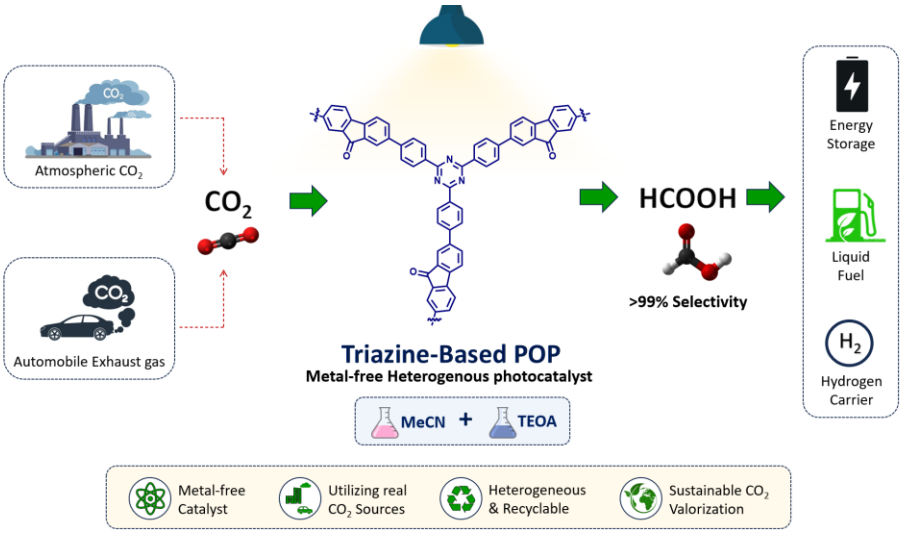

The persistent accumulation of atmospheric CO_2 has emerged as one of the most significant environmental challenges, encouraging the development of sustainable carbon capture and utilization strategies.[1] Photocatalytic CO_2 reduction presents a promising approach for the conversion of CO_2 into value-added chemicals using light as a renewable energy source.[2] Applications of Formic acid spans through fields like hydrogen carrier and energy storage which makes it especially valuable among the products of CO_2 reduction, making it a promising candidate for sustainable, carbon-neutral energy systems.[3] However, many reported heterogenous photocatalysts rely largely on transition metals or expensive metal co-catalysts. [4] Herein, we report a metal-free triazine-based porous organic polymer (POP) catalyst for the photocatalytic conversion of CO_2 to formic acid. The catalyst achieved formic acid production rate of 4.68 mmol g^{-1} h^{-1} with >99% selectivity under mild condition, demonstrating efficient CO_2 reduction without the use of metal-based active sites. Further the catalyst demonstrated practical applicability by producing Formic acid from impure CO_2 sources, achieving 2.3 mmol g^{-1} h^{-1} from automobile exhaust gas and 1.3 mmol g^{-1} h^{-1} in air. These results demonstrate the potential of triazine-based porous organic polymers as sustainable heterogeneous photocatalysts for the efficient and selective conversion of CO_2, maintaining excellent performance even at low CO_2 concentrations.

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Seeing Invisible Hydrides: CEST NMR of the Active State in Ru Pincer Catalysis

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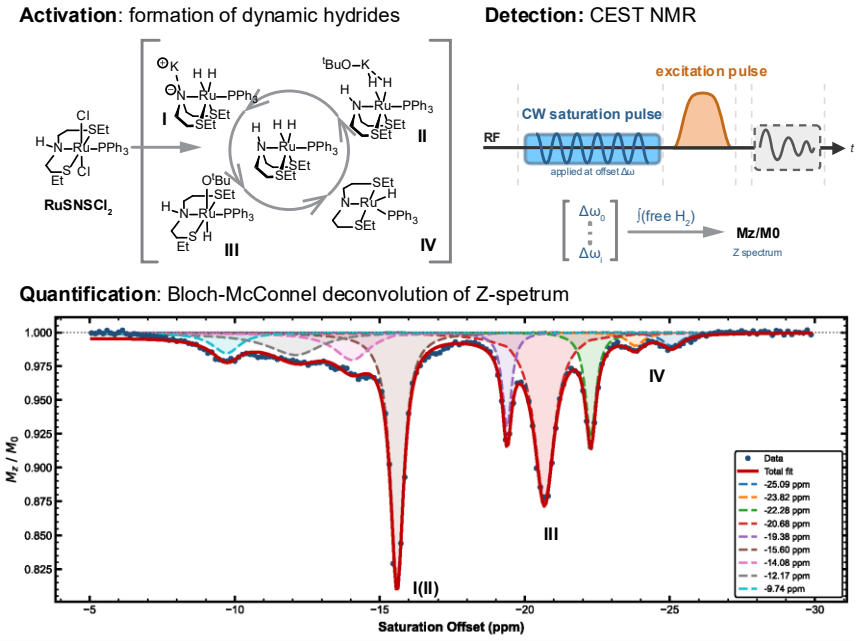

Homogeneous catalysis with metal complexes is often seen as a much simpler case as compared to heterogeneous or biocatalytic systems. Smaller ensemble sizes in combination with easier access to spectral and kinetic data provide more insight into the molecular reaction mechanisms. With the support of computational methods, this should allow for effective predictive modelling of such systems. The main challenge is the correct identification of an active state that typically features short characteristic lifetimes, making it difficult to detect. In this work we demonstrate that this can be addressed by NMR. For a Ru SNS-type pincer complex, a potent hydrogenation catalyst, we demonstrate that under the reaction conditions the complex is transformed into a mixture of *fac*- and *mer*-conformers of mono- and dihydrides.[1] Most of these hydrides are dynamic and are not accessible through thermal NMR measurements. We employ a combination of chemical exchange saturation transfer (CEST, CEST-QUEST) and NOE-based techniques to quantify and to elucidate the structure and dynamics of the hydrides.[2,3] The data shows that the relative concentration of different hydrides is strongly affected by the presence of alcohols, alkoxides and metal cations and changes during the reaction, defining the reaction rate and the final product selectivity.

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