ICIQ
Institut Català d'Investigació Química

ICIQ Summer School 26

BOOK OF ABSTRACTS

20 – 22 July 2026
ICIQ Auditorium Prof. Dr. Kilian Muñiz
Tarragona, Spain

With the support of:

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Presentation

Welcome to the 2026 ICIQ Summer School!

We are pleased to invite you to the 2026 ICIQ Summer School, taking place from July 20–22, 2026, at the Institute of Chemical Research of Catalonia (ICIQ) in Tarragona, Spain.

The ICIQ Summer School is designed to bring together Master's, Doctoral, and Postdoctoral researchers from diverse areas of chemistry and related disciplines, fostering vibrant scientific exchange in an inspiring international environment. Over three intensive days, participants will engage in cutting-edge lectures, interactive discussions, and networking opportunities with leading scientists and fellow early-career researchers.

Our goal is to stimulate critical thinking and collaboration at the frontiers of chemical research, while providing a supportive platform for young scientists to share ideas, broaden perspectives, and build lasting professional connections.

Set in the beautiful Mediterranean city of Tarragona, the Summer School also offers a unique opportunity to enjoy its nearby beaches while immersing yourself in high-level science.

We very much look forward to welcoming you this July for an exciting and enriching scientific experience at ICIQ.

The Organising Committee,

Antonio M. Echavarren – ICIQ, Spain
Luis Escobar – ICIQ, Spain
Judit Martínez – ICIQ, Spain

The Scientific Committee,

Rubén Martín – ICIQ, Spain
Beatriz Prieto-Simón – ICIQ, Spain
Katherine Villa – ICIQ, Spain

General Information

Venue

Institut Català d'Investigacio Química (ICIQ)
Avinguda Països Catalans, 16
43007 Tarragona (Spain)

How to get to Tarragona

Tarragona is a coastal city located in the northeast of Spain, approximately 100 km southwest of Barcelona. It is easily accessible by train, bus, or car from several major cities.

By Train
Tarragona has **two train stations**, so please make sure to check which one your train arrives at:

- **Tarragona City Station (Estació de Tarragona)**:
  Located in the city centre, this station is served by **regional and longdistance trains** from nearby cities such as Barcelona and Valencia. From *Barcelona Sants*, you can take a regional train (lines R15, R16, or R17). The journey takes about 1 hour.
- **Camp de Tarragona Station**:
  This is the **high-speed train (AVE)** station located **9 km outside the city**. It connects Tarragona with **Madrid, Zaragoza, Barcelona**, and other major cities.

  To reach the city centre you'll need to take a **taxi** or **shuttle bus**. For train schedules and tickets, visit the RENFE website.

By Bus
Intercity buses, operated by companies such as Plana, connect Tarragona with cities like Barcelona and Reus. The main bus station is located at **Imperial Tarraco Square**.
For more information: www.busplana.com.

By Plane

- **Reus Airport** is the closest airport (7 km from Tarragona), with connections to some European destinations.
- **Barcelona El Prat Airport** is 90 km away and offers frequent international flights. From there, you can take a train (if you arrive at terminal T1 you must take the shuttle bus to terminal T2 train station, and then take the train to Barcelona-Sants station) or bus to Tarragona.

How to get to ICIQ

The **Institute of Chemical Research of Catalonia (ICIQ)** is located on the **Sescelades Campus**, about 4 km north of the city centre.

By Bus

Local buses from the city centre to ICIQ are operated by EMT Tarragona.
The following lines stop near the institute:

- **Line 5**
- **Line 41**
- **Line 54**

The nearest bus stops are:

- **“Educacional N-240”**
- **“Joan Serra”**

Check www.emtanemambtu.cat for routes and schedules. Tickets can be bought in the same bus.

By Taxi

Taxis are available at various locations across the city. You can also book one by calling:

- **Taxi Tarraco**: +34 642 269 752
- **RàdioTaxis Tarragona**: +34 977 221 414
- **Tarragona City Taxi**: +34 693 303 050

By Car

ICIQ has a very small parking lot. For this reason, we recommend you to park in the adjacents streets.

Language

The official language of the symposium is **English**. Sessions and posters will be presented in this language.

Congress Badge

All participants will receive a name badge upon registration. Please note that access to the conference venue is only allowed with this badge. Badges must be worn at all times during the conference and the dinner. Entry to the meeting rooms and exhibition area will not be allowed to anyone without a badge.

Wi-Fi

Free Wi-Fi internet access is available for the participants of the school.

SSID Guest

Username eventswifi@iciq.es
Password 3Qy7E*9TQycT

Social Events

ICIQ Summer School Social Activity
Date: July, 21st
Place: Clos Montblanc
Ctra. T-242, KM 1, 43422 Barberà de la Conca
Time: 18.30h

Free shuttle will be offered for all the attendees. It will depart from ICIQ at 17.45h.

ICIQ Summer School Dinner
Date: July, 21st
Place: Restaurant El Molí del Mallol
Muralla de Santa Anna 2, Montblanc
Time: 21.00h

If you have any dietary requirement (which should have been indicated on the registration form), please, inform the restaurant staff.

Certificates

Attendance certificates will be sent by email after the school. The certificate will confirm your participation in the event, whether you attended, gave an oral communication, or presented a poster.

If for any reason you do not receive your certificate within a few days after the school, please, do not hesitate to contact us at jmartinez@iciq.es.

Oral Presenters

We strongly recommend that you use the laptop (Windows) provided by the organising committee in the auditorium for your presentation.
Please make sure to send your lecture in advance to jmartinez@iciq.es, or bring it saved on a USB drive on the day of your talk. We kindly ask you to provide the file in both **.ppt and .pdf** formats.

Your presentation should be uploaded to the auditorium's laptop **well in advance of your session**, to ensure that there are no technical issues.

Poster Sessions

Posters should be printed in A0 size (841 x 1189 mm) and in portrait orientation.

Poster	Name	Institution
P1	Christopher Taylor	Universitat de Girona
P2	Laura Velasco	ICIQ
P3	Miguel Uceda	ICIQ
P4	Gala Ogalla	ICIQ
P5	Isik Önder	LMU Munich
P6	Quan Zhang	ICIQ
P7	Maria Martin	ICIQ
P8	Huahua Dong	ICIQ
P9	Yingying Wang	ICIQ
P10	Marta Romero	ICIQ
P11	Farzaneh Hosseine	ICIQ
P12	Yousra Abbad	University Ibn Tofall
P13	Eva Jaramillo	ICIQ
P14	Anna Amanz	ICIQ
P15	Aswin Gopakumar	ICIQ
P16	Yue Ren	ICIQ
P17	Norman Díaz	ICIQ
P18	Angie Bolaños	ICIQ
P19	Bharghab Biswas	ICIQ
P20	Batoul Karim	Institut Polytechnique de Paris
P21	Ricardo Hortigón	ICIQ
P22	Alejandro Delgado	ICIQ

Poster	Name	Institution
P23	Sergio Rodríguez	ICIQ
P24	Luyu Cai	ICIQ
P25	Álvaro Velasco	ICIQ
P26	Hao Lu	ICIQ
P27	María Karla López	Universidad de Alicante
P28	Liangliang Zhang	ICIQ
P29	Huilin Liu	ICIQ
P30	Giona Armellin	ICIQ
P31	Sota Ajiro	The University of Tokyo
P32	Wenhan Zhang	ICIQ
P33	Sergi Danés	ICIQ
P34	Gerard Morell	ICIQ
P35	Shanhnauze Ahsan	ICIQ
P36	Arshad Aranjiyl	ICIQ
P37	Lorenzo Berti	ICIQ
P38	Nick Hermann	ICIQ
P39	Sara Faoro	ICIQ
P40	Hao Wang	ICIQ
P41	Brett Pollard	LMU Munich
P42	Antonio Paparesta	ICIQ
P43	Jijun Xu	ICIQ
P44	Marisol Blanco	ICIQ

Program

Monday, July 20th

09.00 – 09.45 **Registration.** ICIQ Reception

09.45 – 10.00 **Welcome.** Imma Escofet & Antonio M. Echavarren

10.00 – 11.10 **Plenary Speaker 1: Varinder Aggarwal**
Synthesis in a Boron World

11.10 – 12.00 **Invited Speaker 1: Alexander Shafir**
Reaction and structure development using hypervalent iodine

12.00 – 12.50 **Invited Speaker 2: Allegra Franchino**
Repurposing H-bond donors for transition metal catalysis

12.50 – 14.30 **Lunch Break**

14.30 – 15.40 **Plenary Speaker 2: Thomas Carell**
New developments in the field of nucleoside and oligonucleotide therapeutics

15.40 – 16.30 **Invited Speaker 3: Javier Montenegro**
Supramolecular Dynamic Chemistry for membrane transport and Biomimetic Systems

16.30 – 17.30 **Coffee Break and Poster Session**

17.30 – 17.40 **Oral Presentation 1: Elena Borrego**
Novel Gold (I)-Carbenoid Complexes for C-C Bond Formation

17.40 – 17.50 **Oral Presentation 2: Shivaprasad Achary Balahoju**
SET-driven radical mechanism enables metal-free C-X (X = C, N, S) para-functionalisation of nitrobenzene

17.50 – 18.00 **Oral Presentation 3: Mattia Vettori**
Heterogenization of a water-soluble manganese molecular complex unlocks highly efficient CO2 electroreduction to formate

18.00 – 18.10 **Oral Presentation 4: Carla Alamillo**
From Understanding to Innovation: The Power of Mechanistic Insight in Organic Chemistry

18.10 – 18.20 **Oral Presentation 5: Alejandro Cruz**
Deciphering GPCRs activation and modulation. Development of a generic computational approach

18.20 – 18.30 **Oral Presentation 6: Shuai Zhang**
Site-Selective Distal Arylation of Sugars Enabled by Cyclic Acetals

20.30 **Dinner with speakers *(on invitation)***

Tuesday, July 21st

09.00 – 10.10 **Plenary Speaker 3: Jordi Burés**
Past, Present and Future
of Kinetic Analysis

10.10 – 11.00 **Invited Speaker 4: Géraldine Masson**
From Asymmetric Organocatalysis to Photoredox Strategies for Building Complex Molecules

11.00 – 12.00 **Coffee Break and Poster Session**

12.00 – 13.10 **Plenary Speaker 4: Núria López**
Taking CARE of simulations in heterogeneous catalysis

13.10 – 14.40 **Lunch Break**

14.40 – 15.50 **Plenary Speaker 5: Pedro J. Pérez**
Carbon-hydrogen bond activation by organometallics: Towards methane use as a C1-source in chemistry

15.50 – 16.20 **Coffee Break**

16.20 – 16.30 **Oral Presentation 7: Flavia Pedroso**
Photocatalytic Micromotors for S. epidermidis Biofilm Eradication

16.30 – 16.40 **Oral Presentation 8: Thomas Rigotti**
Enantioselective Catalytic Strategies for the Synthesis of Bicyclo[2.1.1]hexanes as Novel Phenyl Bioisosteres

16.40 – 16.50 **Oral Presentation 9: Mingkai Zhao**
Acceleration of Azide-Alkyne Cycloaddition reactions in Octa-amino Bis-calix[4]pyrrole Cages

16.50 – 17.00 **Oral Presentation 10: Meriem Daghmoum**
Thiocarbonyl Difluoride as a Single-Sulfur Atom Transfer Agent: AgSCF3-Mediated Thionation of Amides

17.00 – 17.10 **Oral Presentation 11: José López-Fernández**
Superchaotropic Boron Clusters for Broad-Spectrum Antibiotic Delivery

17.10 – 17.20 **Oral Presentation 12: Davide Rigo**
Synthesis and chemical recycling of crosslinked poly(ether-co-carbonates)

17.20 – 21.00 **Activity:** Winery Tour & Wine Tasting

21.00 **Gala Dinner**

Wednesday, July 22nd

09.30 – 10.20 **Invited Speaker 5: Sílvia Osuna**
Computational Design of Efficient Enzymes Through Coevolution and Correlation-Mediated Allosteric Networks

10.20 – 11.10 **Invited Speaker 6: Daniel Maspoch**
Clip-off Chemistry: breaking bonds, building chemistry

11.10 – 11.40 **Coffee Break**

11.40 – 12.50 **Plenary Speaker 6: David A. Leigh**
Why Nature Chose Catalysis

12.50 – 13.00 **Closing Ceremony and Awards.**
Emilio Palomares & Luis Escobar

Plenary Speakers

Plenary Speaker 1

Varinder K. Aggarwal

University of Bristol,
United Kingdom

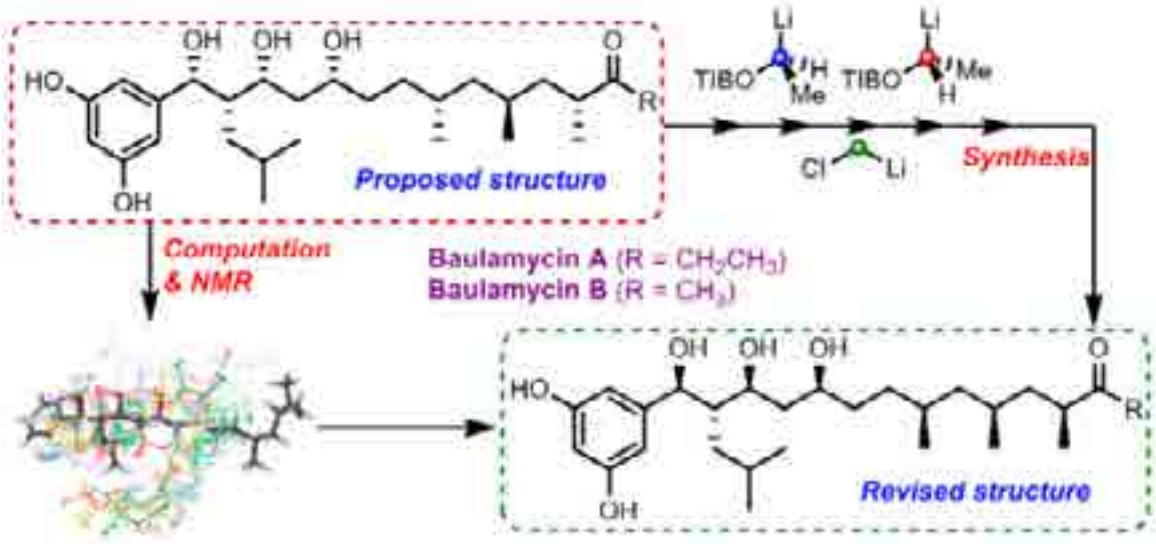
Short Biography

Varinder K. Aggarwal studied chemistry at Cambridge University and received his Ph.D. in 1986 under the guidance of Dr. Stuart Warren. After postdoctoral studies (1986-1988) under Prof. Gilbert Stork, Columbia University, he returned to the UK as a Lecturer at Bath University. In 1991 he moved to Sheffield University, where he was promoted to Professor in in 1997. In 2000 he moved to Bristol University where he holds the Chair in Synthetic Chemistry. He was elected Fellow of the Royal Society in 2012.

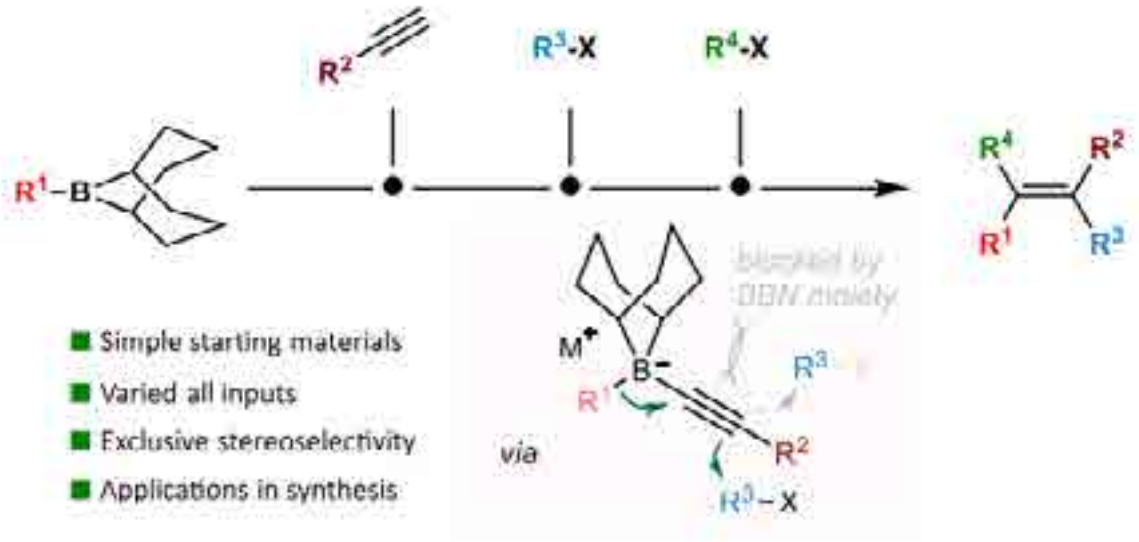
Synthesis in a Boron World

Nature has evolved highly sophisticated machinery for organic synthesis, many of which resemble molecular assembly-line processes. So far chemists have been able to apply this type of approach in the synthesis of peptides, oligonucleotides and polysaccharides but it is much more difficult to apply iterative methodologies to organic synthesis.

Here, we describe the application of iterative homologation of boronic esters using chiral lithiated carbamates and chloromethyllithium enabling us to grow carbon chains with control over both relative and absolute stereochemistry. Application of this strategy to the synthesis of the proposed structure of baulamycin and the real structure will be presented as well as other complex targets.



Cross coupling, particularly Suzuki cross coupling, is one of the most important reactions in medicinal chemistry. Most couplings involve sp2-sp2 bond formation but this invariably leads to flat molecules. With increasing interest in accessing three dimensional space (escape from flatland), there is increasing interest in broadening this coupling reaction to include sp2-sp3 and even sp3-sp3 coupling. In this lecture I will show how new variations of the Zweifel olefination reaction enable sp2-sp3 couplings (alkenes with alkyl boronic esters) and an extension of this reaction which enable aromatics to be coupled with hindered secondary and even tertiary boronic esters. I will also discuss how this chemistry can be applied to the stereocontrolled synthesis of tetrasubstituted alkenes and how we can even extend this work to stereocontrolled sp3-sp3 couplings, where stereochemistry can essentially be dialled in.



References:

1. K. Yeung, R. C. Mykura, V. K. Aggarwal, “Lithiation-Borylation Methodology in the Total Synthesis of Natural Products” Nat. *Synth.*, **1**, 117–126 (2022)
2. J. Wu, P. Lorenzo, S. Zhong, M. Ali, C. P. Butts, E. L. Myers, V. K. Aggarwal, “Synergy of synthesis, computation and NMR reveals correct baulamycin structures” *Nature*, 547, 436, (2017)
3. M. Burns, S. Essafi, J. R. Bame, S. P. Bull, M. P. Webster, S. Balieu, J. W. Dale, C. P. Butts, J. N. Harvey, V. K. Aggarwal, “Assembly-line synthesis of organic molecules with tailored shapes” *Nature*, 513, 183-188, (2014).
4. H. C. Shen and V. K. Aggarwal, Iridium-Catalyzed Stereocontrolled C(sp3)–C(sp3) Cross-Coupling of Boronic Esters and Allylic Carbonates Enabled by Boron-to-Zinc Transmetalation, *J. Am. Chem. Soc.*, **2025**, 147, 5583–5589
5. H. C. Shen, Z. S. Wang, A. Noble, and V. K. Aggarwal, Simultaneous Stereoinvertive and Stereoselective C(sp3)–C(sp3) Cross-Coupling of Boronic Esters and Allylic Carbonates *J. Am. Chem. Soc.*, **2024**, 146, 13719–13726.
6. L. Wei, M. V. Popescu, A. Noble, R. S. Paton, V. K. Aggarwal, Stereocontrolled, Boron-Mediated, Modular Assembly of Tetrasubstituted Alkenes, *Nature*, **2025**, 643, 975–982.

Plenary Speaker 2

Thomas Carell

Ludwig-Maximilians-Universität
München, Germany

Short Biography

Thomas Carell started his academic career studying chemistry at the Universities of Münster and Heidelberg. In 1993, he obtained his doctorate with Prof. H. A. Staab at the Max-Planck Institute of Medical Research.

After postdoctoral training with Prof. J. Rebek at MIT (Cambridge, USA) from 1993 – 1995, Thomas Carell moved to the ETH Zürich (Switzerland) to start an independent group under the mentoring of Prof. F. Diederich. He obtained his Habilitation in 1999.

In 2000, he accepted a full professor position for Organic Chemistry at the Philipps-Universität in Marburg (Germany).

In 2004, he moved to the Ludwig-Maximilians-Universität (LMU) in Munich (Germany) where he is heading a research group with a focus on Chemical Biology and Prebiotic Chemistry focused to analyze the chemistry of epigenetic programming in DNA and RNA.

Thomas Carell is a member of the German National Academy Leopoldina and of the Berlin-Brandenburgische Academy of Arts and Sciences. He is the recipient of the Cross of Merit from the Federal Republic of Germany and since 2019 member of the supervisory board of BASF SE.

New developments in the field of nucleoside and oligonucleotide therapeutics

Nucleosides are a well-established group of therapeutics.

Oligonucleotides establish themselves currently as a novel class of pharmaceuticals.

The latter allow the precise binding to cellular nucleic acids to interfere with splicing or to degrade specific mRNAs. mRNA in turn has started to create a new class of vaccines.

In the lecture I am addressing new aspects in all three areas i) nucleosides, ii) oligonucleotides and iii) mRNA vaccines. I will present a new nucleoside that efficiently reduces the levels of epigenetic mdC in the genome to trigger an epigenetic anti-cancer response. I will present mouse PDX models that show that efficient demethylation can have a profound anticancer effect.[1] In the second part of my lecture, I will present data that allow to deliver oligonucleoside therapeutics efficiently into different cell types.[2,3] The chemistry involves the development of click-adapter molecules that enable an efficient and cost effective one-pot

multiple click linkage of oligonucleotides to different targeting ligands with flexible multiplicity. Finally, I am presenting data that explain why pseudouridine (Y) and 1-methylpseudouridine (1MeY) containing mRNA can escape immune detection. [4,5] Immune silencing of mRNA is a prerequisite for the development of mRNA vaccines and potentially new chemical modifications in RNA are needed to create immune silent RNA therapeutics.[6]

References:

1. F. R. Traube, N. F. Brás, W. P. Roos, C. C. Sommermann, T. Diehl, R. J. Mayer, A. R. Ofial, M. Müller, H. Zipse, T. Carell *Chem*. Eur. J. **2022**, 10.1002/chem.202200640.
2. A. J. Tölke, J. F. Gaisbauer, Y. V. Gärtner, B. Steigenberger, A. Holovan, F. Streshnev, S. Schneider, M. Müller, T. Carell *Angew*. Chem. Int. Ed. **2024**, 10.1002/anie.202405161.
3. E.S. Schönegger, A. Crisp, M. Radukic, J. Burmester, T. Frischmuth, T. Carell *ChemBioChem* **2023**, 10.1002/cbic.202300701.
4. W. Greulich, M. Wagner, M.M. Gaidt, C. Stafford, Y. Cheng, A. Linder, T. Carell, V. Hornung *Cell* **2019**, doi: 10.1016/j.cell.2019.11.001.
5. M. Bérouti, M. Wagner, W. Greulich, I. Piseddu , J. Gärtig, L. Hansbauer, C. MüllerHermes, M. Heiss, A. Pichler, A.J. Tölke, G. Witte, K.-P. Hopfner, D. Anz, M. Sattler, T. Carell, V. Hornung *Cell* **2025**, 10.1016/j.cell.2025.05.032.
6. V. R. Graziano, J. Porat, M. D. Ah Kioon, I. Mejdrová, A.J. Matz, C. G. Lebedenko, P. Chai, J. V. Pluvinage, R. Ricci-Azevedo, A. G. Harrison, S. S. Wright, X. Wang, M. S. Strine, P. Wang, M. R. Wilson, S. K. Vanaja, B. Zhou, F. J. Barrat, T. Carell, R. A. Flynn & V.A. Rathinam *Nature* **2025**, 10.1038/s41586-025-09310-6.

Plenary Speaker 3

Jordi Burés

Institut Català
d'Investigació Química (ICIQ)

Short Biography

Jordi was born and raised in Barcelona. He obtained his undergraduate degree in Chemistry and his PhD at the University of Barcelona, under the supervision of Prof. Jaume Vilarrasa. In 2010, he received a Spanish postdoctoral fellowship to join the group of Prof. Donna Blackmond at The Scripps Research Institute in California. Three years later, he took up a position in the Chemistry Department at Imperial College London as an IC Junior Research Fellow. In 2016, he was appointed as Lecturer at The University of Manchester, where he climbed the academic ladder, eventually becoming Full Professor. In 2024, he joined the ICIQ as an ICREA Research Professor. His current research lines reflect his academic journey, with the development of better synthetic methods guided by reaction mechanistic information.

In 2018, Jordi was awarded the Thieme Chemistry Journals Award; in 2019, the Young Researcher Award from the Spanish Royal Society of Chemistry (RSEQ); in 2020, the Hickinbottom Award from the Royal Society of Chemistry (RSC); and in 2024, the Bristol Myers Squibb Lectureship (Scripps Research). In 2021, Jordi was awarded the FSE Students' Award for "Excellence and Innovation in Teaching and Learning Practice".

Past, Present and Future of Kinetic Analysis

Understanding the molecular mechanisms of synthetic transformations remains one of the central challenges in catalysis and is essential for developing more efficient and robust processes. Kinetic analysis provides some of the most valuable mechanistic evidence, and reaction orders are among its most fundamental and informative outputs. This talk will examine the past, present and future of kinetic analysis.

The first part will revisit classical kinetic methods, which developed in response to the experimental technology available at the time. When collecting concentration–time data was laborious, chemists designed methods that relied on a limited number of measurements, such as initial-rate analysis. We will examine the limitations of these classical approaches and highlight their most common experimental and interpretative pitfalls, particularly when determining and interpreting reaction orders.[1]

The present landscape is defined by advances in reaction monitoring. Collecting many data points throughout a reaction has become relatively straightforward, whereas preparing and performing independent reactions remains experimentally demanding. Reaction Progress Kinetic Analysis (RPKA)[2,3] and subsequent visual kinetic approaches, including time-shift analysis,[4] time

normalization analysis (TNA)[5] and variable time normalization analysis (VTNA) [6,7], emerged in response to this shift. Instead of reducing each experiment to a single initial-rate point, these methods compare the many points contained within complete reaction profiles. They therefore maximise the number of comparisons that can be made between experiments and extract kinetic information across a broad range of concentrations and conversions from only a few strategically designed reactions.

Finally, the continuing increase in computational power and the current revolution in machine learning[8] are opening a new stage in the evolution of kinetic analysis. These developments may help us analyse increasingly complex kinetic datasets, distinguish between competing mechanistic hypotheses and design experiments that provide the greatest amount of mechanistic information. We will explore these emerging possibilities and consider how they may shape the future of kinetic analysis.

References:

1. C. Alamillo-Ferrer, G. Hutchinson and J. Burés, “Mechanistic Interpretation of Orders in Catalyst Greater than One,” Nat. Rev. Chem. 2023, 7, 26–34. DOI
2. D. G. Blackmond, “Reaction Progress Kinetic Analysis: A Powerful Methodology for Mechanistic Studies of Complex Catalytic Reactions,” Angew. Chem. Int. Ed. 2005, 44, 4302–4320. DOI
3. J. S. Mathew, M. Klussmann, H. Iwamura, F. Valera, A. Futran, E. A. C. Emanuelsson and D. G. Blackmond, “Investigations of Pd-Catalyzed ArX Coupling Reactions Informed by Reaction Progress Kinetic Analysis,” J. Org. Chem. 2006, 71, 4711–4722. DOI
4. R. D. Baxter, D. Sale, K. M. Engle, J.-Q. Yu and D. G. Blackmond, “Mechanistic Rationalization of Unusual Kinetics in Pd-Catalyzed C–H Olefination,” J. Am. Chem. Soc. 2012, 134, 4600–4606. DOI
5. J. Burés, “A Simple Graphical Method to Determine the Order in Catalyst,” Angew. Chem. Int. Ed. 2016, 55, 2028–2031. DOI
6. J. Burés, “Variable Time Normalization Analysis: General Graphical Elucidation of Reaction Orders from Concentration Profiles,” Angew. Chem. Int. Ed. 2016, 55, 16084–16087. DOI
7. C. D.-T. Nielsen and J. Burés, “Visual Kinetic Analysis,” Chem. Sci. 2019, 10, 348–353. DOI
8. J. Burés and I. Larrosa, “Organic Reaction Mechanism Classification Using Machine Learning,” Nature 2023, 613, 689–695. DOI

Plenary Speaker 4

Núria López

Institut Català d'Investigació Química (ICIQ),
Spain

Short Biography

Núria López obtained her BSC Chemistry (1995) and her Ph.D. degree in Theoretical Chemistry at the University of Barcelona, Spain (1999). Then she joined the Center for Atomic-scale Materials Physics led by Prof. Jens K. Nørskov (Denmark) as post-doctoral researcher. In 2005 she started her independent career at ICIQ. Her research group focuses on the study heterogeneous photo-electro-catalysis from a theoretical standpoint. In 2010 she was awarded an ERC Starting Grant (2010) and then a ERC Proof-of-concept (2015) by the European Research Council. She was awarded a "Prize for Excellence" by the Real Sociedad Española de Química in 2015 and participated in the consortium that won the RSC's 2022 John Jeyes Award for sustainability. She has collaborated with several industries in Europe to leverage atomistic modelling, participated in more than 10 EU projects, and served in several committees in the European Union, including the most important supercomputing initiatives in Europe (being Chair of PRACE's Steering Committee and INFRAG (EuroHPC-JU)).

Prof. López has an h factor of 94 (GS), has published over 300 published articles and has been included in the Highly Cited Clarivate list of 2025 in Chemistry. She is a pioneer in the introduction of open data practices via ioChem-BD, the computational catalysis database developed at ICIQ.

Taking CARE of simulations in heterogeneous catalysis

I will describe the Artificial Intelligence tools we have been developing over the years to better describe Heterogeneous Catalysis.

Plenary Speaker 5

Pedro J. Pérez

Universidad de Huelva,
Spain

Short Biography

Pedro J. Pérez (Aroche, Spain, 1965) received a Degree in Chemistry from the Universidad de Sevilla in 1987 and a Ph.D. from the same institution in 1991 under the supervision of Prof. Ernesto Carmona. As a postdoctoral Fulbright Scholar, he then joined Prof. Maurice Brookhart's group at UNC-Chapel Hill (USA). In 1993, he accepted an appointment as an Assistant Professor at the newly established Universidad de Huelva (Spain), where he received several promotions before attaining his current position as Professor of Inorganic Chemistry in 2005.

Because the newly created Universidad de Huelva completely lacked research infrastructure, laboratories, and equipment in 1993, Dr. Pérez had to build his independent career from scratch. After three years of raising funds and constructing a laboratory, his independent research work commenced in 1996. Later, in 2010, he became one of the founders and the first Director of the Center for Research in Sustainable Chemistry (CIQSO).

His primary research focuses on developing catalytic systems for the valorization of raw materials, with a special emphasis on highly inert alkanes (CnH2n+2) via metal-catalyzed carbon-hydrogen bond functionalization processes.

Awards/Recognitions/Fellowships

2026 Medal of Honor, University of Huelva.
2026 Elected President of the Huelva Academy of Sciences, Arts and Humanities.
2023 Member of European Academy of Sciences.
2022 Distinguished Career Teaching Award, Faculty of Experimental Sciences, University of Huelva.
2020 Chemistry Europe Fellow.
2019 Member of the Huelva Academy of Science, Arts and Humanities.
2018 Member of the Academia Europaea.
2018 Research Award AIQBE-University of Huelva.
2017 Distinguished Career Research Award, Faculty of Experimental Sciences, University of Huelva.
2016 Medal and Research Award of the Royal Spanish Chemical Society.
2015 Homogeneous Catalysis Award of the Royal Society of Chemistry.
2014 Member of the National Academy of Sciences of Spain.
2014 Fellow of the Royal Society of Chemistry (UK).
2007 Inorganic Chemistry Award, Royal Society of Chemistry of Spain.
1991-1993 Fulbright Scholar.

Carbon-hydrogen bond activation by organometallics: Towards methane use as a C1-source in chemistry

Methane is the main component of natural gas,[1] available in vast amounts in earth crust, which provides a pivotal role for this hydrocarbon as a cornerstone for the future of sustainable chemistry, transitioning from a mere fossil fuel to a valuable feedstock for high-value chemicals. However, due to its high inertness, examples of its chemical modification are scarce, and yet reduced to laboratory-scale transformations.

In this presentation, the historical evolution of methane activation and functionalization through the intermediacy of organometallic complexes will be presented, from early examples and basic concepts to the latest breakthroughs.[2,3] Modern transition-metal catalysts now allow for the precise cleavage of the notoriously inert C–H bond under milder conditions. By bridging past basic milestones with cutting-edge organometallic research, this contribution aims at providing a view of the collective effort yet required to transform this potent greenhouse gas into a sustainable pillar of next-generation chemical manufacturing.

References:

1. Zichittella, G.; Pérez-Ramírez, J. Status and prospects of the decentralised valorisation of natural gas into energy and energy carriers. *Chem. Soc. Rev*. **2021**, 50, 2984-3012. doi: 10.1039/D0CS01506G.
2. Zhao, G.; Drewery, M.; Mackie, J.; Oliver, T.; Kennedy, E. M.; Stockenhuber, M. The Catalyzed Conversion of Methane to Value-Added Products. *Energy Technol*. **2019**, 8, 1900665. doi: 10.1002/ente.201900665.
3. Caballero, A.; Pérez, P. J. Methane as raw material in synthetic chemistry: the final frontier. *Chem. Soc. Rev*. **2013**, 42, 8809-8820. doi: 10.1039/C3CS60120J.

Plenary Speaker 6

David A. Leigh

The University of Manchester,
United Kingdom

Short Biography

David Leigh was born in Birmingham, England, on May 31, 1963. He received his BSc degree in Chemistry in 1984 from the University of Sheffield (UK) followed by a PhD in 1987 under J. Fraser Stoddart (before either of them had made a catenane, rotaxane or knot!). From 1987-1989 Leigh was a postdoctoral fellow at the National Research Council of Canada in Ottawa, Canada, studying carbohydrate-protein interactions. In 1989 he returned to the UK as a Lecturer (Assistant Professor) at the University of Manchester Institute of Science and Technology (UMIST, since 2004 part of the University of Manchester). He moved to become Professor of Synthetic Chemistry at the University of Warwick (1998-2001) and then Forbes Chair of Organic Chemistry at the University of Edinburgh (2001-2012) before returning to Manchester in 2012 where he is now the Sir Samuel Hall Chair of Chemistry, the only named chair in the Department of Chemistry at the University of Manchester (UK), a historic center for the physical sciences (Dalton, Joule, Rutherford, Bragg, Perkin, Robinson, Haworth, Turing, Geim, etc). Since 2016 Leigh has been a Royal Society Research Professor, a position held by a small number of Fellows of the Royal Society, the UK's National Academy of Science and Letters. Since 2018 he is also a Distinguished Professor at East China Normal University, Shanghai. Leigh is a Fellow of the Royal Society (FRS), the Royal Society of Edinburgh (FRSE), an International Honorary Member of the American Academy of Arts and Sciences, a member of the Academia Europaea and an honorary member of the Israel Chemical Society. He is currently President-elect of the Royal Society of Chemistry (RSC), 2026-28 (President, 2028-30).

Leigh is a leading pioneer of molecular ratchet mechanisms (non-equilibrium molecular dynamics) and nanotopology. Landmark examples from Leigh's laboratory include the first synthetic Brownian ratchets (2004-2007). The Leigh group have developed dynamic systems with increasingly complex and functional mechanisms of operation, including an acclaimed synthetic ribosome mimic (2013). In the last decade his group reported the first examples of autonomous chemically fuelled molecular ratchets (2016, 2021 & 2022), used knotting to induce allosteric catalysis (2017), introduced small-molecule robotics (2016) and developed a programmable 'molecular assembler' described in an accompanying Nature N&Vs article as 'Science fiction becomes fact' (2017). The citation of his August Wilhelm von Hofmann Medal from the German Chemical Society (GDCh) states 'If the evolution of life on earth would have needed a competent consultant, he would have been the number one choice' (2024).

Leigh has authored >345 publications, including Nature (11), Science (9), Nat. Chem. (12), PNAS (7), JACS (76) and Angew. Chem. (54). These have accrued >43000 citations, with an h index of 112 (GooSch 28 May 2026). ~1-in-8 of Leigh's papers have been the subject of independent published perspectives ('News & Views' articles) by other leading scientists.

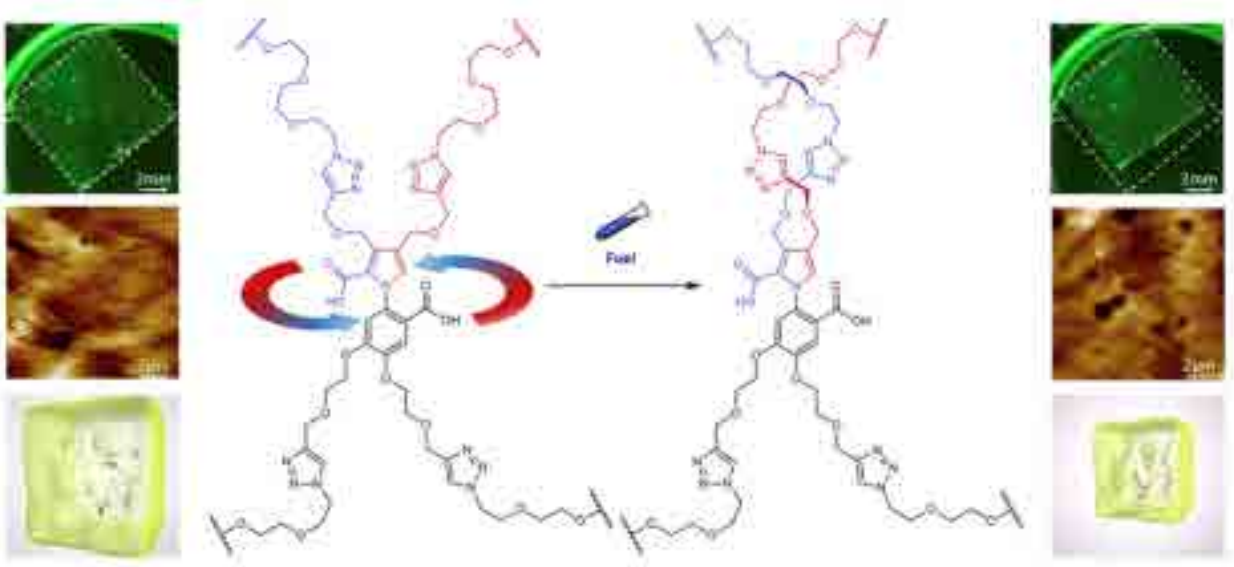
Leigh is also known for activities that merge art with science (video, music, magic, social media, traditional media, www, public lectures). 'Nanobot' [https://bit.ly/2Qw8qRn], a video he commissioned in 2018, generates >1M views per year across platforms. Social media show Leigh's videos being widely used by teachers in high schools [https://bit.ly/36t1nyr], in university courses [https://bit.ly/2MXkzg0], and by the general public. Leigh's molecular 819 knot (Science 2017) appears in the Guinness Book of World Records as 'the world's tightest knot'; his molecularly woven material (Nature 2020) holds the Guinness World Record for 'the finest woven fabric'.

The Leigh group's research contributions have been recognized with a number of scientific awards, including the Royal Society of Chemistry (RSC) Prizes for Supramolecular Chemistry (2003), Interdisciplinary Research (2004), Nanotechnology (2005) and the RSC Merck (2009), Tilden (2010), Pedler (2014), Perkin (2017), Horizon (2023) Prizes, the RSC-Spanish Chemical Society (RSEQ) Prize for Chemistry (2007), the Institute of Chemistry of Ireland Award for Chemistry (2005), German Chemical Society (GDCh) August Wilhelm von Hofmann Medal (2024), American Chemical Society (ACS) Ronald Breslow Award for Achievement in Biomimetic Chemistry (2026), Feynman Prize for Nanotechnology (2007), the International Izatt-Christensen Award in Macrocyclic Chemistry (2007), the EU Descartes Prize for Transnational Research (2007), the ISNSCE (International Society for Nanoscale Science, Computation and Engineering) Nanoscience Prize (2019), Royal Medal (Royal Society of Edinburgh, 2021), and the International Solvay Chair in Chemistry (2028). Leigh is a Clarivate Analytics Highly-Cited Researcher and is listed in Academic Influence's 'Top Influential Chemists 2010-2020'.

Why Nature Chose Catalysis

It seems counter-intuitive that the act of catalysis—simply the acceleration of a chemical reaction—somehow enables work to be done by the catalyst through the transduction of chemical energy from the reaction it accelerates. Yet this is how all of biology is powered.[1,2] Biomolecular motors transduce energy from the reaction they catalyse—generally ATP to ADP—to power the diverse array of tasks required by the cell.[3]

We shall discuss the transduction of chemical energy by a synthetic catalyst to generate force and perform mechanical work.[4] The simplicity of the molecular catalyst reveals the fundamental principles behind how the process occurs. The findings add to the understanding of how biology is powered by chemical energy and provide a blueprint for how to design artificial catalysis-driven molecular nanotechnology.[5] The experimental demonstration of the transduction of chemical energy to perform work against a load provides a minimalist mechanistic illustration of how catalysis-driven molecular motors extract order from chaos.[2]



References:

1. M. Schliwa, G. Woehlke, *Nature* **2003**, *422*, 759.
2. P. W. Hoffmann, *Rep. Prog. Phys*. **2016**, *79*, 032601.
3. S. Amano, S. Borsley, D. A. Leigh, Z. Sun, *Nat. Nanotechnol*. **2021**, *16*, 1057.
4. P.-L. Wang, S. Borsley, M. J. Power, A. Cavasso, N. Giuseppone, D. A. Leigh, *Nature* **2025**, *637*, 594.
5. S. Borsley, D. A. Leigh, B. M. W. Roberts, *Angew. Chem. Int. Ed.* **2024**, *63*, e202400495.

Invited Speakers

Invited Speaker 1

Alexandr Shafir

Institut de Química Avançada de Catalunya (IQAC-CSIC),
Spain

Short Biography

Shafir graduated in Chemistry from Hunter College (CUNY, USA), and obtained his PhD at UC Berkeley, USA (w/ J. Arnold) on redox-active metal complexes based 1,1'-diaminoferrocene ligands. He then joined the S. Buchwald laboratory at MIT to work on Cu-catalyzed C-N and C-O bond-forming reaction, reporting the first room temperature copper-catalyzed C-N coupling protocol, as well as a first ligand-controlled orthogonal copper-catalyzed C-N or C-O coupling. In 2006 A. Shafir received a Ramón y Cajal scholarship and moved to the Universitat Autònoma de Barcelona, where he went on to co-author publications in the fields of catalytic metal nanoparticles. There, he also launched a research program on hypervalent iodine reagents (e.g. JACS 2010), which began a key research topic in his group.

In 2013, Shafir obtained a 5-year Junior Group Leader position at the Institut Català d'Investigació Química (ICIQ) in Tarragona, where he established the Synthetic and Mechanistic Research laboratory. That same year he also represented Spain at the Young Investigator Workshop /EuCheMs (2013). The group's interests involved catalysis and oxidative CH functionalization, particularly using hypervalent iodine reagents. Additionally, the team studied mechanistic aspects of iodane-promoted reactions, and also developed new methods for the synthesis of metal-organic frameworks. Importantly, the group's results led to a very fruitful 3 year-long collaboration and contracts with the international agrochemicals company Syngenta Ltd (UK), with >€270,000 in funding to the research group and a 2019 joint patent. In 2014 the group received funding from the competitive grant (PI: Shafir, MINECO Plan Nacional). In 2017 he received the Thieme Chemistry Journal Award.

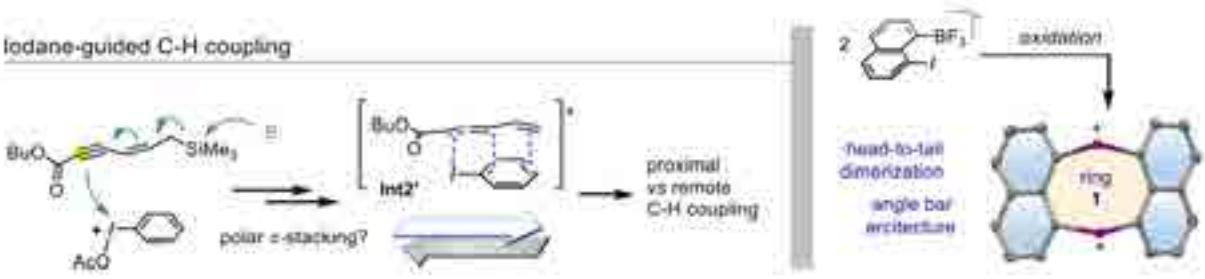
In 2018 Shafir was appointed Cientifico Titular (Tenured Scientist) of CSIC at the IQAC institute in Barcelona. Jointly with prof. A. B. Cuenca, he co-founded the BISI Bonds research group on synthetic methodology, supported through an on-going grant from Spain's MINECO As part of the group's activity, we reported a series of publications on the so-called "iodane-guided" ortho, and, more recently, meta and para C-H coupling reactions (ACIE 2019; ACIE 2020, ChemSci 2021, CHEM 2025). In Nov 2019, Shafir and Cuenca received the Arquímedes Award from the Ministry of Education as supervisors of the year's the best Master Thesis in Chemistry in Spain awarded to Wei Chen; the student's PhD study also received the RSEQ-Lilly award, and the Castells doctoral award from the local chapter of RSEQ.

To help address the societal aspiration towards Circular Economy, as of 2023 the group is part of a "Public-Private" consortium LULYPLAST funded with ~€800.000, aimed to recycle plastic waste through a pyrolysis-upgrade cycle. Recently, our team has also launched a program on boron-doped organic opto-

electronic cores, with early results reflected in a series of publications in the last 2 years (Chem. Sci. 2024, Chem. Sci. 2025, JACS 2026), and in a proof-of-concept grant funded with >250 000 euros on large-scale synthesis of BN-doped materials (IP's: A. Shafir, A. B. Cuenca. As of 2021, Shafir is the vice-president of the Catalan chapter of the Spanish Royal Chemical Society (RSEQ).

Reaction and structure development using hypervalent iodine

Hypervalent organoiodine reagents have become ubiquitous in organic synthesis, both as goto oxidants and as electrophilic group transfer agents. Nevertheless, in recent years several research groups have shown that that the potential of the halogen(III) centers extends way beyond those two applications. This talk will focus our group's recent efforts to discover new reactivity and new molecular architectures based on hypervalent halogen(III) center. With respect to reaction discovery, we have focused on the ability of certain highly reactive λ^3 -C-I-C intermediates to undergo a sigmatropic rearrangement, such that the CAr-Iodine(III) site acts as a reactivity trampoline for aromatic C–H coupling.[1,2] Our recent mechanistic insights into this process will be illustrated based on a rather versatile iodane-guided ortho C–H allylation reaction,[3] and on the newly developed remote C–H functionalization . Additionally, the talk will cover our latest findings on the synthesis and properties of new cyclic scaffolds based on multiple halogen atoms (see the naphthalene-based bis-λ^3-iodane dicationic ring **1**). Beyond their sheer synthetic challenge, these molecules are an interesting platform for new "angle bar" molecular geometries (provided a near-90o C-I-C angle), and for exploring new classes of inter-halogen synergistic effects.[4]



References:

1. W. W. Chen, A. B. Cuenca, A. Shafir, The Power of Iodane-Guided C–H Coupling: A Group-Transfer Strategy in Which a Halogen Works for Its Money. *Angew. Chem. Int. Ed.* **2020***, 59,* 16294.
2. Y. Liang, B. Peng, Revisiting Aromatic Claisen Rearrangement Using Unstable Aryl Sulfonium/Iodonium Species: The Strategy of Breaking Up the Whole into Parts. *Acc. Chem. Res.* **2022***, 55,* 2103.
3. a) W. W. Chen, A. Cunillera, D. Chen, S. Lethu, A. López de Moragas, J. Zhu, M. Solà, A. B. Cuenca, A. Shafir, *Angew. Chem. Int. Ed.* **2020***, 59*, 20201; b) J. D. Martín-Bernardos, K. Golob, W. W. Chen, O. A. Luongo, I. Sedó, A. B. Cuenca, A. Shafir, *Chem* **2025***, 11*, 102546.
4. a) W. W. Chen, M. Artigues, M. Font-Bardia, A. B. Cuenca, A. Shafir, Cyclic Homo- and Heterohalogen Di-λ^3-diarylhalonium Structures. *J. Am. Chem. Soc.* **2023***, 145*, 13796–13804;b) with Wei Chen, *Manuscript in preparation*, **2026**.

Invited Speaker 2

Allegra Franchino

Durham University,
United Kingdom

Short Biography

Allegra's training in homogeneous catalysis, focused on transition metals and bifunctional ligands, started during her degree at the University of Milan (under the guidance of Prof. Cesare Gennari, including an Erasmus semester at RWTH Aachen, and continued during her PhD studies at the University of Oxford with Prof. Darren Dixon (2013–2017).

After a brief stint in industry, in 2018 she joined the Echavarren group at ICIQ, supported by a 3-year MSCA COFUND fellowship. She then spent a year in the Morandi lab at ETH Zurich, working on iron catalysis and amination reactions.

Allegra moved to Durham University in September 2022, and is now Associate Professor there. Her group works on combining transition-metal catalysis, organocatalysis and mechanistic studies for the selective synthesis of added-value compounds. Since joining Durham, she has secured over €2.0m in funding, including a UKRI Future Leaders Fellowship.

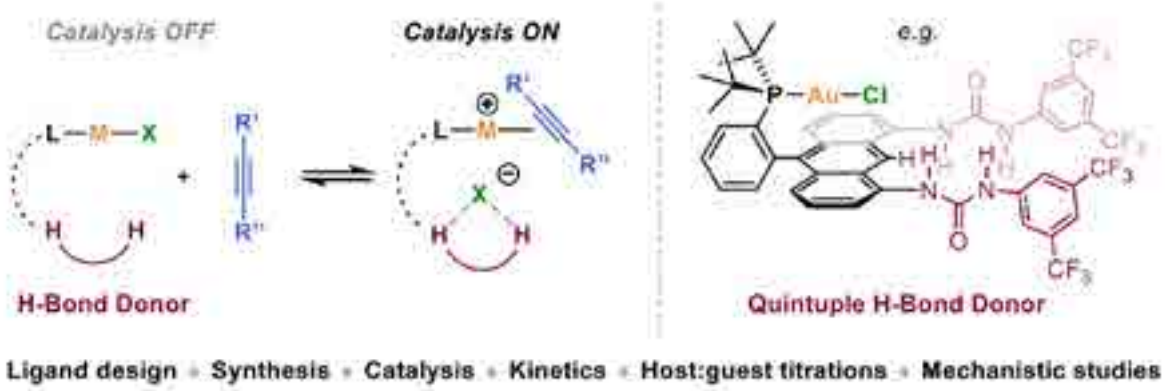
Repurposing H-bond donors for transition metal catalysis

In this talk, I will describe our efforts to pioneer conceptually new strategies that combine transition metal catalysis (chloride scavenging for precatalyst activation) and supramolecular chemistry (H-bond donors for anion binding).

Gold catalysis provides access to a remarkable array of complex products. However, the use of silver salts to activate gold(I) chloride precatalysts can be problematic, due to Ag(I) light sensitivity, hygroscopicity, redox activity and interference with the desired gold chemistry, which would otherwise be water- and air-tolerant. Self-activating gold(I) chloride complexes have emerged as a promising alternative, but still suffer from much lower activity and narrower applicability than silver salts, as Au–Cl cleavage is rate limiting.[1,2]

Addressing these limitations, we have recently reported a self-activating Au(I) chloride complex with a modified Buchwald ligand that incorporates a supramolecular chloride receptor: a 1,8-anthracene bisurea quintuple H-bond donor. Detailed mechanistic studies show that, in the presence of a coordinating product, the exceptional chloride binding ability of the bisurea unlocks a zwitterionic catalyst resting state where the Au–Cl bond has been cleaved. This significantly reduces barriers for catalysis and enables for the first time H-bond donors to compete with inorganic chloride scavengers in terms of activity and generality.[3]

Unpublished results from our group focus on novel multidentate H-bond donors that are no longer tethered to the ligand, able to activate various metal–pseudohalide bonds and applicable to enantioselective reactions.[4]



References:

1. A. Franchino, M. Montesinos-Magraner, A. M. Echavarren, *Bull. Chem. Soc. Jpn.* **2021**, *94*, 1099–1117.
2. J. Carlos Pérez-Sánchez, R. P. Herrera, M. C. Gimeno, *Chem. Eur. J.* **2024***, 30*, e202401825.
3. R. Parolin, T. J. Blundell, A. Franchino, *Angew. Chem. Int. Ed.* **2026***, 65*, e23431.
4. A. Brion, R. Parolin, A. Franchino, *in preparation*.

Invited Speaker 3

Javier Montenegro

Universidade de Santiago
de Compostela,
Spain

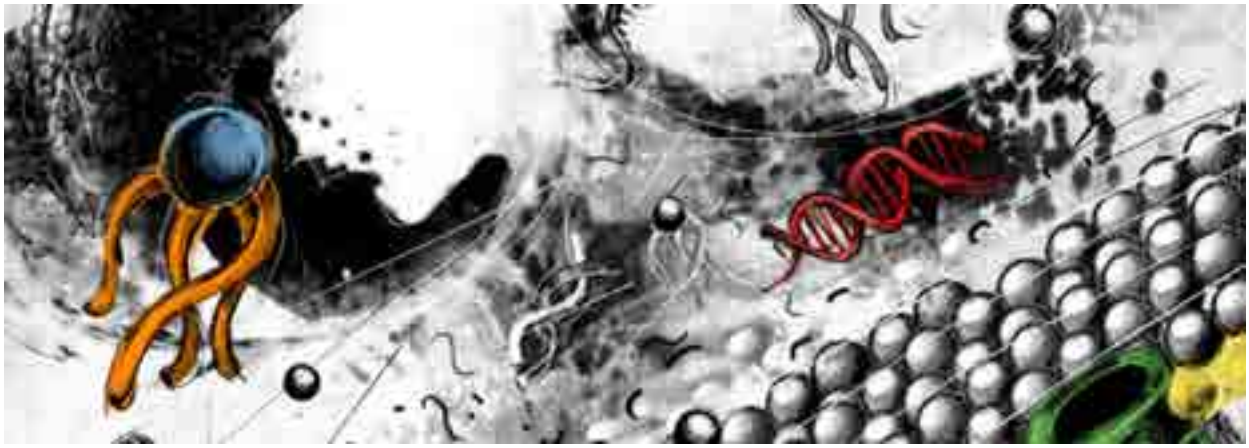
Short Biography

Javier Montenegro received his master degree (2003) and PhD (2009) from the University of Santiago de Compostela, under the direction of Prof. Susana López, working in the field of synthetic retinoids and their evaluation as artificial pigments in bacteriorhodopsins. In 2005 he was a visiting scientist in the group of Prof. Steven Ley at Cambridge University (Total Synthesis). In 2007 he was a visiting scientist at the Scripps Research Institute (La Jolla) working with Prof. Reza M. Ghadiri in prebiotic chemistry and supramolecular dynamic polymers. In 2009 he moved to the University of Geneva for postdoctoral studies with Prof. Stefan Matile in biosensing and synthetic transport systems. In 2012 he returned to Spain to the Organic Chemistry Department at the University of Santiago de Compostela and the CIQUS. He was then promoted to Profesor Titular (2020) and Oportunius Distinguished Research Profesor (2021). Javier sits at the advisory board of ChemSystemsChem and Supramolecular Materials. He has achieved competitive funding from international fuding aganecies including Pathfinder and Transition grants from the EIC, La Caixa health grant and one International Traingin Network. He has supervised 11 PhD students and 14 Postodoctoral associates with prestigous funding including 5 Marie Curies and 5 JdC. He has received different prestigious awards including the Juan de la Cierva (2012), the Ramón y Cajal (2015), the ERC Staring grant (2015), a Young Investigator Grant of the Human Frontier Science Program (2017), the JSP Fellow 52th Bürgenstock Conference (2017), the Prize of Young Investigators of the Spanish Royal Society of Chemistry (2018), the Prize of Young Research Group Leaders in Chemical Biology of the RSEQ (2019) and the ERC Synergy grant (2025).

Supramolecular Dynamic Chemistry for membrane transport and Biomimetic Systems

Our research group is interested in the application of supramolecular chemistry to understand and manipulate biology. [1,2] Our work philosophy is based in the importance of weak and noncovalent forces to control the shape and the topology of biomolecules, which are governed by the principles described by supramolecular chemistry. These supramolecular lessons can then be applied to control the properties and function of biomolecules. We believe that by modulating the shape we can mimic, control and improve functional behaviour. With focus in supramolecular interactions for artificial membranes and tubular composites, we

investigate the construction of synthetic systems for controlling and emulating biology and life-like soft systems. [3-8]



References:

1. Fuertes, A.; Juanes, M.; Granja, J.R.; Montenegro, J. *Chem. Commun.* **2017***,* 53, 7861–7871.
2. Lostalé-Seijo, I.; Montenegro, J. Nat. Rev. Chem. 2018, 2, 258–277. b) Pérez-Pérez, M.; Fuertes, A.; Montenegro, J. *Curr. Opin. Chem. Biol.* **2025***,* 78, 102497.
3. Gallego, I.; Ramos-Soriano, J.; Méndez-Ardoy, A.; Cabrera-González, J.; Lostalé-Seijo, I.; Illescas, B.M.; Reina, J.J.; Martín, N.; Montenegro, J. *Angew. Chem. Int. Ed.* **2022**, 61, e202210043.
4. Fernández-Caro, H.; Méndez-Ardoy, A.; Montenegro, J. *Nanoscale* **2022**, 14, 3599–3608.
5. Insua, I.; Bergueiro, J.; Méndez-Ardoy, A.; Lostalé-Seijo, I.; Montenegro, J. *Chem. Sci.* **2022**, 13, 3057–3068. b) Insua, I.; Cardellini, A.; Díaz, S.; Bergueiro, J.; Capelli, R.; Pavan, G.M.; Montenegro, J. *Chem. Sci*. **2023**, 14, 14074–14081.
6. Bayón-Fernández, A.; Méndez-Ardoy, A.; Álvarez-Lorenzo, C.; Granja, J.; Montenegro, J. J. *Mater. Chem*. B **2023**, 11, 606–617. b) Folgar-Cameán, Y.; Torralba-Maldonado, D.; Fulias-Guzmán, P.; Pazo, M.; Máximo-Moreno, I.; Royo, M.; Illa, O.; Montenegro, J. J. *Mater. Chem. B* **2025**, 13, 3365–3373. c) García Coll, J.; Ali, L.M.A.; Montenegro, J.; Bettache, N.; Ulrich, S. *Chem. Commun*. **2025**, 61, 4050–4053.
7. Barba-Bon, A.; Salluce, G.; Lostalé-Seijo, I.; Assaf, K.I.; Hennig, A.; Montenegro, J.; Nau, W.M. *Nature* **2022**, 603, 637–642. b) Chen, Y.; Barba-Bon, A.; Grüner, B.; Winterhalter, M.; Aksoyoglu, M.A.; Pangeni, S.; Ashjari, M.; Brix, K.; Salluce, G.; Folgar-Cameán, Y.; Montenegro, J.; Nau, W.M. J. *Am. Chem. Soc*. **2023**, 145, 13089–13098. c) Salluce, G.; Folgar-Cameán, Y.; Barba-Bon, A.; El Anwar, S.; Grüner, B.; Lostalé-Seijo, I.; Nau, W.M.; Montenegro, J. *Angew. Chem. Int. Ed.* **2024**, e202404286.
8. Van der Meel, R.; Wender, P.A.; Merkel, O.M.; Lostalé-Seijo, I.; Montenegro, J.; Miserez, A.; Laurent, Q.; Sleiman, H.; Luciani, P. *Nat. Rev. Mater*. **2025**, 10, 587–609.

Invited Speaker 4

Géraldine Masson

Centre National de la Recherche Scientifique (CNRS),
France

Short Biography

Géraldine Masson received her Ph.D. in organic chemistry from Joseph Fourier University (Grenoble, France) in 2003 under the supervision of Dr. Sandrine Py and Prof. Yannick Vallée. She then moved to the University of Amsterdam (The Netherlands) as a Marie Curie postdoctoral fellow, working with Prof. Jan van Maarseveen and Prof. Henk Hiemstra.

In 2005, she joined the CNRS as a researcher in the group of Prof. Jieping Zhu at the Institut de Chimie des Substances Naturelles (ICSN). She established her independent research activity in 2011 and has led the POWER group (Photocatalysis and Organocatalysis With Efficient Reactivity) since 2012. She was promoted to CNRS Research Director (DR2) in 2014 and to DR1 in 2020. In 2021, she became Co-Director of the joint CNRS–SEQENS laboratory HitCat, and since 2025 she serves as Deputy Director of ICSN.

She has served as Deputy Editor of ACS Organic & Inorganic Au since 2021 and as Associate Editor of The Journal of Organic Chemistry (ACS) since 2019.

Her research focuses on the development of innovative catalytic methodologies for the synthesis of optically active, biologically relevant molecules, with particular emphasis on asymmetric organocatalysis and photoredox catalysis.

From Asymmetric Organocatalysis to Photoredox Strategies for Building Complex Molecules

This lecture will first address advances in asymmetric enantioselective synthesis, highlighting how asymmetric organocatalysis can be used to build complex chiral molecules.[1] Particular emphasis will be placed on its application to natural product synthesis, through the total synthesis of exotine A and B. Key stereocontrolled transformations enabling the efficient and selective construction of these architectures will be discussed.[2]

In a second part, I will present complementary approaches based on visible-light photoredox catalysis.[3]

This will include stereoselective Smiles-type rearrangements directed by a chiral auxiliary,[4] as well as photocatalyst-free decarboxylative borylation of amino redox-active esters.[5] These methodologies enable the selective installation of aryl groups at otherwise challenging positions and the efficient incorporation

of boron motifs, providing access to β-arylpropamides and α-aminoboron derivatives under mild conditions.

Overall, the combination of asymmetric catalysis and radical-based strategies provides versatile tools for the synthesis of complex and functionally rich molecules.

References:

1. Selected reviews: (a) Courant, T.; Masson, G. J. *Org. Chem.* **2016***, 81*, 6945. (b) Varlet, T.; Masson, G. *Chem. Commun.* **2021***, 57*, 4089. (c) Bouchet, D.; Varlet, T.; Masson, G. *Acc. Chem. Res.* **2022***, 55*, 3265.
2. In preparation.
3. Selected reviews: (a) Prier, C. K.; Rankic, D. A.; MacMillan, D. W. C. *Chem. Rev.* **2013***, 113*, 5322. (b) Romero, N. A.; Nicewicz, D. A. Chem. Rev. 2016, 116, 10075. (c) Douglas, J. J.; Sevrin, M. J.; Stephenson, C. R. J. *Org. Process Res. Dev.* **2016***, 20*, 1134.
4. (a) Ma, W.-Y.; Leone, M.; Derat, E.; Retailleau, P.; Reddy, C. R.; Neuville, L.; Masson, G. *Angew. Chem. Int. Ed.* **2024**, e202408154. (b) Di Terlizzi, L.; Nicchio, L.; Montinho-Inacio, E.; Tiwari, N.; Derat, E.; Retailleau, P.; Fagnoni, M.; Neuville, L.; Protti, S.; Masson, G. *JACS Au* **2025***, 5*, 4972.
5. (a) Serafino, A.; Pierre, H.; Le Vaillant, F.; Boutet, J.; Guillamot, G.; Neuville, L.; Masson, G. *Org. Lett.* **2023***, 25*, 9249. (b) *In preparation*.

Invited Speaker 5

Sílvia Osuna
Universitat de Girona,
Spain

Short Biography

Sílvia Osuna received her PhD in 2010 from the University of Girona (UdG) at the Institut de Química Computacional (IQC). In 2010, she moved to the group of Prof. Houk at the University of California, Los Angeles (UCLA) with a Marie Curie postdoctoral fellowship to work on the computational design of enzymes. Sílvia is now an ICREA research professor and part-time full professor at UdG. Her group was created thanks to the awarded 2015 European Research Council project – Starting grant project and focuses on the development of new computational tools and approaches for computational enzyme design. Sílvia has been recently awarded the Fundación Banco Sabadell science and engineering award 2025, Biotrans Junior award 2025, the 2023 Young Spanish National Award in Chemistry, 2021 EuChemS lecture award, among others. Her group is currently funded by a European Research Council project – Consolidator Grant, ERC- Proof of Concept grants, and one I+D Spanish MINECO project.

Computational Design of Efficient Enzymes Through Coevolution and Correlation-Mediated Allosteric Networks

Enzymes exist as an ensemble of conformational states, whose populations can be altered through substrate binding, allosteric interactions, post-translational modifications, and even by introducing mutations into their sequence. In many enzymatic systems, full catalytic potential is only retained when in the presence of binding partners, either from additional proteins to generate heterocomplexes or from the formation of homo-oligomers.[1] Despite progresses and recent advances in generative models for protein design,[2] designing efficient enzymes and predicting oligomeric assemblies presenting a tight communication for enhancing a specific catalytic function remains challenging. Such tightly intertwined enzymatic assemblies modulate the conformational heterogeneity of the systems and allow the adoption of the multiple catalytically relevant conformational states needed for catalysis.[3] In this talk, we will explore our developed computational pipelines that integrate AlphaFold2 with quantum mechanics and molecular dynamics simulations to guide enzyme design and foster protein assembly, thereby enabling the cooperative interactions and conformational transitions crucial for enhanced catalytic performance. [3-5] We will also discuss how our approach, which combines coevolutionary analysis

and correlation-mediated allosteric networks, can be used to redesign enzymes and modify protein–protein interfaces for improved catalytic activity.[3, 5] Over the years, our work with diverse enzyme systems has generated strong evidence that rational design strategies can effectively yield active enzyme variants.[5] Moreover, we demonstrate that the current challenge of predicting distal active sites to enhance functionality in computational enzyme design can ultimately be met. [3]

References:

1. Goodsell, DS; Olson, AJ. Structural Symmetry and Protein Function. *Annu Rev Biophys* **2000***, 29*, 105-153
2. Casadevall, G.; Duran, C.; Osuna, S. AlphaFold2 and Deep Learning for Elucidating Enzyme Conformational Flexibility and Its Application for Design, *JACS Au* **2023**, 3, 1554.
3. Osuna, S. The challenge of predicting distal active site mutations in computational enzyme design, *WIREs Comput Mol Sci*. **2020**, e1502.
4. Casadevall, G.; Duran, C.; Estévez-Gay, M.; Osuna, S. Estimating conformational heterogeneity of tryptophan synthase with a template-based AlphaFold2 approach, *Prot. Sci*. **2022**, *31*, e4426.
5. Duran, C.; Kinateder, T.; Hiefinger, C.; Sterner, R.; Osuna, S. Altering Active-Site Loop Dynamics Enhances Standalone Activity of the Tryptophan Synthase Alpha Subunit, *ACS Catal.,* **2024***, 14,* 16986–16995
6. Duran, C.; Hiefinger, C.; Kinateder, T.; Poveda, A.; Uhl, P.; Jiménez-Barbero, J.; Sterner, R.; Osuna, S., Designing functional dimeric enzymes from impaired monomers through coevolution and correlationguided reprogramming of allosteric networks, **2026** *submitted for publication*.

Invited Speaker 6

Daniel Maspoch

Institut Català de Nanociència i Nanotecnologia (ICN2), Spain

Short Biography

Dr. Daniel Maspoch is an ICREA Research Professor and Group Leader at the Catalan Institute of Nanoscience and Nanotechnology (ICN2) and Autonomous University of Barcelona (UAB, Spain). His main research interests focus on clip-off chemistry, reticular chemistry and materials, and delivery systems. He is the author of over 230 articles, has filed 16 patents (4 of which have been licensed), signed 4 technology transfer contracts, developed 3 technologies currently available on the market, and is the co-founder of the spin-off company Ahead Therapeutics. In recent years, he has received prestigious European Research Council ERC-Consolidator, Proof-of-Concept (x2), and ERC-Advanced Grants. He has also been appointed as a Corresponding Academician of the Royal Spanish Academy of Science and has received several awards, including the Gold Medal of the Royal Spanish Society of Chemistry (2026), the Research Excellence Award from the Catalan Society of Chemistry (2025), the Hermanos Elhuyar Hans Goldschmidt Lecture from the German Chemical Society (2024), the prestigious Rei Jaume I Award (2023), and the Research Excellence Award from the Royal Spanish Society of Chemistry (2020).

Clip-off Chemistry: breaking bonds, building chemistry

Historically, innovations in synthetic methods and chemical reactions have transformed how scientists design and synthesize molecules and materials. Indeed, novel reactions or synthetic strategies not only enable access to previously unattainable structures but also inspire new paradigms for constructing materials that address global social, economic, and industrial challenges.

In this talk, I will introduce the concept and recent advances in Clip-off Chemistry. This approach is based on the design and synthesis of novel molecules and materials with welldefined compositions and structures via bond cleavage within molecular frameworks. Clip-off Chemistry thus represents a new synthetic methodology in which programmed, selective disassembly leads to the formation of new molecules and materials. This molecular disassembly is achieved through chemical reactions; in a first approach, via ozonolysis, which enables the cleavage of organic building blocks or linkers through direct breaking of alkene or alkyne bonds. I will present the fundamental principles of Clip-off Chemistry and recent examples of molecules and structures obtained through controlled bond fission in porous reticular materials.

Oral Communications Abstracts

Novel Gold (I)-Carbenoid Complexes for C-C Bond Formation

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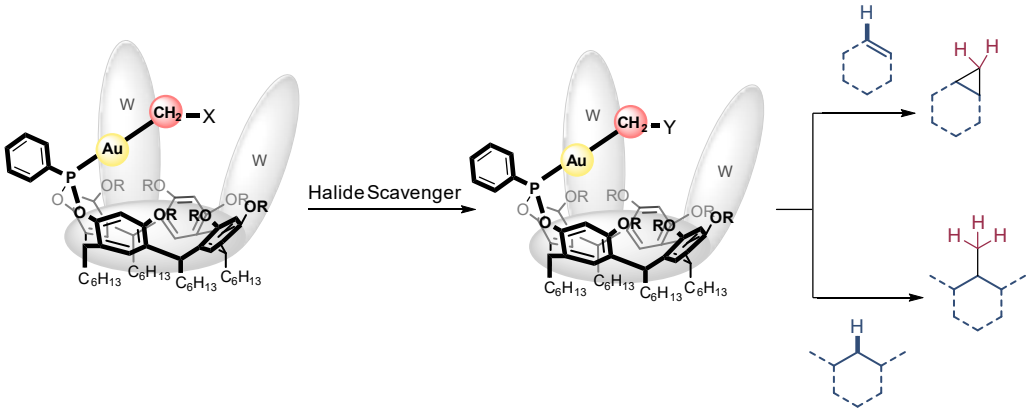
The development of supramolecular systems that emulate enzymatic activity represents a promising strategy to enhance the selectivity and efficiency of catalytic transformations. In this context, gold(I) cavitands based on resorcin[4]arene scaffolds have demonstrated catalytic properties in various processes, offering new routes for supramolecular catalysis.[1]

Over the past decade, carbenes have been proposed as key intermediates in a wide range of goldcatalyzed transformations.[2] However, knowledge regarding gold(I) carbenoid species remains limited, despite their reactivity being similar to that of carbene counterparts and their potential as attractive alternatives to otherwise non-isolable species.[3] In 2017, our group described the synthesis of easily accessible gold carbenoid with bulky ligand as gold(I) carbene equivalents in solution.[4]

In this contribution, we report the synthesis of novel chloromethyl gold (I)-cavitand complexes and their ability to promote C-C bond formation upon activation with a variety of chloride scavengers.



References:

1. a) M. P. Schramm, M. Kanaura, K. Ito, M. Ide, T. Iwasawa *Eur. J. Org. Chem.* **2016**, 813-820. b) N. Endo, M. Kanaura, M. P. Schramm, T. Iwasawa Eur. J. Org. Chem. 2016, 2514-2521.c) I. Martín-Torres, G. Ogalla, J. M. Yang, A. Rinaldi, A. M. Echavarren *Angew. Chem. Int. Ed.* **2021**, *60*, 9339-9344.
2. a) Y. Wang, M. E. Muratore, A. M. Echavarren *Chem. Eur. J.* **2015**, *21*, 7332-7399. b) R. J. Harris, R. A. Widenhoefer *Chem. Soc. Rev.* **2016**, *45*, 4533-4551. c) M. Navarro, D. Bourissou *Adv. Organomet. Chem.* **2021**, *76*, 101-144.
3. a) H. Lebel, J.F. Marcoux, C. Molinaro, A. B. Charette *Chem. Rev.* **2003**, *103*, 977-1050. b) H. Gessner *Chem. Commun.* **2016**, *52*, 12011–12023.
4. J. M. Sarria Toro, C. García-Morales, M. Raducan, E. S. Sminova, A. M. Echavarren *Angew. Chem. Int. Ed.* **2017**, *56*, 1859-1863.

SET-driven radical mechanism enables metal-free C-X (X = C, N, S) para-functionalisation of nitrobenzene

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Achieving selective C-H activation and bond formation in aromatic molecules remains a central task in organic chemistry. Conventional strategies rely on metal catalysts, pre-functionalized reagents, or harsh conditions, thereby increasing synthetic complexity and waste. Radical-based approaches offer a compelling alternative thanks to their unique reactivity patterns, enabling transformations under comparatively mild conditions. Here, by leveraging a single electron transfer (SET) process between Lewis pairs, we report a general radical-based mechanism that affords the one-pot regioselective C-X (X=C, N, and S) functionalisation of bare nitrobenzene.1 Detailed NMR, EPR, and XRD spectroscopies coupled to DFT studies show that after SET, the resulting pair of radicals engages in a cross-coupling reaction, which, after hydride abstraction, leads to the formation of para-functionalised product under mild conditions. These findings demonstrate that SET to nitrobenzene is far more accessible than previously appreciated,2 with a wide variety of carbanions, amides, alkoxides, organophosphides, and thiolates as compatible partners, positioning the broader class of nitroaromatics as versatile platforms for harnessing radical-pair reactivity in synthesis and expanding the scope of metal-free functionalisation strategies. More broadly, they highlight that nitro groups cannot always be regarded as innocent functionalities in the presence of anionic species, with important implications for reaction design and mechanistic interpretation.

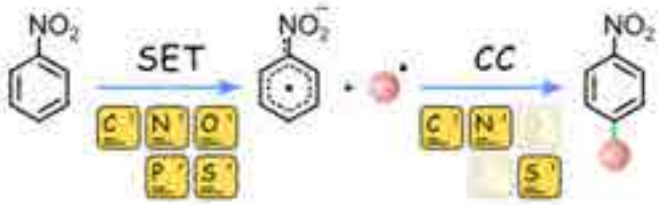

Figure 1: SET-mediated radical ion-pair formation and para-selective functionalization of nitrobenzene.

Acknowledgements: ERC-StG-2023, RadicalProtON (101116089), Basque Government grant (IT1584-22).

References:

1. Balahoju, S. A.; Bhattacharjee, N.; Lezama, L.; Lopez, X.; Salcedo-Abraira, P.; Rodríguez-Diéguez, A.; Reta, D. *ACS Omega* **2025**, *10* (22), 23798–23807.
2. Zhao, Y.; Zhu, H.; Sung, S.; Wink, D. J.; Zadrozny, J. M.; Driver, T. G. *Angew. Chem. Int. Ed.* **2021**, *60* (35), 19207–19213.

Heterogenization of a water-soluble manganese molecular complex unlocks highly efficient CO2 electroreduction to formate

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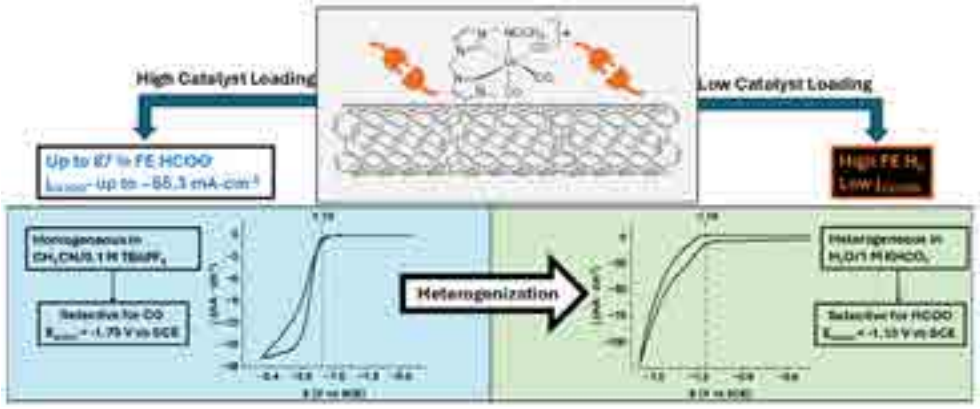
Molecular coordination complexes have been key platforms for understanding the chemistry behind CO2 electroreduction and for designing efficient catalysts for its conversion.1 However, molecular CO2-to-formate electrocatalysis in water that combines high rate, selectivity, and durability remains rare. Here, we report an earth-abundant Mn(I) bis-N-heterocyclic carbene complex whose reactivity is profoundly altered upon immobilization on multi-walled carbon nanotubes (MWCNTs). In homogeneous organic media, the catalyst selectively produces CO via CO2 coordination at Mn(-I) anionic intermediate, while the formate pathway proceeds through a Mn(I)–hydride route that generates a Mn(I)–formate intermediate highly stable in organic solvents, thereby preventing selective formate production.2 Upon heterogenization, product selectivity switches from CO to formate and the catalytic onset potential improves substantially, with an onset shift of ~600 mV relative to homogeneous operation. In CO2-saturated aqueous bicarbonate, the Mn/MWCNT hybrid cathode achieves formate partial current densities up to j = –65.3 mA·cm^{-2}, TOF(formate) up to 5917 h^{-1}, and Faradaic efficiency up to 88% in an H-cell, while maintaining excellent durability (TON up to 2.7 × 10^4 over 8 h at 50 mA·cm^{-2}). Electrochemical analysis, combined with isotopic labelling experiments and in situ/ex situ spectroscopy (including XAS) provides evidence-based constraints indicating that immobilization at the MWCNT/water interface promotes both Mn–H formation and reduction of the Mn–formate intermediate, enabling efficient formate production in aqueous electrolyte. This work shows that heterogenization on nanostructured carbon can fundamentally reshape the redox landscape and product selectivity of molecular catalysts in water, unlocking catalytic pathways inaccessible in homogeneous media.



References:

1. Franco, F.; Rettenmaier, C.; Jeon, H. S.; Roldan Cuenya, B. Transition metal-based catalysts for the electrochemical CO2 reduction: from atoms and molecules to nanostructured materials. *Chem. Soc. Rev.* **2020**, *49* (19), 6884-6946, 10.1039/D0CS00835D. DOI: 10.1039/D0CS00835D.
2. Fernández, S.; Franco, F.; Martínez Belmonte, M.; Friães, S.; Royo, B.; Luis, J. M.; Lloret-Fillol, J. Decoding the CO2 Reduction Mechanism of a Highly Active Organometallic Manganese Electrocatalyst: Direct Observation of a Hydride Intermediate and Its Implications. *ACS Catal.* **2023**, *13* (15), 10375-10385. DOI: 10.1021/acscatal.3c01430.

From Understanding to Innovation: The Power of Mechanistic Insight in Organic Chemistry

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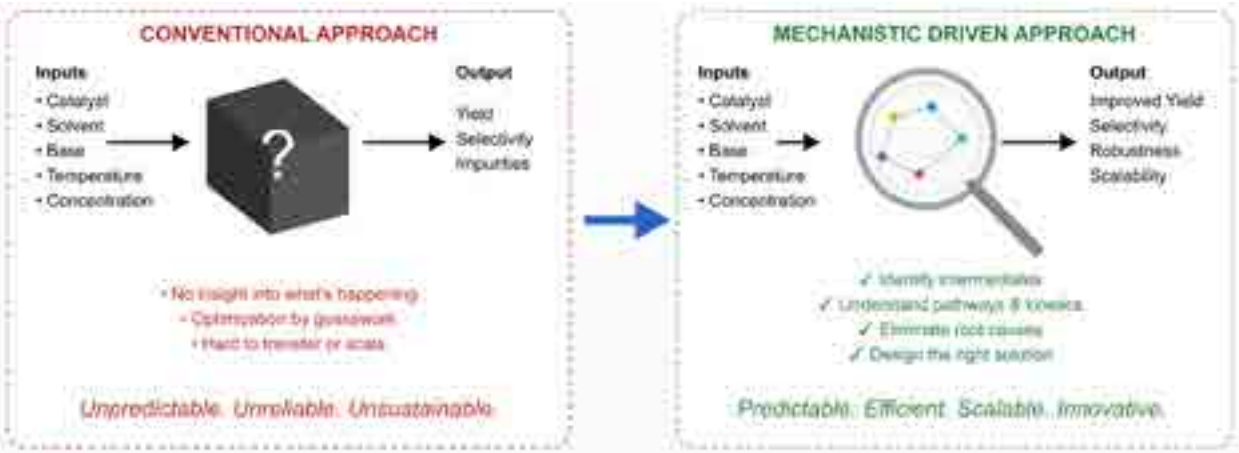
Many challenges in synthetic chemistry eventually reach a point where empirical optimisation alone is no longer sufficient. When reaction performance, selectivity, robustness, or scalability cannot be improved through conventional screening approaches, progress depends on a fundamental understanding of the underlying reaction mechanism. In this presentation, I will discuss how a mechanistically driven study can take ownership of complex projects that have stalled due to a lack of molecular-level understanding.

Through selected case studies, I will illustrate how the combination of experimental investigation with mechanistic reasoning,we can uncover the origins of inefficiencies and design rational solutions that are unlikely to be accessible through trial-and-error approaches, which can be infinite. Mechanistic understanding not only explains what is happening in a reaction but also provides the predictive power necessary to drive innovation, accelerate development, and unlock opportunities that would otherwise remain hidden.



Deciphering GPCRs activation and modulation. Development of a generic computational approach

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G protein-coupled receptors (GPCRs) are a superfamily of integral membrane proteins constituted by 7 transmembrane (TM) α-helices which mediate most cellular responses to external stimuli, giving rise to one of the most outstanding receptors families in the human body. Indeed, GPCRs constitute the largest family of druggable proteins in the human genome and malfunction of their associated signal transduction processes is one of the underlying causes of many human pathologies.Despite all this, only a small fraction of the possible druggable GPCRs has been exploited pharmacologically. Therefore, gaining insight, at both structural and molecular level, into how GPCRs participate in signal transduction processes and how these receptors are modulated is of utmost importance to develop effective pharmacological treatments, ideally without side effects, against GPCRsassociated pathologies. However, this supposes a major challenge since GPCRs are not simple on/off switches due to the fact that there is a preexisting equilibrium between their different states, associated with distinct conformational ensembles and functions, which can be modulated by ligand binding.

For this reason, we developed a generic computational approach that allows studying in a comprehensive way GPCRs transitions between different endpoint states, modulated or not by allosteric and orthosteric ligands[1-2]. Specifically, this methodology allows calculating the free energy profiles for activation processes of GPCRs and their derived complexes combining the usage of targeted molecular dynamics (TMD) simulations to generate the intermediate structures of a given activation process, with the protein-dipole Langevin-dipole (PDLD) method and our refined coarse-grained (CG) model for GPCRs to calculate the binding and conformational free energy contributions, respectively. This methodology has been successfully applied to Cannabinoid receptor 1 (CB1R)[3], Sphingosine 1-phosphate receptor 1 (S1PR1)[1] and CXC chemokine receptor 4 (CXCR4)[2] getting a deeper understanding of their activation conformational landscape and regulation. One of the main milestones achieved has been the rational design of the first small-molecule CXCR4 agonist (see Figure 1) identifying transition states of its activation process along with key resiudes and structural features that give rise to such barriers.

Figure 1. Scheme of the rational design of the first small-molecule CXCR4 agonist by the dual-moiety strategy. HL82624 is constituted by a binding moiety, derived from HF51116 which occupies CXCR4 major pocket and provides affinity, and a signalling moiety, derived from SDF-1α which occupies CXCR4 minor pocket and triggers GPCR activation favoring W94 and E288 active-state side-chain conformations. (Extracted from ref 1)

References:

1. Cruz, A. and Warshel, A. *J. Chem. Inf. Model.* **2025**, *65*, 16, 8637–8652
2. Zhou, J. *et al*. J. *Am. Chem. Soc.* **2026**, *148*, 20, 20545–20554
3. Cruz, A. and Warshel, A. *Proteins* **2024**, *93*, 4, 763–785

Site-Selective Distal Arylation of Sugars Enabled by Cyclic Acetals

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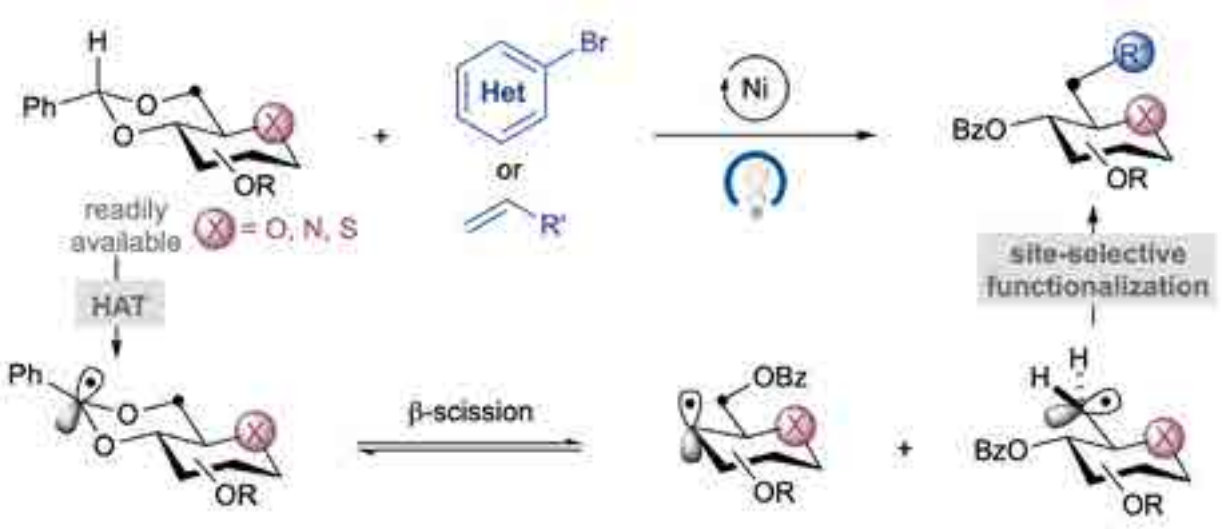
Herein, we describe a photoinduced Ni-catalyzed protocol that leverages the potential of cyclic acetals as vehicles for accessing glycosides bearing carbon–carbon linkages distal to the anomeric position. This method offers a new gateway to elusive compounds with high site selectivity, providing new opportunities in sugar-based therapeutics with lipophilic side chains.



References:

1. S. Zhang, J. Ordóñez, C. Blanco, L. Talavera, N. Kasdekar, E. Gómez-Bengoa, D. Crich, R. Martin, *J. Am. Chem. Soc.* **2026**, accepted.
2. C. Romano, L. Talavera, E. Gómez-Bengoa, R. Martin, *J. Am. Chem. Soc.* **2022**, *144*, 11558–11563.
3. S. K. Kariofillis, S. Jiang, A. M. Żurański, S. S. Gandhi, J. I. Martinez Alvarado, A. G. Doyle, *J. Am. Chem. Soc.* **2022**, *144*, 1045–1055.
4. G. Wang, C. C. Ho, A. Zhou, Y. -J. Hao, J. Lv, J. Jin, Z. Jin, Y. R. Chi, *J. Am. Chem. Soc.* **2024**, *146*, 824-832.

Photocatalytic Micromotors for S. epidermidis Biofilm Eradication

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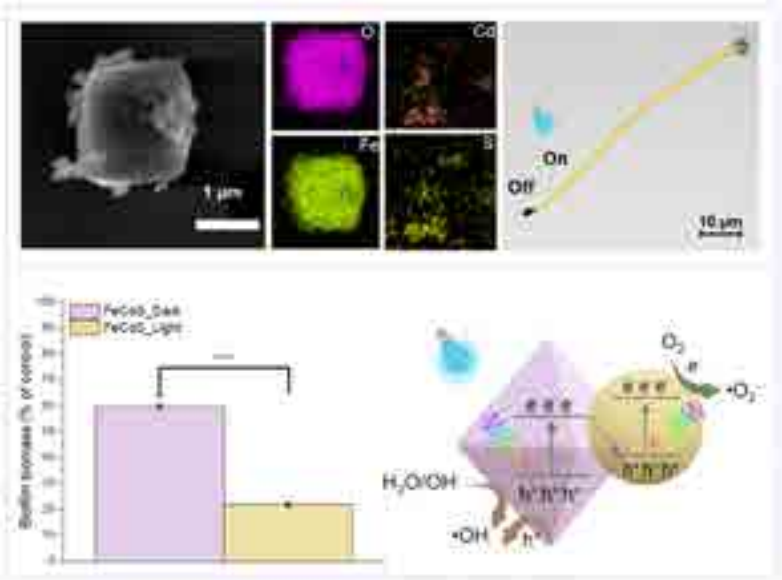
Antimicrobial resistance (AMR) is the capacity of pathogenic microorganisms to resist medications that were once effective against them. AMR has escalated into a critical global health crisis, causing millions of deaths each year and driving up healthcare costs worldwide1,2. In particular, biofilms are particularly difficult to eradicate because their dense extracellular matrix hinders the penetration of antimicrobial agents and protects embedded bacteria from external stresses. Current strategies to combat AMR emphasize the responsible use of antibiotics, investing in research and innovation for new treatments, and reinforcing the guidelines for infection prevention and control in healthcare settings1,2. Among emerging solutions, photocatalytic micromotors (PMNMs) represent a promising frontier for overcoming AMR resistance and achieving precise pathogen targeting3-5. Here, we investigate FeCdS-based photocatalytic micromotors for the disruption and removal of Staphylococcus epidermidis biofilms, a major cause of chronic and medical device-associated infections. Upon visible-light irradiation, these micromotors generate reactive oxygen species while simultaneously exhibiting self-propelled motion. The combination of photocatalytic activity and active transport is expected to enhance interactions with the biofilm matrix and improve bacterial inactivation compared with passive systems. Our results demonstrate that light-activated FeCdS PMNMs significantly degrade biofilm structure and exhibit superior antimicrobial activity compared to both dark controls and conventional therapies. These findings demonstrate the potential of PMNMs in combating biofilm-associated infections and contribute to the development of alternative antimicrobial approaches to address challenges associated with antimicrobial resistance.



References:

1. The Lancet, *Lancet Microbe* **2025**, 6, 100947.
2. G. Chen, W. Chang, M. Qiu, et al., *Mater. Chem. Front*. **2025**, 9, 772–792.
3. Y. Chen, J. M. Gonçalves, R. Ferrer Campos, K. Villa, *Small* **2024**, 2410901.
4. Z. Wu, Y. Chen, D. Mukasa, O. S. Pak, W. Gao, *Chem. Soc. Rev*. **2020**, 49, 8088–8112.
5. Z. Jiang, L. Fu, C. Wei, Q. Fu, S. Pan, *J. Nanobiotechnol.* **2023**, 21, 388.

Enantioselective Catalytic Strategies for the Synthesis of Bicyclo[2.1.1]hexanes as Novel Phenyl Bioisosteres

Thomas Rigotti[a]*, Pablo Garrido-García[a], Carla Pérez-Sánchez[a], Silvia Ortega-Gutiérrez[b], Mar Martín-Fontecha[b], Israel Fernández[b], Álvaro Somoza[c], Mariola Tortosa[a]

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Bicyclo[2.1.1]hexanes are bridged bicyclic scaffolds with well-defined exit vectors that are becoming increasingly popular building blocks in medicinal chemistry since they represent saturated bioisosteres of phenyl rings.[1,2] In this context, the development of enantioselective strategies that enable the obtainment of such hydrocarbon frameworks with control of the tridimensionality is highly desirable.[3] Herein we disclose the development of unprecedented enantioselective catalytic approaches to obtain differently disubstituted bicyclo[2.1.1]hexanes (Figure 1).[4,5] These enantioenriched sp^3-hybridized skeletons serve as appropriate mimics of *ortho*- and *meta*-substituted phenyl rings, representing versatile building blocks for the construction of a variety of drug analogues. An improvement of physicochemical properties and better pharmacokinetic profiles have been observed upon replacement of a phenyl ring for a saturated scaffold. Remarkably, retention of the biological activity for the bicyclo[2.1.1]hexane-containing analogues toward the specific molecular receptors targeted by the original drugs has been confirmed. Moreover, their cytotoxicity in a panel of cancer cell lines was evaluated, observing markedly differential effects for the two enantiomers and, in some cases, a substantial improvement over the corresponding sp^2-based drugs. This showcased that the control of the absolute configuration has an impact on the biological properties of the bioisostere-containing drug analogues, opening new avenues for lead optimization in drug discovery.

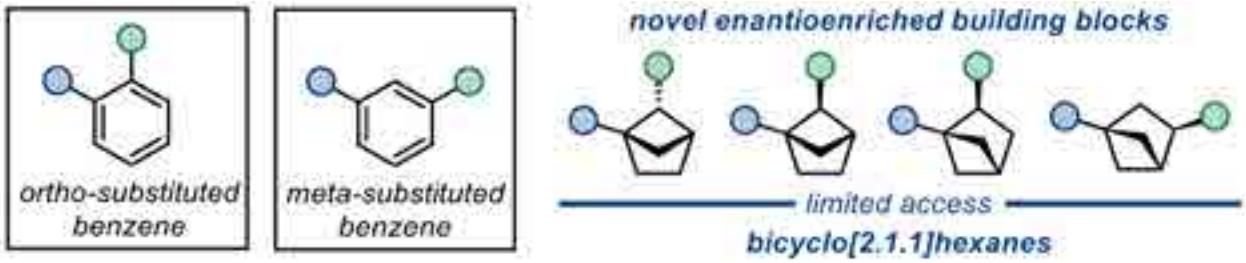

Figure 1. Developed catalytic strategies for the synthesis of differently substituted enantioenriched bicyclo[2.1.1]hexanes.

References:

1. P. K. Mykhailiuk, *Org. Biomol. Chem.* **2019**, *17*, 2839-2849.
2. M. A. M. Subbaiah, N. A. J. Meanwell, *J. Med. Chem.* **2021**, *64*, 14046-14128.
3. J. Tsien, C. Hu, R. R. Merchant, T. Qin, *Nat. Rev. Chem.* **2024**, *8*, 605-627.
4. P. Garrido-García, I. Quirós, P. Milán-Rois, S. Ortega-Gutiérrez, M. Martín-Fontecha, L. A. Campos, Á. Somoza, I. Fernández, T. Rigotti, M. Tortosa, *Nat. Chem.* **2025**, *17*, 734-745.
5. C. Pérez-Sanchez, P. Garrido-García, D. Fernández, D. González-Pinardo, S. Ortega-Gutiérrez, M. Martín-Fontecha, I. Fernández, T. Rigotti, M. Tortosa, *Nat. Synth.* **2026**, DOI:10.1038/s44160-026-01048-x.

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Acceleration of Azide-Alkyne Cycloaddition reactions in Octa-amino Bis-calix[4]pyrrole Cages

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Inspired by nature's strategies, chemists have developed molecular and supramolecular containers that mimic certain features of enzymes. Similar to enzymes' active sites, the inclusion of two reacting substrates within the confined space of a synthetic molecular flask increases their effective local concentration. The confinement process can also arrange and orient the reacting groups of the substrates in a geometry resembling that of the reaction's transition state. Our group recently reported the acceleration of azide-alkyne cycloadditions[1,2,3] and Diels–Alder reactions[4] in the cavity of a self-assembled [4+2] octa-imine bis-calix[4]pyrrole cage. However, the imine bonds present two main limitations: (1) the rigidity they impart to the cage structure, and (2) their intrinsic reduced stability in water, which has hindered further studies on these octa-imine cages in aqueous media. Herein, we report the synthesis of octa-amino bis-calix[4]pyrrole cages **1** and **2**. The complete reduction of the eight imine bonds to amino groups using $NaBH_4$ gives the more flexible octa-amino cage **1** soluble in organic solvents. The hydrolysis of the eight ethyl ester groups at the lower rim of the calix[4]pyrrole units in **1** with NaOH allows isolation of the water-soluble octa-amino cage **2** as a sodium salt. Both cages form highly thermodynamically and kinetically stable ternary hetero-complexes with azide and alkyne pyridine *N*-oxide guests. The cages accelerate the cycloaddition reaction of the confined substrates and selectively produce the 1,4-triazole isomer. The analysis of the kinetic data using an elaborated kinetic model yielded the rate constants for the confined reaction in chloroform ($k_{intra} = 6.0 \pm 1.5 \times 10^{-6}$ s^{-1}) and in a water solution ($k_{intra} = 8.0 \pm 2.2 \times 10^{-5}$ s^{-1}), along with the acceleration factors determined as effective molarities ($EM_{kin} = k_{intra}/k_{bulk}$).

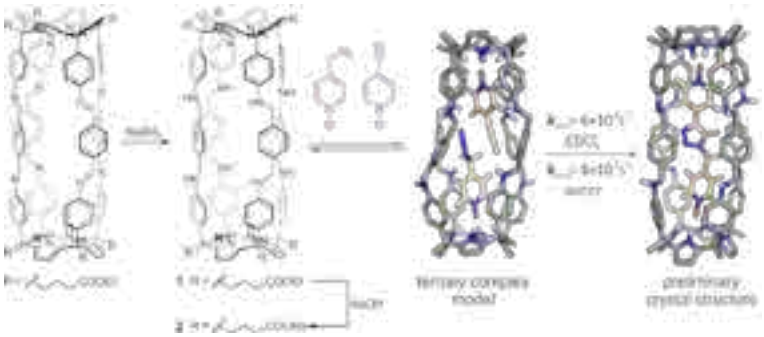

Figure 1: Synthesis of cages **1** and **2**, equilibrium of formation of the ternary complex (Michaelis), and confined reaction occurring in the cavity of cages **1** and **2**, producing the 1,4-triazole isomer.

References:

1. Li, Y.; Mirabella, C. F. M.; Aragay, G.; Ballester, P. *JACS Au* **2025**, *5*, 902–912.
2. Li, Y.; Aragay, G.; Ballester, P. *Chem. Sci., 2025, 16*, 14534-14543.
3. Li, Y.; Aragay, G.; Ballester, P. *Nat. Commun.*, **2026**. https://doi.org/10.1038/s41467-026-72315-w.
4. Huang, J.; Ballester, P. *J. Am. Chem. Soc.* **2025**, *147*, 13962–1397

Thiocarbonyl Difluoride as a Single-Sulfur Atom Transfer Agent: AgSCF3-Mediated Thionation of Amides

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Thioamides occupy a central role in organic synthesis, medicinal chemistry, and materials science, acting as stable amide bioisosteres and versatile intermediates in catalysis.[1] Traditional thionation methods often rely on toxic and malodorous sulfurizing reagents such as Lawesson's reagent or phosphorus decasulfide,[2] typically under harsh conditions.

Herein, we report a practical and operationally simple synthetic strategy for amide thionation using silver trifluoromethylthiolate ($AgSCF_3$) as a latent sulfur-transfer reagent. Upon activation by a Lewis acid, $AgSCF_3$ generates thiocarbonyl difluoride (TCF, $S{=}CF_2$) in situ, which acts as a single-sulfur atom transfer agent, enabling the selective conversion of amides into their corresponding thioamides. The methodology exhibits broad substrate scope, including aryl, heteroaryl, aliphatic, and cyclic amides, as well as drug-derived derivatives, with high functional group tolerance. The resulting thioamides display versatile reactivity, serving as valuable building blocks in synthesis and catalysis. Mechanistic investigations, including two-chamber trapping experiments, support a Lewis-acid-mediated TCF release followed by a formal [2+2] cycloaddition–cycloreversion sequence with the amide carbonyl.

Overall, this work uncovers a previously unrecognized reactivity mode of TCF, enabled by $AgSCF_3$, that operates beyond a multi-atom transfer platform,[3] delivering a broadly applicable thionation method that addresses key shortcomings of classical methods.

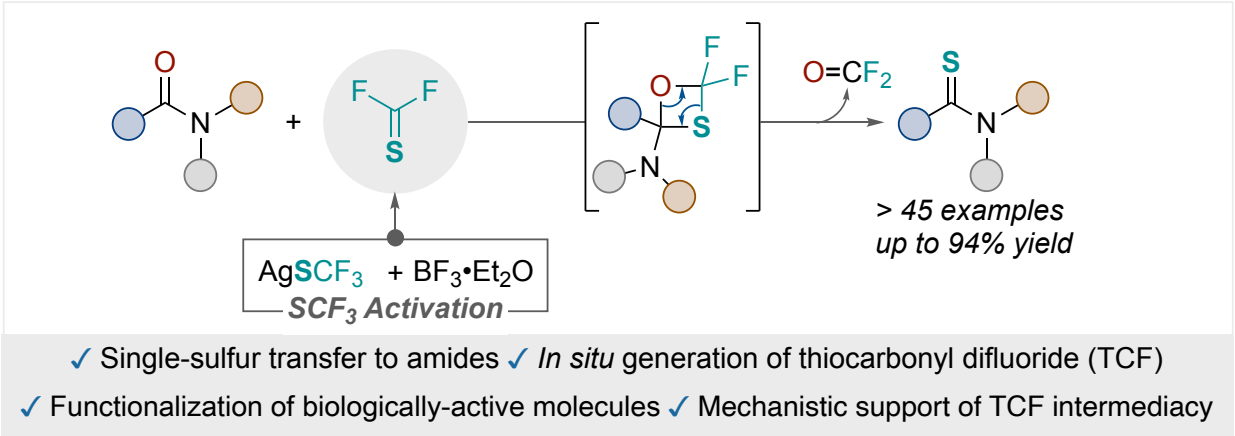

Figure 1. AgSCF3-mediated amide to thioamide conversion

References:

1. T. N. Hansen, C. A. Olsen, *Chem. Eur. J.* **2024**, *30*, e202303770.
2. V. Polshettiwar, M. P. Kaushik, *J. Sulfur Chem.* **2006**, *27*, 353–386.
3. (a) T. Scattolin, K. Deckers, F. Schoenebeck, *Angew. Chem. Int. Ed.* **2017**, *56*, 221–224. (b) T. Scattolin, A. Klein, F. Schoenebeck, *Org. Lett.* **2017**, *19*, 1831–1833. (c) T. Scattolin, K. Deckers, F. Schoenebeck, Org. Lett. 017, 19, 5740–5473. (d) M. Zhang, S. Chen, Z. Weng, *Org. Lett.* **2018**, *20*, 481–484.

Superchaotropic Boron Clusters for Broad-Spectrum Antibiotic Delivery

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As an alternative to conventional amphiphilic delivery systems, superchaotropic boron clusters have recently emerged as a robust platform for the transmembrane transport of bioactive cargos.[1] Their superchaotropic nature facilitates the translocation of hydrophilic cargoes across lipid bilayers by promoting their desolvation. Unlike traditional systems, these boron-based carriers can penetrate the lipid bilayers and release the cargo within the intracellular environment without compromising either membrane integrity or cargo stability. Moreover, boron clusters can be chemically functionalized to fine-tune their transport efficiency and toxicity profiles.[2]

Inspired by the behavior of boron clusters, this work explores whether superchaotropic carriers could broaden the therapeutic scope of antibiotics that are only active against Gram-positive bacteria by enhancing their efficacy and enabling their activity against Gram-negative pathogens bearing a double-membrane barrier. This strategy may provide a promising platform for the development of new antibacterial therapies to combat the growing threat of antimicrobial resistance worldwide.[3]

This work presents the design and synthesis of a novel dodecaborate cluster platform capable of overcoming biological barriers. The resulting platform was conjugated with natural antibiotics such as vancomycin, erythromycin and novobiocin, which are only active against Gram-positive bacteria. These conjugates have been evaluated for their ability to cross the outer membrane of Gram-negative pathogens (Figure 1) and for enhanced antibacterial activity in Gram-positive bacterial infections, highlighting these platforms as versatile carriers for next-generation antibacterial therapies.

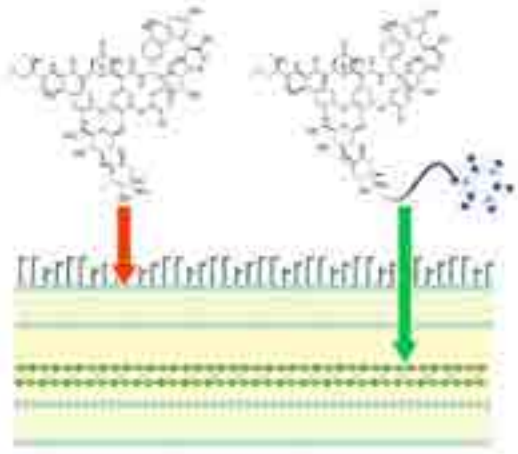

Figure 1. Schematic representation of the transmembrane transport of antibiotic Vancomycin in Gram-negative bacteria mediated by superchaotropic boron cluster conjugation.

References:

1. A. Barba-Bon, G. Salluce, I. Lostalé-Seijo, K. I. Assaf, A. Hennig, J. Montenegro, W. M. Nau. *Nature* **2022**, *603* (7902), 637–642.
2. G. Salluce, Y. Folgar-Cameán, A. Barba-Bon, I. Nikšić-Franjić, S. El Anwar, B. Grüner, I. Lostalé-Seijo, W. M. Nau; J. Montenegro. *Angew. Chem. Int. Ed.* **2024**, *63* (23), e202404286.
3. R. Kumari, I. Saraogi. *ChemPhysChem,* **2025**, *26*, e202401057

Synthesis and chemical recycling of crosslinked poly(ether-co-carbonates)

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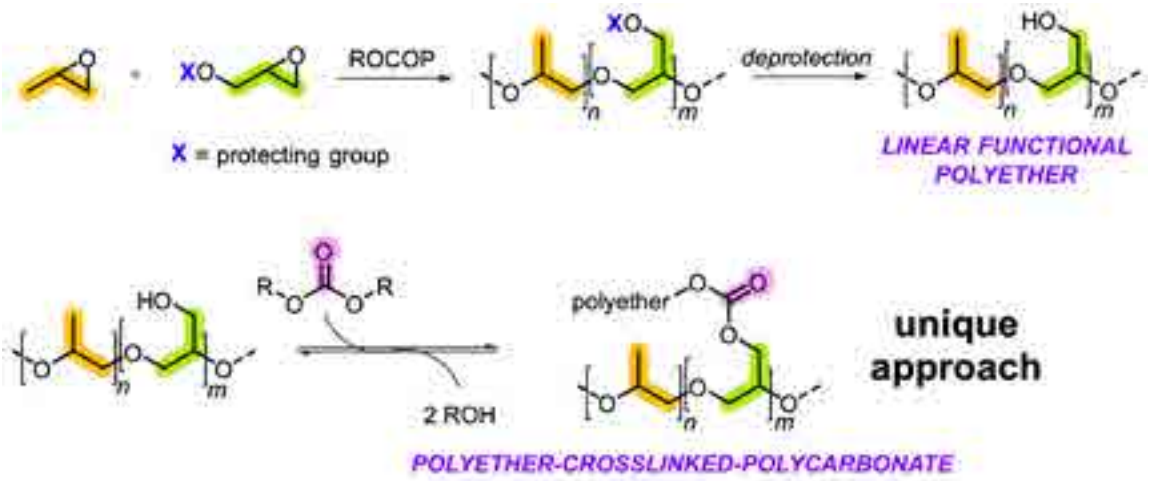
Plastic pollution and recycling are global problems posing an imminent challenge to mankind.[1] One option to mitigate these environmental issues is the development of sustainable routes to biobased plastics (i.e., bioplastics)[2] and their concomitant recycling/upcycling.[3] The chemical recycling of plastics is key especially for thermosets (crosslinked polymers) as inherently they cannot be recycled with conventional "melt-and-reshape" methods. Polyethers and polycarbonates are a class of polymers interconnected by C-O and C-C bonds which are used in a wide variety of applications.[4,5]



The presence of C-O based (ether and carbonate) bonds within the polymer architecture provides better bio/photo/chemo-based degradability compared to, for instance, conventional rubbers and polyolefins. This makes the development of polyether/carbonates with reversible crosslinks very attractive in the context of sustainable development. We thus envisioned to prepare polyethers with suitable (reversible) carbonate crosslinking groups that can be installed via a novel and modular synthesis approach using an in house developed catalytic system.[6] The obtained crosslinked poly(ether-co-carbonates) could be chemically recycled via methanolysis with no appreciable loss of properties/performance detected after recycling.

References:

1. https://www.unep.org/plastic-pollution#:~:text=Every%20minute%2C%20the%20equivalent%20of,-up%20in%20landfills%20or%20dumped (accessed on 27/01/2026)
2. S. Spierling, S. Springer, S. Albrecht, C. Herrmann, H.-J. Endres et al. J. Clean. Prod. 2018, 185, 476-491.
3. L. D. Ellis, N. A. Rorrer, K. P. Sullivan, G. T. Beckham et al. Nat. Catal. 2021, 4, 539–556.
4. J. Herzberger, K. M. Worm, F. R. Wurm, H. Frey et al. Chem. Rev. 2016, 116, 2170–2243.
5. H. Wang, F. Xu, Z. Zhang, M. Feng, M. Jiang, S. Zhang, RSC Sustainability, 2023, 1, 2162-2179.
6. C. J. Whiteoak, N. Kielland, V. Laserna, A. W. Kleij et al. J. Am. Chem. Soc. 2013, 135, 1228–1231.

Poster Abstracts

Adding PLP-like Functionalities to the Genetic Code

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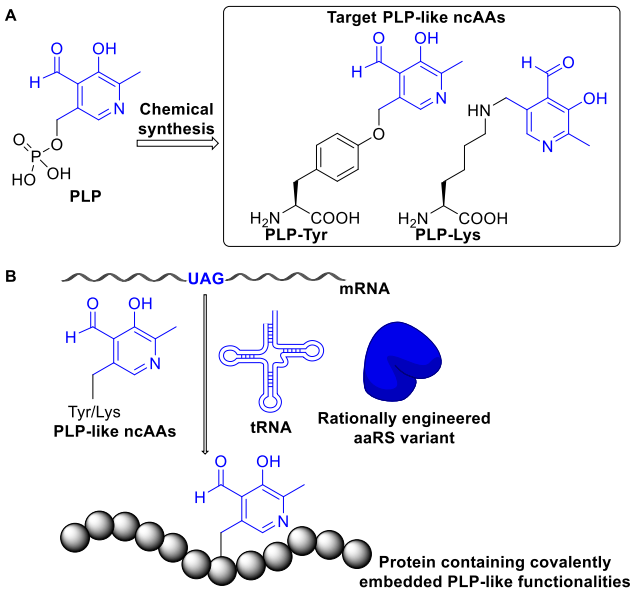
Abstract text: Pyridoxal-5'-phosphate (PLP)-dependent enzymes are a well-studied class of enzymes which exploit a highly versatile cofactor to catalyse a diverse breadth of transformations, including transaminations, racemizations, decarboxylations and eliminations (1). However, the modest operational stability of PLPdependent enzymes can restrict their usage in industrial settings. Industrial processes can require the exogenous addition of costly PLP to the reaction medium or the optimisation of PLP-binding through enzyme engineering (2). Engineering aminoacyl-tRNA synthetases (aaRSs) for chemically synthesised non-canonical amino acids (ncAAs) with side-chains designed to mimic PLP (Fig. A) could enable these functionalities to be covalently embedded at user-defined positions within protein backbones (Fig. B) (3). By following a computational approach involving AlphaFold2/3, quantum mechanics, molecular dynamics and correlation and coevolutionary analysis (4-6), we aim to rationally engineer highly efficient and selective aaRS variants, thereby avoiding the time and effort inputs associated with classical selection-based approaches (3). Ultimately, we envisage that this study could enable the cost-effective production of PLP-dependent enzymes with improved activity and stability profiles to facilitate their usage in industrial applications.



References:

1. 1. J.F. Rocha, A.F. Pina, S.F. Sousa, N.M.F.S.A. Cerqueira, *Catal. Sci. Technol.* 2019, **9**, 4864-4876.
2. D.R. Padrosa, R. Alaux, P. Smith, I. Dreveny, et al. *Front. Bioeng. Biotechnol.* 2019, **7**, 1-13.
3. C.C. Liu, P.G. Schultz, *Annu. Rev. Biochem.* 2010. **79**, 413-44.
4. G. Casadevall, C. Duran, S. Osuna, *JACS Au* 2023, **3**, 1554–1562.
5. S. Osuna, *Comput. Mol. Sci.* 2021,**11**, e1502.
6. G. Casadevall, J. Casadevall, C. Duran, S. Osuna, *Protein Eng. Des. Sel*. 2024, **37**, gzae005.

Novel phthalocyanine-based complexes for compartmentalized photocatalytic CO2 reduction

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Access to affordable and sustainable energy is a key objective for sustainable development, as recognized by the United Nations.[1] In this context, artificial photosynthesis is a very promising technology to produce renewable fuels from abundant feedstock such as water and CO_2, using sunlight as a source of energy. However, achieving a fully integrated and efficient artificial photosynthetic system remains a challenge. The two half reactions involved, namely water oxidation and CO_2 reduction, together with efficient light-harvesting and charge separation, represent chemical and technological challenges in themselves.[2] Further understanding and new system development is needed to advance the field.[3] One promising approach involves designing artificial systems that mimic the compartmentalization and spatial organization found in natural photosynthesis. Polymeric vesicles (polymersomes), self-assembled vesicles with high structural and chemical versatility, offer a robust platform to confine catalytic functions within distinct environments, separated by a membrane. This design can enhance reaction efficiency and stability by minimizing undesired side reactions and enabling directional charge transport.[3]

Herein, we report the development of a novel phthalocyanine-based cobalt complex for photocatalytic CO_2 reduction to CO with over 88 % selectivity when using a Cu-based photosensitizer under blue light irradiation (**Figure 1**). To enhance the stability and selectivity of this photocatalytic system, both the new cobalt phthalocyanine catalyst and a new Ir-based photosensitizer have been anchored to the membrane of a polymersome, resulting in the first example of a polymersome-based system for compartmentalized photocatalytic CO_2 reduction to methane in aqueous solutions. The effect of the polymersome confinement of both the catalyst and the photosensitizer allows to tune the selectivity of the photocatalytic reaction to obtain only CO_2 reduction derived products in water, suppressing the normally competing hydrogen evolution reaction.[4] Mechanistic studies are ongoing to rationalize these differences in reactivity between homogeneous and heterogenized systems.

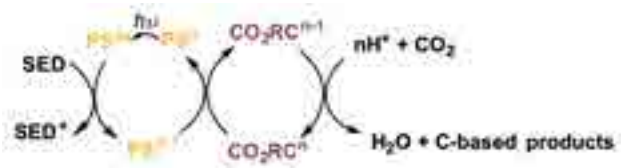

Figure 1. General scheme of the photocatalytic system for CO_2 reduction to C-based products. This approach consists of the combination of a photosensitizer (PS), a CO_2 reduction catalyst (CO_2RC), and a sacrificial electron donor (SED).

References:

1. C. Das Neves Gomes, *et al. Angew. Chem. Int. Ed.* **2012**, *51*, 187-190.
2. a) B. Zhang, *et al. Chem. Soc. Rev.* **2019**, *48*, 2216-2264. b) Z. Codolà, *et al. J. Am. Chem. Soc.* **2019**, *141*, 323-333. c) N. Kato, *et al. Joule* **2021**, *5*, 687-705.
3. a) E. Boutin, *et al. Chem. Soc. Rev.* **2020**, *49*, 5772-5809. b) A. Pannwitz, *et al. Chem. Soc. Rev.* **2021**, *50*, 4833-4855. c) L. Velasco-Garcia, C. Casadevall. *Commun. Chem.* **2023**, *6*, 263.
4. L. Velasco-Garcia, E. J. Espinoza-Suárez, J. R. Morelos-Pérez, K. Nassif, S. Plana, C. Casadevall, *Manuscript submitted*.

Exotic intermediate radicals in non-classic photoredox chemistry for transformation of challenging chemical building blocks

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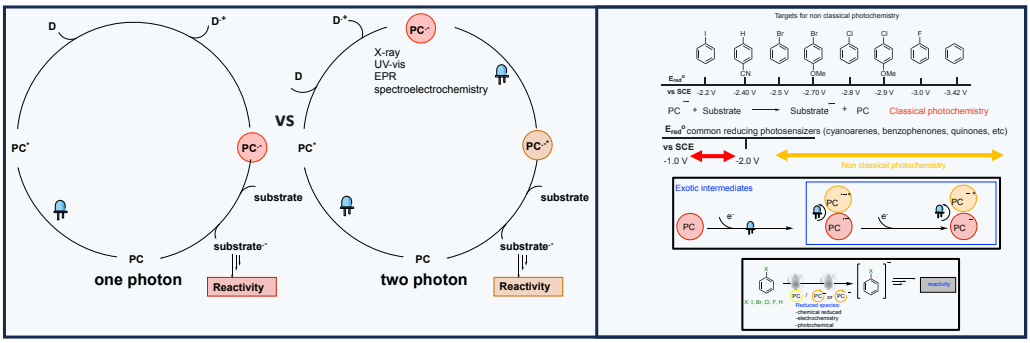
Keywords: Photosensitizers; excited radicals; Photoredox catalysis; single-electron transfer; unlocking photochemical reactions

Classical photosensitizers (**PS**), upon excitation with light (**PS***), become enhanced reductants and oxidants capable of undergoing single-electron transfer (**SET**) with an electron donor or acceptor. This process forms a radical intermediate species (**PS$^{\bullet+/-}$**), in which the photosensitizer has gained or lost one electron. The radical intermediate typically undergoes a second SET, reacting with a substrate in a quenching oxidant/reductant process to regenerate the ground-state photosensitizer, thereby completing the catalytic cycle. However, the radical reduced/oxidized species (**PS$^{\bullet+/-}$**) can itself undergo a second photon excitation to form an excited radical state (**PS$^{\bullet+/-*}$**), possessing even more extreme redox properties and enabling access to novel reactivity pathways.

In this work, an exotic radical intermediate as photosensitizer is used for overcoming challenging reactions which are limited thermodynamically by high redox potentials. Their reactivity has been tested against halogenated aryls which are common blocks difficult to reduce (-3.0 V vs SCE) and activation of this bond C-X (X: Br,Cl,F; BDE_{C-F}: 130 kcal/mol) is of great importance in pharmaceutical chemistry, green chemistry and material science. Their reactivity has been tested as well with unreactive benzene which is well known for the birch reaction ($Ered_{benzene}$: -3.42 vs SCE). Classical methods include using a metal alkali and large volumes of NH3(liq.) procedures that can be dangerous and time consuming in preparation.

Scheme 1.



References:

1. [1] Lloret-Fillol J, Pascual D, Fernandez S, Sun S, Dubed Bandomo GC, Martin-Diaconescu V, et al. Unravelling the Super-Reductive State of Iridium Photoredox Catalysts . ChemRxiv. 2023; This content is a preprint and has not been peer-reviewed.
2. Pfund, B.; Wenger, O. S. Excited Organic Radicals in Photoredox Catalysis. JACS Au 2025, 5 (2), 426–447. “This abstract is part of the Grant (PREP2022-000208), funded by MICIU/AEI/10.13039/501100011033 and by the FSE+.”

“This abstract is part of the Grant (PREP2022-000208), funded by MICIU/AEI/10.13039/501100011033 and by the FSE+.”

Mechanistic Insights into Confined Gold(I) Carbenoids in C–C Bond Forming Reactions

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Gold(I) cavitands based on resorcin[4]arene scaffolds have emerged as promising systems for supramolecular catalysis, enabling selective catalytic transformations.[1] Recent experimental studies in our group have shown that chloromethyl gold(I)-cavitand complexes promote C–C bond formation upon activation with chloride scavengers, likely through highly reactive gold(I) carbenoid intermediates.[2–4]

In this work, density functional theory (DFT) calculations were performed to investigate the reaction mechanism of these transformations. The computational results provide insight into the formation and reactivity of the formed species, as well as the influence of the cavitand environment on the reaction pathway and intermediate stabilization. The calculated energy profiles support the experimentally observed reactivity and contribute to a deeper understanding of these supramolecular gold-mediated processes.

Figure 1. Gold(I)-Carbenoid Cavitands for C–C bond formation.

References:

1. a) M. P. Schramm, M. Kanaura, K. Ito, M. Ide, T. Iwasawa *Eur. J. Org. Chem.* **2016**, 813-820. b) N. Endo, M. Kanaura, M. P. Schramm, T. Iwasawa *Eur. J. Org. Chem.* **2016**, 2514-2521.c) I. Martín-Torres, G. Ogalla, J. M. Yang, A. Rinaldi, A. M. Echavarren *Angew. Chem. Int. Ed.* **2021**, *60*, 9339-9344.
2. a) Y. Wang, M. E. Muratore, A. M. Echavarren *Chem. Eur. J.* **2015**, *21*, 7332-7399. b) R. J. Harris, R. A. Widenhoefer *Chem. Soc. Rev.* **2016**, *45*, 4533-4551. c) M. Navarro, D. Bourissou *Adv. Organomet. Chem.* **2021**, *76*, 101-144.
3. a) H. Lebel, J.F. Marcoux, C. Molinaro, A. B. Charette *Chem. Rev.* **2003**, *103*, 977-1050. B) H. Gessner *Chem. Commun.* **2016**, *52*, 12011–12023.
4. 4. J. M. Sarria Toro, C. García-Morales, M. Raducan, E. S. Sminova, A. M. Echavarren *Angew. Chem. Int. Ed.* **2017**, *56*, 1859-1863.

Novel Epigenetic Sequencing Methods for 5-methyldeoxycytidine

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Abstract not uploaded

Meta-C–H Cyclopropenylation of Pyridines through oxazino pyridine intermediates with CPCs

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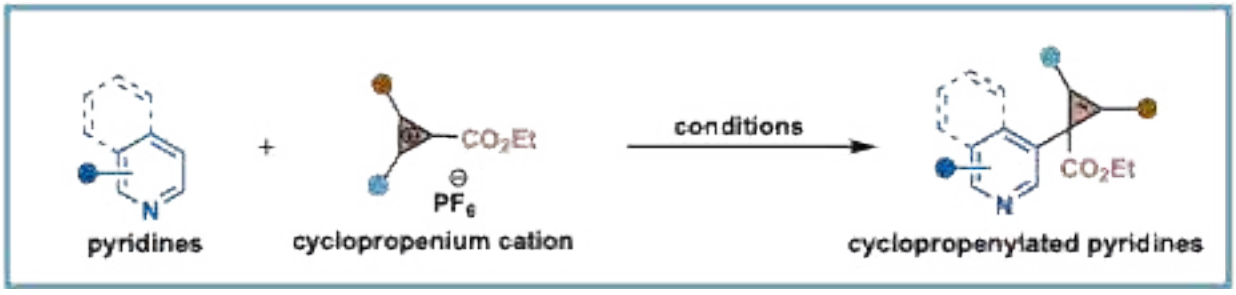
Cyclopropenes are versatile building blocks in organic synthesis that can serve as precursors of cyclopropanes or alternative complex cores.[1] However, despite its potential utility as three-dimensional scaffold with four defined exit vectors for pendant functionality, the cyclopropene ring remains largely underexplored in medicinal chemistry, due to the lack of suitable precursors and mild reaction conditions, together with their inherent instability. In 2023, we reported the first late-stage cyclopropenylation of aromatic C–H bonds with CPCs and demonstrated that cyclopropenes can enhance the metabolic stability of drug molecules. However, the applicability of this strategy to pyridine-containing systems is limited by the nucleophilicity of the pyridine nitrogen.[2,3] We present here a broadly applicable strategy for the late stage meta-selective cyclopropenylation of pyridines with cyclopropenium cations through a redox-neutral dearomatization-rearomatization strategy developed by Studer group.[4] The reaction features wide substrate scope, compatibility with structurally diverse CPCs, including drug like and ligand derived scaffolds. Moreover, the resulting cyclopropene motifs serve as versatile handles for further diversification, highlighting the utility of cyclopropenium chemistry in heterocycle functionalization and enabling new opportunities in medicinal chemistry and chemical biology.



References:

1. a) M. Rubin, M. Rubina, V. Gevorgyan, *Chem. Rev.* **2007**, *107*, 3117; b) Z.-B. Zhu, Y. Wei, M. Shi, *Chem. Soc. Rev.* **2011**, *40*, 5534; c) L. A. Wessjohann, W. Brandt, T. Thiemann, *Chem. Rev.* **2003**, *103*, 1625. d) R. D. Row, J. A, Prescher, *Acc. Chem. Res.* **2018**, *51*, 1073.
2. H.-F. Tu, A. Jeandin, M. G. Suero, *J. Am. Chem. Soc.* **2022**, *144*, 16737-16743.
3. a) H.-F. Tu, A. Jeandin, C. Bon, C.Brocklehurst, F. Lima, M. G. Suero, *Angew. Chem. Int. Ed.* **2023**, *62*, e202308379. b) A. Faraone, M. Balletti, A. Jeandin, H.-F- Tu, V. A. Ikonnikova, L. S. Sojka, M. G. Suero, *Angew. Chem. Int. Ed.* **2025**, e202518939.
4. H. Cao, Q. Cheng, A. Studer, *Science* **2022**, *378*, 779–785.

Heterogeneous Catalysis as a Tool to Study Nonclassical Nonlinear Effects

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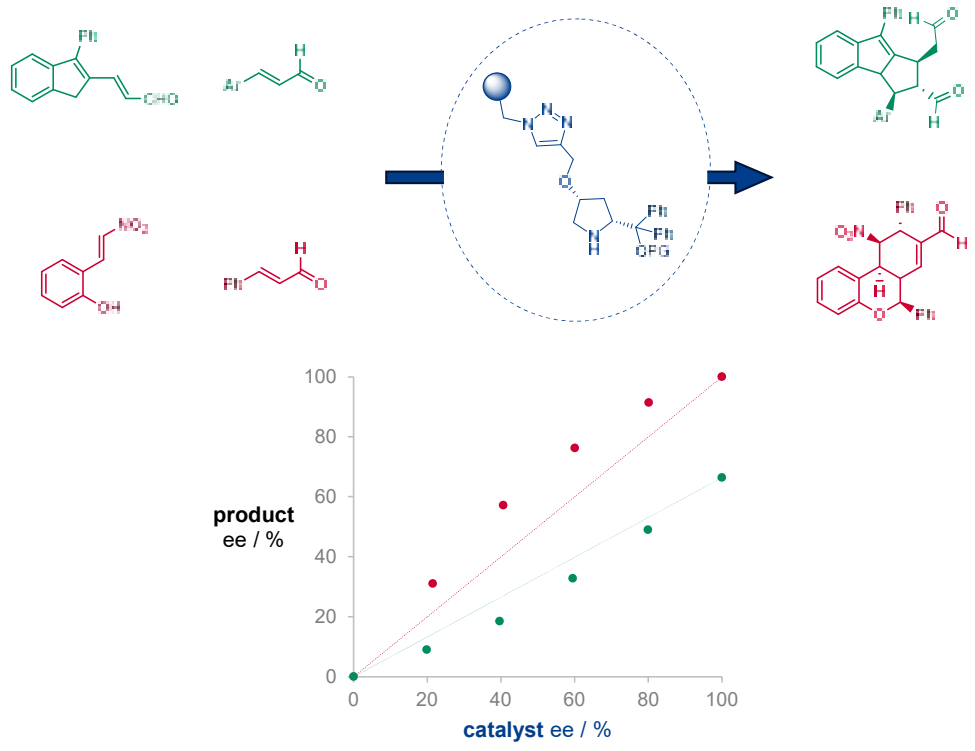
Nonlinear effects (NLEs), defined as deviations from a linear correlation between catalyst and product enantiomeric excess, are commonly attributed to catalyst aggregation or the involvement of multiple catalyst species. However, cascade processes that generate several stereocenters have recently emerged as a source of nonclassical NLEs that do not require the direct interaction between two molecules of catalyst.

Here, we employ catalysts immobilized on polymeric resins as a mechanistic tool to confirm this non-conventional mechanism to generate NLE. The spatial separation of enantiomers across different resin beads, together with the sparse distribution of catalytic sites within the polymer matrix, makes the simultaneous participation of multiple catalyst molecules very unlikely. The persistence or disappearance of NLEs using immobilised catalysts is therefore diagnostic of the nonclassical NLE not attributed to the interaction between two or more molecules of catalyst.



References:

1. C. Ali, D. G. Blackmond, J.Burés, *ACS Catal.* **2022**, 12, 10, 5776–5785.
2. J. Yu, D. G. Blackmond, *ACS Catal.* **2025**, 15, 3890–3897.
3. D. McLeod, J. A. Izzo, D. K. B. Jørgensen, R. F. Lauridsen, K. A. Jørgensen, *ACS Catal.* **2020**, 10, 10784–10793.
4. P. Kotame, B. -C. Hong. J. -H. Liao, *Tetr. Lett.* **2009**, 50, 704–707.

Hybrid light/electrical-driven micromotors with switchable propulsion modes

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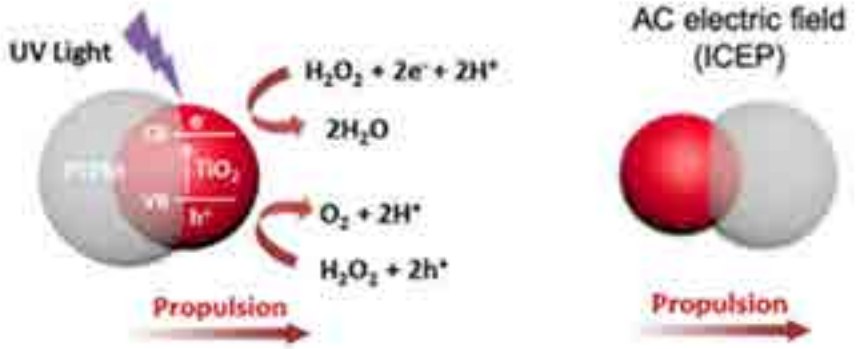
Micromotors with switchable propulsion modes are highly desirable for versatile microscale manipulation, yet most existing designs rely on a single driving stimulus and lack directional reversibility[1-3]. Electric or optical stimuli alone often fall short in providingflexible control over swimming directionin complex environments, while real-time visualization and tracking of mciroswimmer remains challenging in the absence of intrinsic luminescence[4]. Against these limitations, dual light/electric-responsive luminescent microswimmers with programmable directional switching represent an appealing solution to expand the functional scope of micromotor systems. Here, we report hybrid light/electric-driven snowman-like TiO_2-PTPM micromotors with switchable propulsion modes and intrinsic fluorescence emission. Under light irradiation, photocatalytic reactions steer the micromotors toward the TiO_2 hemisphere, whereas applied electric fields reverse locomotion toward the PTPM side via dielectrophoretic force. Selective Pt deposition on one particle end further enables controllable rotational motion within H_2O_2 solution[5]. In addition, fluorescent dyes incorporated into the PTPM segment endow the micromotors with luminescent property for in-situ motion tracking. Such dual-stimuli-responsive luminescent micromotors with tunable moving behaviours provide a flexible platform for microscale manipulation.



References:

1. X. Chen, X. Chen, M. Elsayed, H. Edwards, J. Liu, Y. Peng, H. P. Zhang, S. Zhang, W. Wang, A. R. Wheeler, *ACS Nano* **2023**, *17*, 5894–5904.
2. S. E. Ghellab, M. Al-salihi, X. Zhou, L. Lei, D. Yan, *Adv. Funct. Mater.* **2025**, *35*, 202504218.
3. X. Lv, S. Du, C. Zhou, W. Wang, H. Wang, Z. Zhang, *ChemNanoMat* **2021**, *7*, 902–905.
4. U. Töpfer, M. R. Bailey, S. Schreiber, F. Paratore, L. Isa, *ACS Nano* **2025**, *19*, 39210–39219.
5. Z. Xiao, S. Duan, P. Xu, J. Cui, H. Zhang, W. Wang, *ACS Nano* **2020**, *14*, 8658–8667.

Mechanistic Insights into TBD-Catalysed Polymer Recycling and Monomer Synthesis for a Circular CO2-Based Polymer Economy

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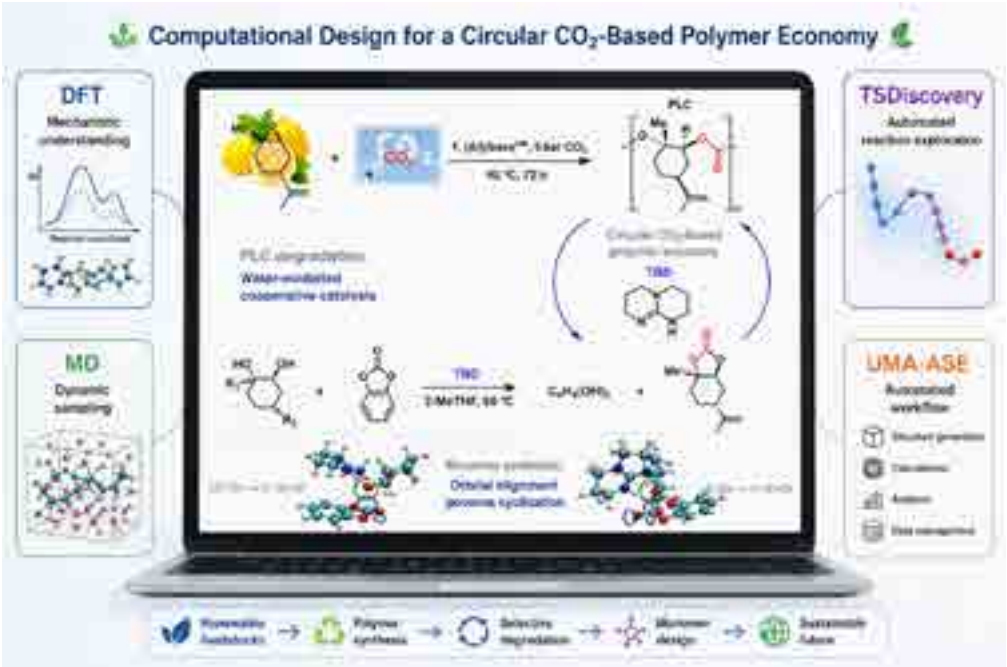
The transition towards a circular and carbon-neutral economy requires sustainable approaches to both polymer recycling and the synthesis of CO_2-based materials. Poly(limonene carbonate) and abbreviated as PLC, derived from renewable limonene oxide and CO_2, is a promising platform for circular plastics but its development relies on understanding the molecular origins of catalyst-controlled reactivity. Using density functional theory (DFT), molecular dynamics (MD) and automated computational workflows, we have investigated two TBD-catalysed transformations relevant to CO_2-based polymers.[1,2] The calculations reveal that PLC degradation[1] proceeds through a water-mediated cooperative catalytic mechanism involving catalyst-assisted water activation. In addition, cyclic carbonate formation is governed by favourable orbital alignment rather than simple geometric proximity during ring closure. These findings provide molecular-level design principles for both polymer recycling and monomer synthesis, and demonstrate how modern computational tools can accelerate the development of sustainable materials for a circular CO_2-based polymer economy.



References:

1. D. H. Lamparelli, A. Villar-Yanez, L. Dittrich, J. Rintjema, F. Bravo, C. Bo, A. W. Kleij, *Angew. Chem. Int. Ed.* **2023**, *62*, e202314659. https://doi.org/10.1002/anie.202314659
2. A. Villar-Yanez, C. Manservisi, D. Rigo Author, N. Kulbacka, C. Bo, A. W. Kleij, *ChemRxiv* **2025**, https://chemrxiv.org/doi/full/10.26434/chemrxiv-2025-3xlnv

Hidden Pathways in Cp*Co-Catalyzed Nucleophilic Couplings

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Over the past decade, Cp*CoIII catalysts have emerged as powerful tools for directed C–H functionalization reactions.[1]

While their reactivity toward electrophilic partners is well established, nucleophilic C–H coupling processes remain rare and their underlying mechanisms are poorly understood.[2,3] In this work, we identify key mechanistic features governing Cp*Co-mediated carbon–carbon bond formation, revealing unexpected complexity across both transmetalation and reductive elimination steps.

Using well-defined cobaltacyclic intermediates as mechanistic platforms, we show that transmetalation can proceed via distinct, additive-dependent pathways. Notably, in contrast to prevailing paradigms for Cp*TM systems, where nucleophilic C–R couplings typically require an oxidatively-induced reductive elimination from high-valent intermediates,[4] we reveal that C–C bond formation can occur directly from Cp*Co(III) species.

These results revise the current mechanistic landscape of Cp*TM-mediated nucleophilic couplings and highlight a fundamentally distinct reactivity profile of cobalt compared to its noble metal counterparts, opening newopportunities for nucleophilic C–H functionalization.

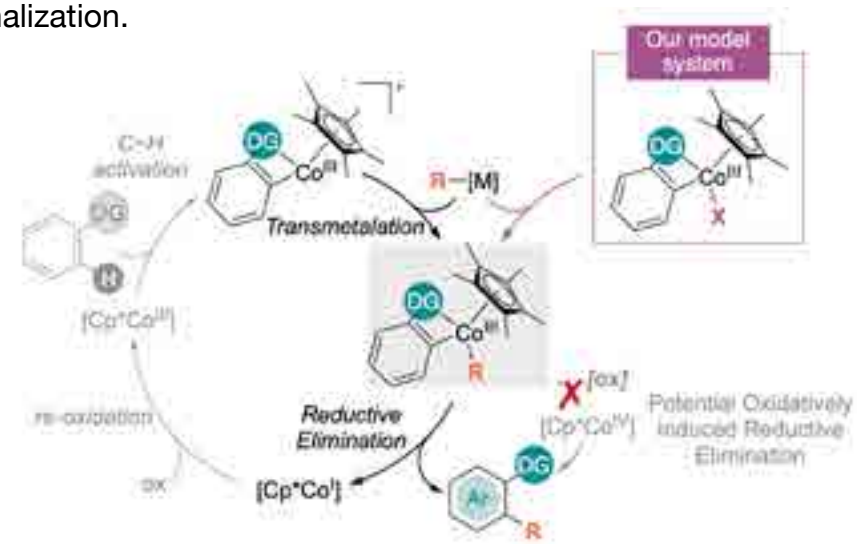

Figure 1. C–H nucleophilic coupling mechanism.

References:

1. P. Gandeepan, T. Müller, D. Zell, G. Cera, S. Warratz, L. Ackermann. *Chem. Rev.* **2019**, *119*, 2192.
2. (a) T. Gensch, F. J. R. Klauck, F. Glorius. *Angew. Chem. Int. Ed.* **2016**, *55*, 11287. (b) X. G. Liu, Q. Li, H. Wang. Adv. Synth. Catal. 2017, 359, 1942. (c) S. D. Friis, M. J. Johansson, L. Ackermann. *Nat. Chem.* **2020**, *12*, 511.
3. S. López-Resano, S. Martínez de Salinas, F. A. Garcés-Pineda, A. Moneo-Corcuera, J. R. Galán-Mascarós, F. Maseras, M. H. Pérez-Temprano. *Angew. Chem. Int. Ed.* **2021**, *60*, 11217.
4. J. Kim, K. Shin, S. Jin, D. Kim, S. Chang. *J. Am. Chem. Soc.* **2019**, *141*, 4137.

Technetium-Based Polyoxometalates: Building Blocks and Oxidation States

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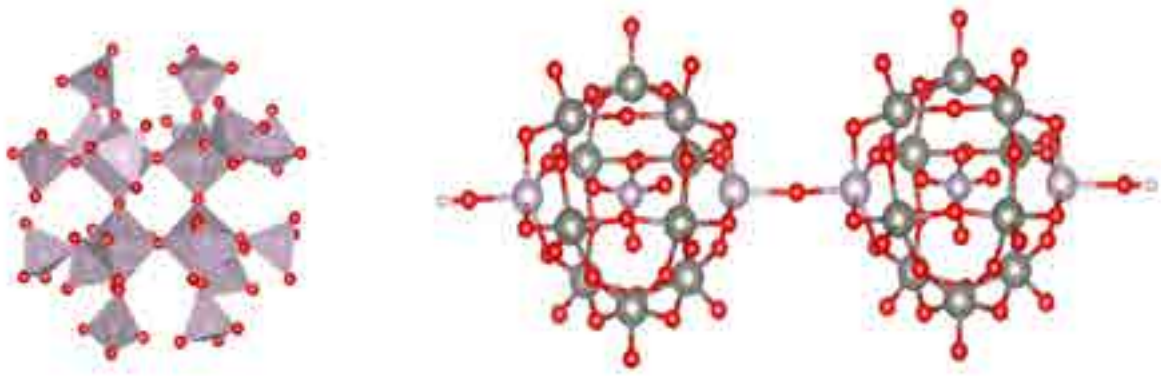
Polyoxometalates (POMs) are a prominent class of metal-oxygen cluster anions primarily composed of early transition metals (e.g., Mo, W, and V) in high oxidation states. The integration of computational approaches with experimental investigations has become increasingly important for elucidating the structural and electronical properties of Tc-containing POM systems.

In our recent work, we investigated cyclic Tc(V) metal-oxo tetrameric species and evaluated their relative stabilities in comparison on with the corresponding Re(V) analogues [1].

In this contribution, we further extend our computational studies to dimeric architectures of the type POM-Tc-O-Tc-POM. By correlating experimentally determined crystallographic geometries with density functional theory (DFT)-optimized structures, we aim to elucidate the most plausible oxiddation state and electronic configuration of Tc in newly proposed Tc-based Keggin-type polyoxometalates frameworks.



References:

1. J. Bustos, M. Shohel, A. G. Buzanich, L. Zakharov, J. Buils, M. Segado-Centellas, C. Bo, M. Nyman, *Chem. Eur. J.* **2025***, 31*, e202404144.

Review of Rare Earth-Based Phosphate Materials (2019–2025): Synthesis, Characterization and Applications

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Rare earth-based phosphate materials ($REPO_4$, where RE = La–Ce and Y) have attracted significant attention owing to their remarkable thermal stability, chemical durability, optical properties, and structural versatility. During the period 2019–2025, extensive research has focused on developing advanced rare earth phosphate materials with tailored morphologies and enhanced functional performances. This review summarizes recent progress in the synthesis, characterization, and applications of rare earth phosphate materials.

Recent studies reveal that rare earth phosphates exhibit excellent performance in a wide range of applications. In optics and photonics, $REPO_4$ materials demonstrate efficient luminescence and energy-transfer properties suitable for phosphors, lasers, and light-emitting devices. Their high thermal and radiation stability make them promising candidates for nuclear waste immobilization and advanced ceramic technologies. Furthermore, rare earth phosphates have shown potential in heterogeneous catalysis, environmental remediation, phosphorus recovery, and energy-related applications. Emerging investigations also explore their role in magnetic, sensing, and biomedical systems.

Overall, the literature published between 2019 and 2025 highlights the growing importance of rare earth phosphate materials as multifunctional inorganic compounds. Future research should focus on scalable synthesis strategies, structure–property relationships, and the development of sustainable applications to further expand their technological impact.

References:

1. S. Chong, B. J. Riley, X. Lu et al., *RSC Adv.* **2024**, *14*, 18978–19000.
2. Y. Ji, P. M. Kowalski, P. Kegler et al., *Front. Chem.* **2019**, *7*, 197.
3. M. R. Rafiuddin, G. Donato, S. McCaugherty et al., *ACS Omega* **2022**, *7*, 39482–39490.

Enantioselective, site-selective Ni-catalyzed β- & γ- alkylation of unsaturated amides

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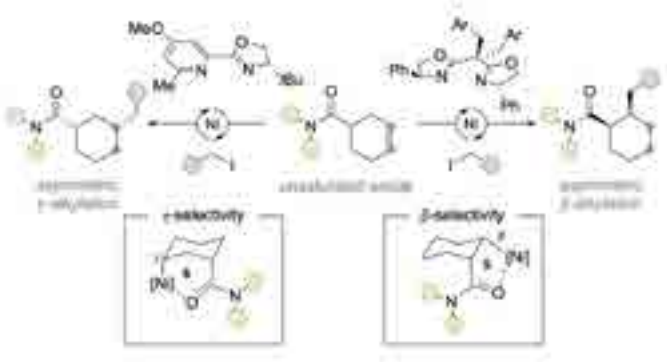
The use of catalysts to control the synthesis of architecturally complex and enantiopure molecules has become an essential tool in contemporary organic chemistry, chemical biology, medical chemistry and material science.[1] Undoubtedly, metal-catalyzed cross-coupling reactions that promote the functionalization of abundant sp^3 C–H bonds have offered innovative solutions for forging sp^3 architectures.[2] Among these, Ni-catalyzed chain-walking of simple olefins has recently gained considerable momentum as a powerful and practical alternative to conventional sp^3 C–H functionalization strategies. Nevertheless, the extention of this strategy to its enantioselective version remains relatively unexplored, with scarce examples being reported in literature. In this project, we aimed at unravelling the potential that nickel catalysis offers for enabling enantioselective interrupted chain-walking scenarios for forging new sp^3–sp^3 architectures (**Scheme 1**).

On the basis of the known expertise of the Martin group in Ni catalysis and chain-walking reactions and the observations regarding this transformation, we expect that the ligand backbone would exert a non-negligible influence on dictating whether β- or γ-selectivity is obtained by populating a mechanism consisting of either the intermediacy of five- or six-membered nickelacycles.[3] We hypothesize that the nature of the ligand backbone will be critical for dictating whether five- or six-membered nickelacycles are formed, thus favoring the formation of sp^3 architectures with either β- or γ-selectivity. We have recently conducted preliminary experiments that holds considerable promise for enabling the targeted transformation based on the utilization of either pyridine oxazoline or bis-oxazoline ligands.



Scheme 1. Ni-Catalyzed β- and γ-Alkylation of Unsaturated Amides via Interrupted Chain-Walking.

References:

1. T. Cernak, K. D. Dykstra, S. Tyagarajan, P. Vachal, S. W. Krska. *Chem. Soc. Rev.* **2016**, *45*, 546-576.
2. R. Jana, T. P. Pathak, M. S. Sigman. *Chem. Rev.* **2011**, *111*, 1417-1492.
3. J. Rodrigalvarez, H. Wang, R. Martin. *J. Am. Chem. Soc.* **2023**, *145*, 3869-3874

Lewis Acid-Catalyzed Functionalization of Indoles with Hydrazones

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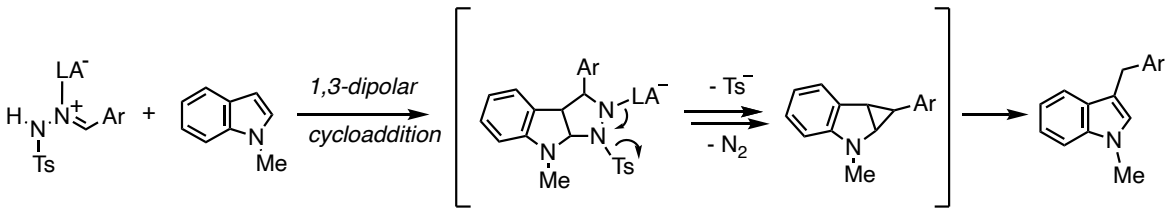
Indoles are among the most important heterocycles in nature and in pharmaceutical compounds. We have developed an efficient methodology for the functionalization of indoles by a formal 1,3-dipolar cycloaddition with N-substituted aryl tosyl hydrazones catalyzed by Lewis acids, leading finally to 3-benzyl indoles.

The reaction proceeds by formation of a pyrazoline intermediate that gives rise to a cyclopropane, as previously shown in our total synthesis of the lundurines [1], following early work by Padwa in intramolecular reactions of hydrazones with alkenes [2]. This is an alternative to the formation of cyclopropane-fused indoles by reactions with metal carbenes. Application of this chemistry to the difunctionalization of indoles at C2 and C3 will be also presented.



References:

1. Kirillova, M. S.; Muratore, M. E.; Dorel, R.; Echavarren, A. M. *J. Am. Chem. Soc.* **2016**, *138*, 3671–3674.
2. Padwa, A.; Ku, H. *J. Org. Chem.* **1980**, *45*, 3756–3766

Low Overpotential, High Impact: NiO Catalysts for Alkaline Media Electrolysis

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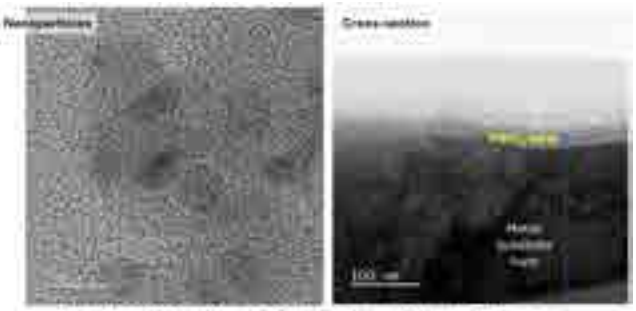
Keywords: Electrocatalysis, Doped NiO, HER, OER, Electrolysis, Green Hydrogen

Background and motivation. Efficient hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) catalysts are critical for the advancement of green hydrogen production technologies and achieving global sustainability goals. Alkaline and anion exchange membrane (AEM) water electrolyzers are promising for cost-effective hydrogen generation; however, the development of stable, scalable, and high-performance bifunctional electrocatalysts remains a challenge. Ni-based oxides have demonstrated significant potential for HER and OER in alkaline media due to their intrinsic activity and cost-effectiveness. To overcome limitations in activity and durability, this study focuses on the ultrafast flash combustion (FC) synthesis of doped NiO directly grown on Ni-foam (Figure 1). This method provides precise tunability of material properties, resulting in a highly robust and efficient electrocatalyst.[1–4]

Materials and methods. Modified NiO was synthesized via an ingeniously developed rapid FC method, optimizing the fuel/metal ratio to achieve precise stoichiometry and a porous, robust structure on Ni-foam. HER and OER activities were tested in 1 M Fe-free KOH using a three-electrode setup. Durability was evaluated in an NREL zero-gap flow cell anion exchange membrane electrolyzer under real-world conditions.

Results and discussion. The modified NiO catalyst exhibited ultra-low overpotentials of 70 mV at 25°C and 30 mV at 70°C for HER at 100 mA cm^{-2} in 1 M Fe-free KOH, and 70 mV at 10 mA cm^{-2} for OER (a record-breaking value known so far) in 1 M KOH at 25°C. In zero-gap flow cell electrolyzers, it demonstrated stable, resilient performance over extended operation (300 h+) making as obtained FC electrodes ideal for industrial applications. Characterizations (XRD, SEM, TEM, EDX, TGA, DSC, ICP-OES as well as operando Raman and operando XAS) revealed that optimized doping enhanced the electronic structure, facilitated active species formation, and supported a porous, well-adhered morphology for improved mass transport and activity. Or in other words, engineered electrode architecture performs better than material composition itself.



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References:

1. Bucci, A.; Lloret-Fillol, J.et al. *J. Mater. Chem. A* **2021**, *9* (21), 12700–12710.
2. Rao, R. R.; Lloret-Fillol, J.; Stephens, I. E. L.; Durrant, J. R. et al. *J. Am. Chem. Soc.* **2022**, *144* (17), 7622–7633.
3. Rao, R. R.; Bucci, A.; Gopakumar, A.; Stephens, I. E. L.; Lloret-Fillol, J.; Durrant, J. R. et al. *ACS Catal.* **2024**, *14* (15), 11389–11399.
4. Bucci, A.; Lloret-Fillol, J. US20230250538A1, August 10, **2023**. https://patents.google.com/patent/US20230250538A1/en.

Cu-catalyzed stereodivergent decarboxylative amination of bicyclic carbamates: Access to cyclobutane-1,3-diamine synthons

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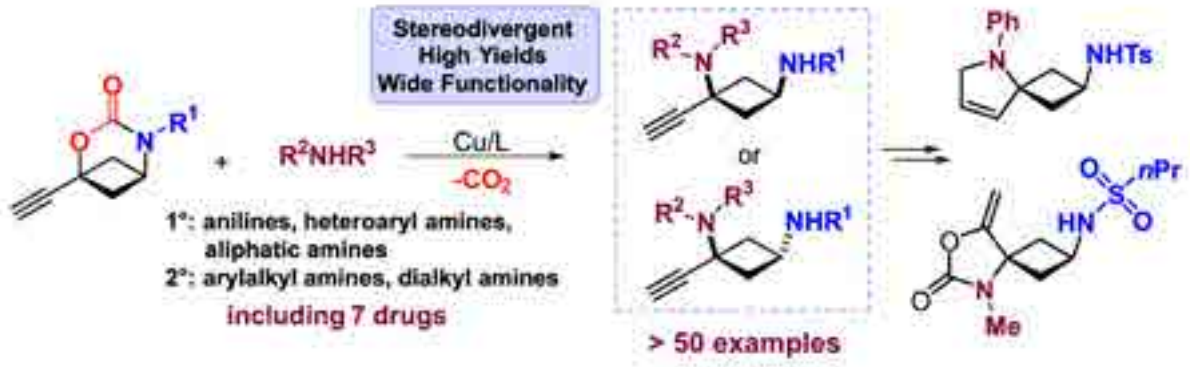
Cyclobutane fragments are considered significant to the design and synthesis of bioactive molecules, and in new drug discovery.[1] In recent years, a variety of functionalized cyclobutanes have been successfully obtained using bicyclobutane (bcb) as a starting point.[2] Due to limitations of the bcb structure and the requirement of a step-wise synthesis, streamlined access to a range of stereodefined cyclobutane-1,3-diamines has so far been elusive.[3] At present, the common synthetic methods towards aminated cyclobutanes require multiple steps using stoichiometric approaches while suffering from a lack of functional diversity and/or providing a single stereo-isomeric product. A catalytic procedure that provides access to diaminated scaffolds in a stereodivergent way using the same catalytic process remains unexplored. Here, we show that a Cu-mediated approach allows to convert 2-oxa-4-azabicyclo[3.1.1]heptan-3-one derivatives into trisubstituted cyclobutane-1,3-diamines in high yield and chemo-selectivity. Both cis and trans diastereomers could be selectively obtained by simple solvent control, and in typically high isolated yields of >80%.



References:

1. K. Majima, M. Yamano, J. Org. Chem. 2021, 86, 11464-11471.
2. A. Maity, K. Balanna, C. G. Daniliuc, A. Studer, Chem. Sci. 2025, 16, 7264-7269.
3. D Dmytro, S. Radchenko, S. O. Pavlenko, O. O. Grygorenko, D. M. Volochnyuk, S. V. Shishkina, O. V. Shishkin, I. V. Komarov, J. Org. Chem. 2010, 75, 5941–5952.

Rh(II)-Catalyzed Enantioselective Aryl C-H Bond Benzylation

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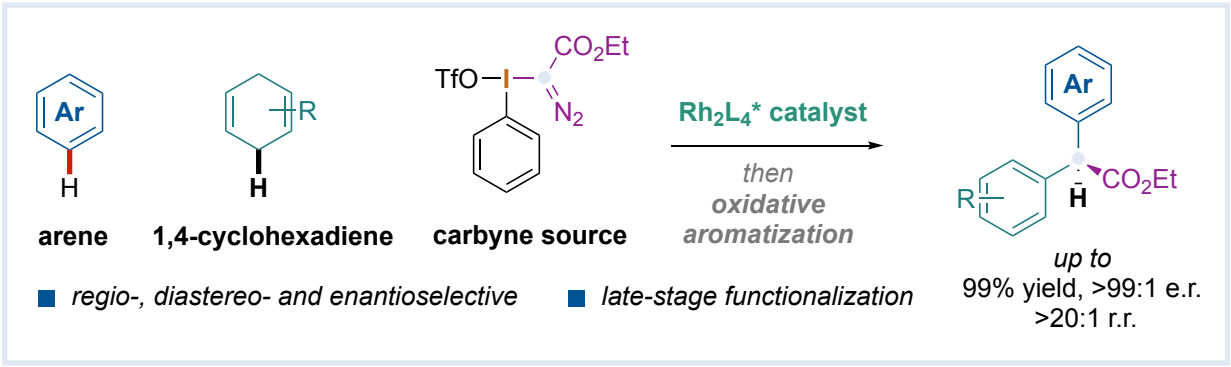
Chiral di(hetero)arylmethane motifs are prevalent in a wide range of bioactive compounds and pharmaceuticals.[1,2] Asymmetric benzylation of aryl C–H bonds represent a powerful strategy for accessing these structures.[3–5] However, non-directed asymmetric benzylation of aromatic C–H bonds – especially in complex settings – remains largely underexplored.

Herein, we present the first catalytic methodology for the regio-, and enantioselective late-stage functionalization of di(hetero)arylmethanes via double C–H functionalization, combining hypervalent iodine reagents, 1,4-cyclohexadienes, and paddlewheel dirhodium carboxylate catalysts (Scheme 1). Central to this work is the catalytic generation of a chiral donor/acceptor Rh(II)-carbene via para-selective electrophilic aromatic substitution with chiral Rh(II)-carbynoids.[6] This approach enables the construction of new chiral centers directly from aryl C-H bonds in aromatic feedstocks and drug molecules through a carbyne transfer platform, offering access to an unexplored chemical space that remains challenging to achieve with existing methods.



Scheme 1. Rh(II)-Catalyzed Enantioselective Aryl C-H Bond Benzylation.

References:

1. U. Gulati, R. Gandhi, J. K. Laha *Chem Asian J.,* **2020***, 15*, 3135-3161.
2. D. Ameen, T. J. Snape Med. *Chem. Commun.,* **2014***, 4*, 893-907.
3. B. Ma, J. Wu, L. Liu, J. Zhang *Chem. Commun.,* **2017***, 53*, 10164-10167.
4. W. Xu, R. Paira, N. Yoshikai *Org. Lett.,* **2015***, 17*, 4192-4195.
5. L. Ackermann, S. Barfüsser, C. Kornhaass, A. R. Kapdi *Org. Lett.,* **2011***, 13*, 3082-3085.
6. E. Palomo, A. Krech, Y. J. Hsueh, Z. Li, M. G. Suero *J. Am. Chem. Soc.,* **2025***, 147*, 13120-13125.

Boundary-guided motion of photoactive microswimmers at light-defined interfaces

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The successful design of steerable microswimmers capable of precise light-induced motion holds exciting potential for applications ranging from drug delivery and cargo transport to environmental remediation and the development of artificial life-like systems[1]. However, most photoactive microswimmers exhibit random trajectories and limited steering capabilities (Fig. 1A). Current strategies to overcome this limitation typically rely on multi-component architectures[2] or on the application of external fields[3], which often results in complex system configurations. As a result, achieving precise control over both direction and velocity remains a major challenge.

Here, we employ single-component photocatalytic microswimmers synthesized by a hydrothermal reaction. Their motion is driven by a photoinduced chemical reaction, enabled by efficient charge separation at a surface heterojunction between distinct crystallographic facets[4]. Using static and dynamic light patterns generated by a digital micromirror device (DMD), we demonstrate that structured illumination can create virtual boundaries that guide photocatalytic microswimmers without requiring physical confinement or auxiliary external fields (Fig. 1B). At light–dark interfaces, partial illumination induces asymmetric photocatalytic activity across the microswimmer surface, generating persistent reorientation that redirects propulsion along the boundary. We achieve programmable control over microswimmer trajectories, robust guidance across complex light geometries, adaptability to time-dependent patterns, and simultaneous, independent manipulation of multiple microswimmers.

Moreover, boundary-guided motion enables programmable cargo transport through light-controlled capture and release (Fig. 1C). Overall, this work establishes an all-optical strategy for activating, directing, and dynamically reconfiguring microswimmer motion, representing a significant step toward adaptive and autonomous microsystems capable of rapidly responding to evolving environments.

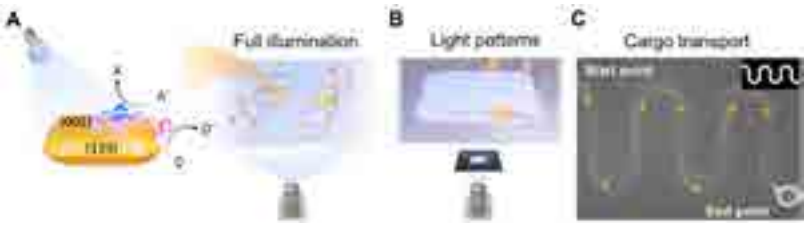

Figure 1: (A) Schematic illustration of facet-dependent photocatalytic reactions on $BiVO_4$, showing spatial separation of oxidation and reduction sites, moving under uniform illumination conditions, resulting in curved trajectories. **(B)** Illustration of a microswimmer moving under structured illumination, showing guided motion along light-defined boundaries. **(C)** Cargo transport along a serpentine light-defined pathway.

References:

1. Chen, D. E. Fan, P. Fischer, A. Ghosh, K. Göpfrich, R. Golestanian, H. Hess, X. Ma, B. J. Nelson, T. Patiño Padial, J. Tang, K. Villa, W. Wang, L. Zhang, A. Sen, S. Sánchez, *Nat. Nanotechnol.* **2025***, 20*, 990–1000.
2. K. Villa, *Chem. Commun.* **2023***, 59*, 8375–8383.
3. Y. Chen, J. M. Gonçalves, R. Ferrer Campos, K. Villa, *Small* **2025**, 21, 2410901.
4. S. Heckel, C. Bilsing, M. Wittmann, T. Gemming, L. Büttner, J. Czarske, J. Simmchen, *Adv. Sci.* **2022**, 9, 2105009.

Carbanion-Ligated Ruthenium Monomeric and Oligomeric Catalysts for Efficient & Selective Organic Electrocatalytic oxidation

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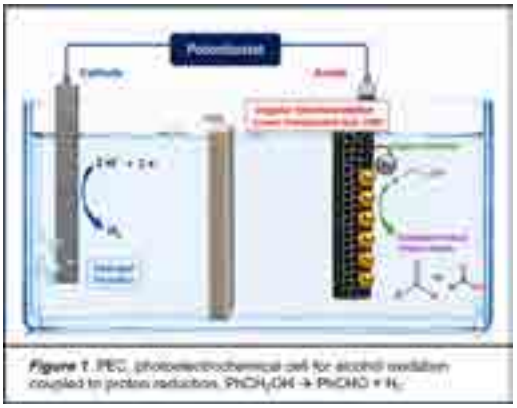
The oxygen evolution reaction (OER) is widely employed as the anodic half-reaction in electrolyzers and artificial photosynthetic systems. However, its sluggish kinetics and large overpotential requirements significantly compromise the overall energy efficiency of these processes. Replacing OER with the electrooxidation of organic substrates constitutes an attractive alternative, as these transformations typically require lower overpotentials while simultaneously generating value-added chemicals. However, efficient and selective organic electrooxidation under mild conditions remains challenging, particularly at neutral pH where proton-coupled electron transfer (PCET) processes are kinetically demanding.



Herein, we present a family of monomeric and oligomeric ruthenium complexes featuring carbanion-based auxiliary ligands and a catalytically active [Ru–O] unit. The electronic properties of these complexes are tailored to promote the selective oxidation of organic substrates under mild conditions. Furthermore, the molecular catalysts can be immobilized onto graphitic materials through supramolecular (CH–π and π–π) interactions, enabling the preparation of hybrid electrodes that operate efficiently in heterogeneous media.

This molecular and hybrid catalyst platform provides a versatile strategy for selective organic electrocatalytic oxidations under mild conditions and highlights the potential of carbanion-supported ruthenium complexes for sustainable electrochemical transformations.

References:

1. Badalyan, A.; Stahl, S. S. Cooperative Electrocatalytic Alcohol Oxidation with Electron-Proton-Transfer Mediators. *Nature,* **2016***, 535*, 406–410.
2. Hoque, M. A.; Llobet, A. et al., Water Oxidation Electrocatalysis Using Ruthenium Coordination Oligomers Adsorbed on Multiwalled Carbon Nanotubes. *Nat. Chem.,* **2020***, 12*, 1060–1066.
3. Gil-Sepulcre, Llobet, A. et al., Surface-Promoted Evolution of Ru-bda Coordination Oligomers Boosts the Efficiency of Water Oxidation Molecular Anodes. *J. Am. Chem. Soc.,* **2021***, 143,* 11651–11661.
4. Ranu, K.; Llobet, A. et al., Supramolecular Rebound Healing Mechanism Enhances the Performance of Graphitic Hybrid Monomeric and Oligomeric Molecular Anodes. *ACS Catal.,* **2026***, 16*, 464–477.

Bis(iminophosphorane)phosphine NPN CoII Complex for Hydrosilylation reactions

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Catalysis plays a central role in modern synthetic chemistry by enabling efficient and selective transformations under mild conditions. Among these, hydrosilylation has emerged as a powerful and versatile strategy for the reduction of unsaturated bonds, providing straightforward access to valuable organosilicon intermediates.[1] This methodology benefits from the use of readily available, easy-to-handle silane reagents and generates products that can be further functionalized.

This reaction, which is used at the industrial level, mainly rely on platinum catalysts.[2] However, the development of catalysts based on earth-abundant metals as sustainable alternatives has gained a significant attention.[3] Achieving performances comparable to noble metal systems generally requires careful ligand design.

For such reductive transformations, electron rich ligands can be very favourable. Given our interest for iminophosphoranes (P=N) which are ylide type electron rich N based ligands, we studied the potential of mixed ligands associating iminophosphoranes with other coordinating moiety (pyridine, phosphine…)[4,5] having complementary electronic properties to develop hydrosilylation catalysts.

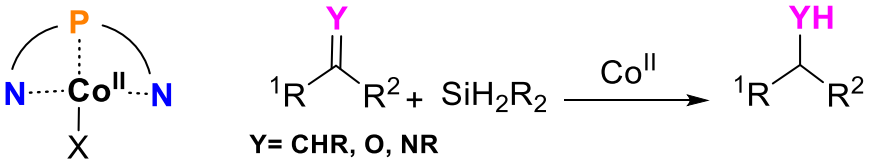

Figure 1. Co-catalyzed hydrosilylation reactions

In this work, we present the synthesis of an unprecedented bis(iminophosphorane) phosphine (NPN) ligand, as well as the synthesis and characterization of its Co^{II} complexes and discuss their catalytic activity in the hydrosilylation of various functional groups including olefins[6] and polar bonds. (Figure.1)

References:

1. D. Troegel, J. Stohrer, *Coord. Chem. Rev.* **2011**, 255, 1440–1459.
2. J. L. Speier, J. A. Webster, G. H. Barnes, *J. Am. Chem. Soc.* **1957**, 79, 974–979.
3. L. D. de Almeida, H. Wang, K. Junge, X. Cui, M. Beller, *Angew. Chem. Int. Ed.* **2021**, 60, 550–565.
4. S. E. García-Garrido, A. Presa Soto, J. García-Álvarez, *Adv. Organomet. Chem.* **2022**, 77, 105–168.
5. I. Popovici, C. Barthes, T. Tannoux, C. Duhayon, N. Casaretto, A. Monari, A. Auffrant, Y. Canac, *Inorg. Chem*. **2023**, 62, 2376–2388.
6. I. Popovici, Y. Chen, S. Bourcier, N. Casaretto, A. Auffrant, *Dalton Trans*. **2025**, 54, 15705.

Ni-Catalyzed Suzuki-Miyaura Coupling of (Hetero)Aryl Halides with Polyfluorinated Boronic Esters

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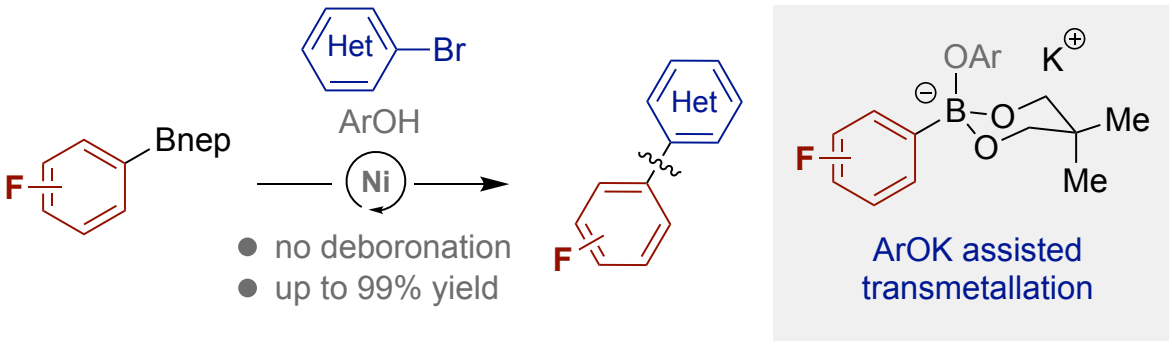
Electron-deficient polyfluorinated boron reagents have found little echo in Ni-catalyzed Suzuki-Miyaura reactions1 due to their proclivity for competing deboronation under basic conditions2 and their inherent difficulty to enable transmetallation events3. Herein, we describe a Ni-catalyzed blueprint that enables the coupling of a broad range of electron-deficient polyfluorinated boronic esters and (hetero)aryl halides, including challenging substrate combinations. The strategy does not take recourse to specialized ligands, but rather the utilization activated phenols as additives, offering not only a particularly facile transmetal-lation via the intermediacy of tetracoordinated boronates, but also suppressing parasitic deboronation events.



References:

1. Hu, Q.-H. Adv. *Synth. Catal.* **2016**, *358*, 2072–2076.
2. Lloyd-Jones, G.C. *J. Am. Chem. Soc.* **2021**, *143*, 14814–14826.
3. Denmark, S.E. *J. Am. Chem. Soc.* **2018**, *140*, 4401–4416.

Dual Co/Photoredox-Catalyzed Regio- and Stereoselective Synthesis of Highly Functional 1,3-Dienes

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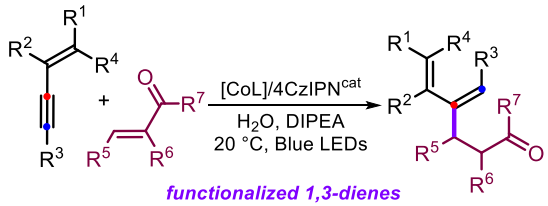
Keywords: *1,3-dienes, dual Co/photoredox catalysis, C-C coupling, α,β-unsaturated carbonyls.*

The synthesis of highly functionalized 1,3-dienes has long been an important target in organic chemistry due to their versatility in applications and presence in numerous complex bioactive compounds.[1] The nature of these structures is dictated by the degree of substitution and their functionalization, but the presence of various substituents increases the synthetic challenge. It has been therefore a challenge to develop synthetic methodologies and facilitate the rapid assembly of complex 1,3-diene synthons.[2]

Here, we present a dual Co/photoredox catalytic coupling of 1,3-enynes and α,ß-unsaturated aldehydes and ketones providing access to highly functional 1,3-diene synthons through a regio- and stereoselective carboncarbon coupling process. The scope of the process features diverse functionalized scaffolds with a high degree of molecular complexity. The synthetic utility of these 1,3-dienes is demonstrated including a one-pot approach using an alkynyl cyclic carbonate as a 1,3-enyne precursor offering direct access to the 1,3-diene product. Mechanistic analysis involving control reactions, deuterium labeling studies and DFT calculations are in line with the in-situ formation of a Co^{III}-H species and an outer-sphere coupling scenario, in which a regio- and stereoselective conversion occurs between a dienyl radical and an unsaturated carbonyl species.[3]



functionalized 1,3-dienes
33 examples, yield up to 94%
high stereo- and regio-control
outer-sphere radical attack

References:

1. a) M. de Paolis et al., Stereoselective Alkene Synthesis, Springer, Berlin Heidelberg 2012, pp. 87–146. b) C. Jiang et al., Chem. Commun. 2021, 57, 5710–5713. c) P. Hubert et al., Adv. Synth. Catal. 2020, 362, 5532–5575. d) S. Chen et al., Nat. Commun. 2024, 15, 5479.
2. W. Ai, R. Zhong, X. Liu, Q. Liu, Chem. Rev. 2018, 119, 2876–2953.
3. B. L. Tóth, A. Delgado, D. Ghorai, D. Meneses, A. García-Camacho, M. Vicent-Morales, J. Benet-Buchholz, I. Funes-Ardoiz, A. W. Kleij, Angew. Chem. Int. Ed. 2026, 65, e22561. DOI: 10.1002/anie.202522561.

Gold(I)-catalyzed Cyclization of Functionalized Alkenynes: Access to Chromene Derivates

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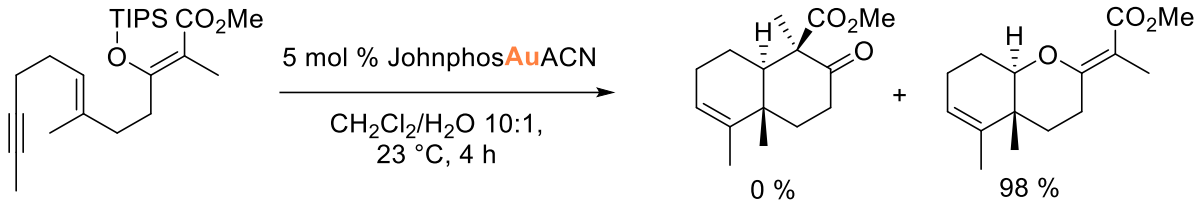
Gold-catalyzed alkyne-alkene reactions constitute a powerful strategy for the construction of complex molecules under mild conditions.[1,2] In the present work, we explored the intramolecular cyclization of a functionalized alkenyne precursor originally designed for the synthesis of fused decalin derivatives. Notably, instead of the anticipated bicyclic decalin system, the reaction selectively afforded a chromene scaffold through a competitive cyclization pathway promoted by the gold(I) catalyst (Scheme 1).



Scheme 1. Reaction scheme.

The reaction proceeds with the intramolecular cyclization (6-endo-dig) of the 1,5-enyne catalyzed for gold(I) catalyst followed by intramolecular nucleophilic attack of the oxygen atom and subsequent protodeauration to furnish the chromene scaffold in good yield. Ongoing computational and experimental studies are aimed at understanding the factors governing the observed chemoselectivity.

The methodology provides straightforward access to chromene scaffolds, a privileged structural motif frequently encountered in natural products and biologically active compounds.

References:

1. Dorel, R.; Echavarren, A. M., *Chem. Rev.* **2015**, *115*, 9028–9072.
2. Rong, Z.; Echavarren, A. M. *Org. Biomol. Chem.* **2017**, *15*, 2163–2167.

Gold(I)-catalyzed Enantioselective Biscyclopropanation of 1,6-Enynes

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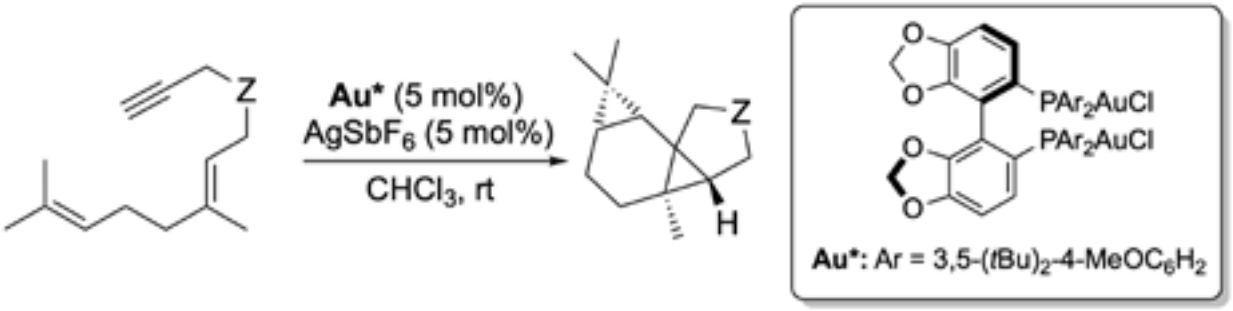
The enantioselective gold(I)-catalyzed bicyclopropanation of 1,6-dienynes[1-3] was achieved using the chiral dinuclear gold catalyst (R)-DTBM-SEGPHOS$(AuCl)_2$, efficiently building enantioenriched fused tetracyclic frameworks. The desired compounds were obtained in moderate yields with good enantioselectivities. DFT calculations support the experimentally observed enantioselectivity.



References:

1. Nieto-Oberhuber, C.; Muñoz, M. P.; Buñuel, E.; Nevado, C.; Cárdenas, D. J.; Echavarren, A. M. *Angew. Chem. Int. Ed.* **2004**, *43*, 2402–2406.
2. Sethofer, S. G.; Mayer, T.; Toste, F. D. *J. Am. Chem. Soc.* **2010**, *132*, 8276–8277.
3. Rong, Z.; Echavarren, A. M. *Org. Biomol. Chem.* **2017**, *15*, 2163–2167.

Ni-Catalyzed Decarbonylative Hydroxylation with N_2O

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Nitrous oxide (N_2O) is a potent greenhouse gas and ozone-depleting substance with an atmospheric lifetime of ≈120 years.[1] Its use as oxygen transfer is particularly appealing, as it generates N_2 as bydeproduct. While early work by Hillhouse[2] demonstrated the viability for promoting O–insertion into Ni-(II)-alkyl complexes, recent studies have extended N_2O-mediated oxygenation to aryl halides[3] and sp^2 C–H bonds via 1,4-Ni shift events.[4] Herein, we disclose the first example of a N_2O-mediated oxygenation event by means of C–C bond cleavage and Ni catalysts.

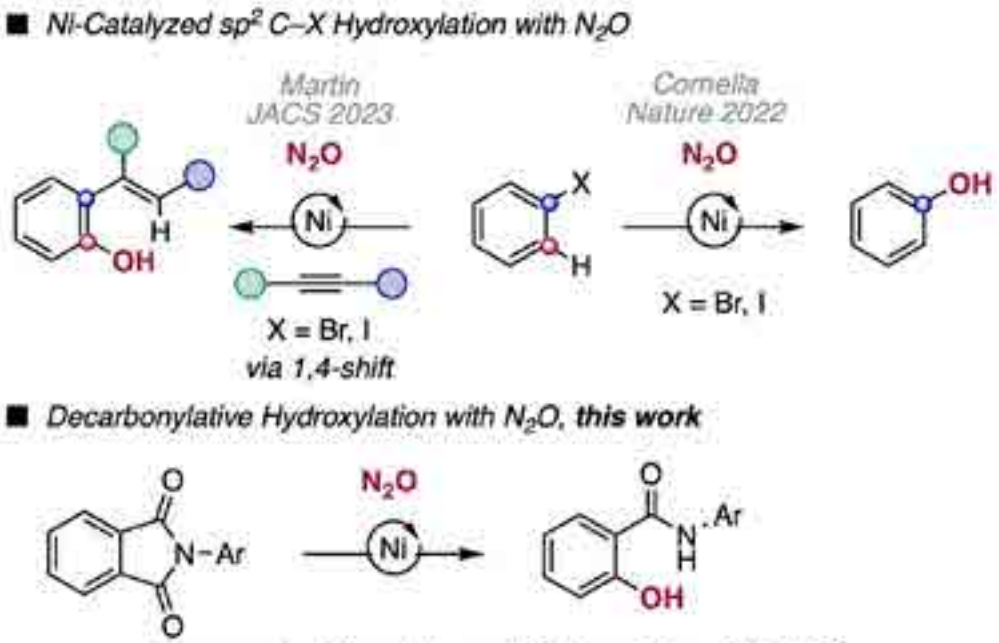

Figure 1. Ni-catalyzed O-transfer with N_2O

References:

1. H. Tian, et al. *Nature* **2020**, *586*, 248–256.
2. P.T. Matsunaga, G. L. Hillhouse, A. L. Rheingold J. *Am. Chem. Soc.* **1993**, *115*, 2075–2077.
3. F. LeVaillant, A. Mateos Calbet, S. González-Pelayo, E. J. Reijerse, S. Ni, J. Busch, J. Cornella. *Nature* **2022**, *604*, 677–683.
4. H. Zhang, J. Rodrigalvarez, R. Martin. *J. Am. Chem. Soc.* **2023**, *145*, 17564–17569.

Theoretical Study of CO_2 Hydrogenation to Methanol on In_2O_3/ZrO_2

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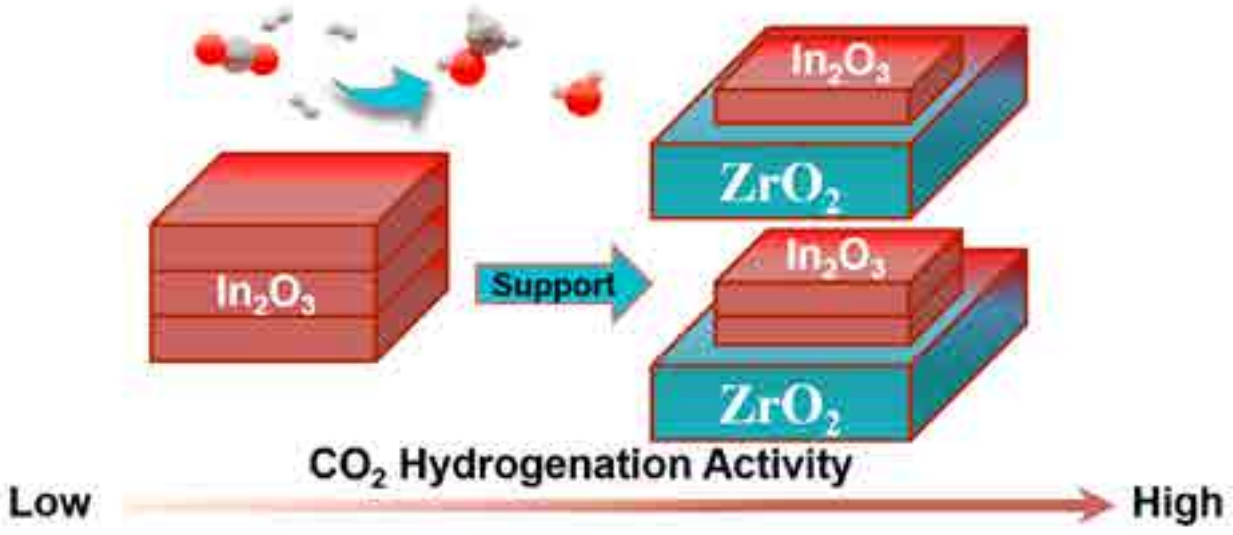
CO_2 hydrogenation to methanol reaction ($CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O$) presents significant application potential in carbon capture and utilization, as it can both reduce the consumption of fossil fuel resources and promote carbon emission reduction and carbon neutrality. Indium oxide-based catalysts have been widely used in the hydrogenation of CO_2 to methanol, In_2O_3 is prone to over-reduction and subsequent deactivation under reaction conditions.[1,2] Recent studies have demonstrated that supporting In_2O_3 on ZrO_2 can yield highly active InOx nanolayers for methanol synthesis.[3,4] Nevertheless, the underlying mechanism of how ZrO_2 influences In_2O_3 remains elusive. To explore the specific impact of the ZrO_2 support, we contruct heterojunction models featuring In_2O_3 nanolayers supported on different crystalline phases of ZrO_2 (c-ZrO_2, m-ZrO_2 and t-ZrO_2). Density functional theory (DFT) simulations are systematically performed to investigate the surface structures and the complete CO2 hydrogenation mechanisms over the In_2O_3/ ZrO_2 catalyst. By comparing the differences in surface structures and reaction pathways between pristine In_2O_3 and In_2O_3/ ZrO_2 heterojunctions, we aim to construct mutiple descriptors to elucidate the intrinsic role of the ZrO_2 support. This work will provide critical insights that are highly significant for guiding the rational design of high-performance catalysts for CO_2 hydrogenation.



References:

1. A. Tsoukalou, P. M. Abdala, D. Stoian, *J. Am. Chem. Soc.* **2019**, *141,* 13497-13505.
2. A. Cao, Z. Wang, H. Li and J. K. Nørskov, *ACS Catal.,* **2021**, *11*, 1780-1786.
3. H. Eliasson, Y.-T. Chiang, T. P. Araújo, *Adv. Mater.,* **2025**, *37*, 2419859.
4. L. Xu, Q. Wang, Q. Gu, S., *Angew. Chem. Int. Ed.,* **2025**, *64*, e202508091.

Influence of precursor chemistry and carbonization temperature on the structure and catalytic performance of N,S-functionalized ZIF-8-derived carbons

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Metal organic frameworks (MOFs) have emerged as attractive precursors for the preparation of functionalized carbon materials owing to their high porosity, tunable composition, and ability to partially transfer structural features to the resulting carbon framework (1, 2). These characteristics enable the generation of heteroatom-doped carbons with a unique combination of textural properties, chemical composition, and surface functionality (3, 4). In this work, carbon materials were synthesized from pristine ZIF-8 and from ZIF-8 partially modified through ligand exchange with a nitrogen and sulfur rich molecule, followed by carbonization at 750 and 900 °C. This strategy enabled the controlled incorporation of heteroatoms into the precursor and allowed investigation of how their evolution during pyrolysis influences the structure and catalytic performance of the resulting carbons.

The precursors and carbon materials were characterized by X-ray diffraction (XRD), N_2 and CO_2 adsorption, Raman spectroscopy, FTIR, SEM, TGA-MS, and XPS. Precursor modification progressively alters the structure and porosity of ZIF-8, whereas the carbonization temperature controls both the evolution of the carbon framework and the final heteroatom speciation. Consequently, materials carbonized at 900 °C display a more developed sp^2 network, enhanced electronic connectivity, and a more favorable integration of heteroatoms within the carbon matrix.

Catalytic performance was evaluated in the transfer hydrogenation of p-chloronitrobenzene using hydrazine as hydrogen donor. Carbons obtained at 900 °C exhibited significantly higher activity than their counterparts carbonized at 750 °C. In particular, C3.1-0.2-900, derived from a precursor with a ligand exchange degree of 27.6%, achieved complete conversion within 90 min and displayed the highest initial reaction rate while maintaining 100% selectivity toward p-chloroaniline. In contrast, materials carbonized at 750 °C showed conversions below 54%, substantially slower kinetics, and, in some cases, the formation of secondary products associated with hydrodehalogenation and N-N coupling pathways.

The catalytic behavior is therefore dictated not only by porosity or overall elemental composition, but mainly by the structural organization of the carbon matrix and the chemical environment of the incorporated heteroatoms, both of which are governed by precursor chemistry and carbonization temperature. This work establishes a direct structure-activity relationship in MOF-derived carbons and highlights the potential of controlled precursor modification as a strategy for the development of efficient metal-free catalysts for transfer hydrogenation reactions.

References:

1. Figueroa-Quintero L, Villalgordo-Hernández D, Delgado-Marín JJ, Narciso J, Velisoju VK, Castaño P, et al. *Small Methods.* **2023**,7.
2. Dai Y, Jiang C, Xu M, Bian B, Lu D, Yang Y. *Applied Catalysis A: General*. **2019**, 580, 158–66.
3. Yao J, Wang L, Xie D, Jiang L, Li J, Fang X. *Frontiers in Chemistry*. **2022**, 101000680
4. Villalgordo-Hernández D, Grau-Atienza A, García-Marín AA, Ramos-Fernández EV, Narciso *J. Materials*. **2022**,15.

Photoinduced Nickel-Catalysed Enantioconvergent sp^3–sp^3 Coupling of Unactivated Olefins and Aziridines

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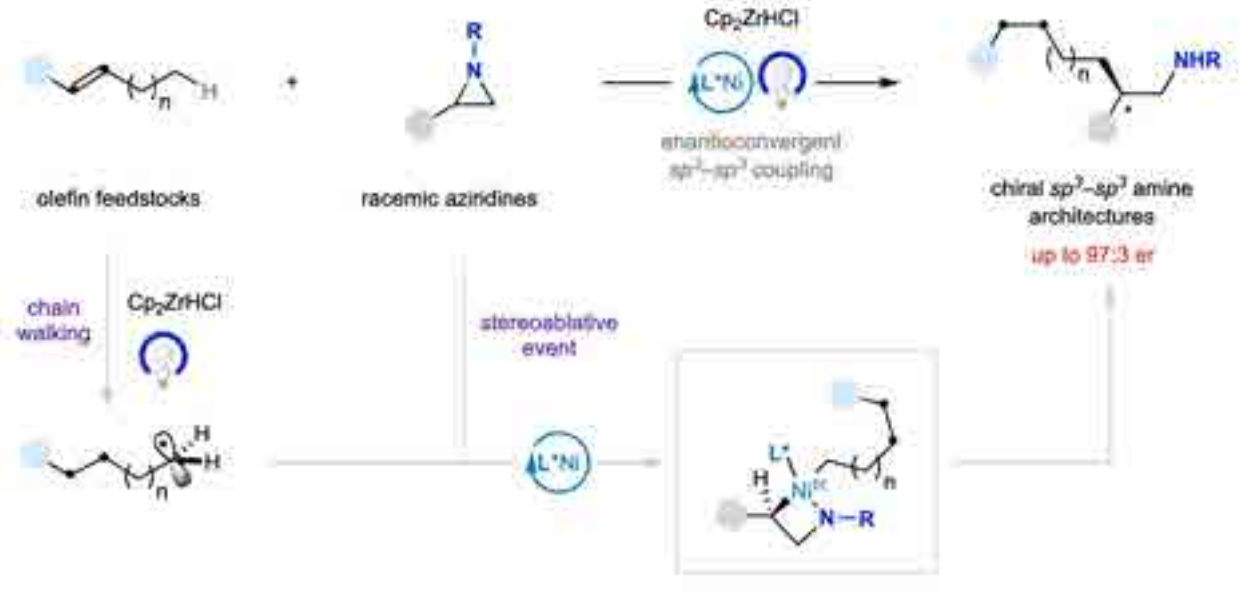
Catalytic sp^3–sp^3 bond-forming reactions have found considerable echo in both academic and pharmaceutical laboratories. This is largely due to the observation that a higher content in sp3 hybridized carbons has recently shown to improve several molecular attributes that contribute to clinical success. Although the ready availability of unactivated olefins and aziridines makes them ideal precursors to forge enantioenriched sp^3–sp^3 architectures with added-value amine functions, an enantioconvergent catalytic scenario of these counterparts has not yet been realized in the cross-coupling arena. Herein, we describe a mild and broadly applicable photoinduced blueprint that uncovers the potential of unactivated terminal and even internal olefins as latent carbogenic sp^3 nucleophiles. This strategy enables the enantioselective construction of amine-containing sp^3–sp^3 architectures with racemic aziridines, facilitated by a nickel catalyst in combination with a chiral biimidazole ligand, even in the context of late-stage diversification of advanced synthetic intermediates.



References:

1. L. Zhang, H. Wang, T.G. Santiago, W.-J. Yue, R. Martin, *Nat. Catal.* **2025**, *8*, 348–356.
2. L. Zhang, H. Liu, T.G. Santiago, R. Martin, *J. Am. Chem. Soc.* **2025**, *147*, 44048–44054.

Dual Catalytic Enantioconvergent Carbamoylation of Aziridines

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In recent years, Ni-catalyzed enantioconvergent reactions of racemic alkyl electrophiles have gained significant momentum in synthetic organic chemistry. Among them, the enantioconvergent transformations of racemic aziridines have garnered particular attention due to their potential to provide direct access to enantioenriched β-functionalized aliphatic amine architectures[1]. Herein, we disclose an enantioconvergent carbamoylation of racemic aziridines enabled by a dual catalytic strategy[2]. This method provides a new approach for the synthesis of highly enantioenriched β-amino amides from simple precursors, under mild conditions, with broad applicability including late-stage diversification of advanced intermediates and excellent enantioselectivity. Preliminary studies with well-defined nickel complexes support a mechanism proceeding via carbamoyl organometallic intermediates.

References:

1. Zhang, L.; Wang, H.; Santiago, Tomás G.; Yue, W.-J.; Martin, R. *Nat. Cat.* **2025**, *8*, 348-356.
2. Zhang, L.; Liu, H.; Santiago, T. G.; Martin, R. *J. Am. Chem. Soc.* **2025**, *147*, 44048–44054.
3. Li, L.; Hu, Z.; Ren, S.; Arndtsen, B. A.; Chu, L. *J. Am. Chem. Soc.* **2025**, *147*, 28206–28214.
4. CuestaGalisteo, S.; Schörgenhumer, J.; Hervieu, C.; Nevado, C. *Angew. Chem., Int. Ed.* **2024**, *63*, No. e202313717.

Regio- and Stereoselective Dual Co/photocatalyzed Synthesis of Diene Diols

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The merger of transition metal catalysis and photoredox catalysis has been on the rise in the development of synthetic methodologies.[1] More recently, the progress has been extended to first-row (transition) metals, of which cobalt represents an intriguing case[2,3,4]. A dual catalytic strategy involving photochemistry does not only alleviate the need for a stoichiometric (heterogeneous) reductant such as Zn, but it can also deliver alternative, unknown coupling scenarios. Herein, we discuss the synthesis of branched 1,5 dienes bearing a quaternary center and two alcohol end-groups (cf., formation of diene-diols). We further discuss our advances in terms of ligand-controlled, regio-divergent decarboxylative homocoupling of vinyl cyclic carbonates (VCCs).[5]

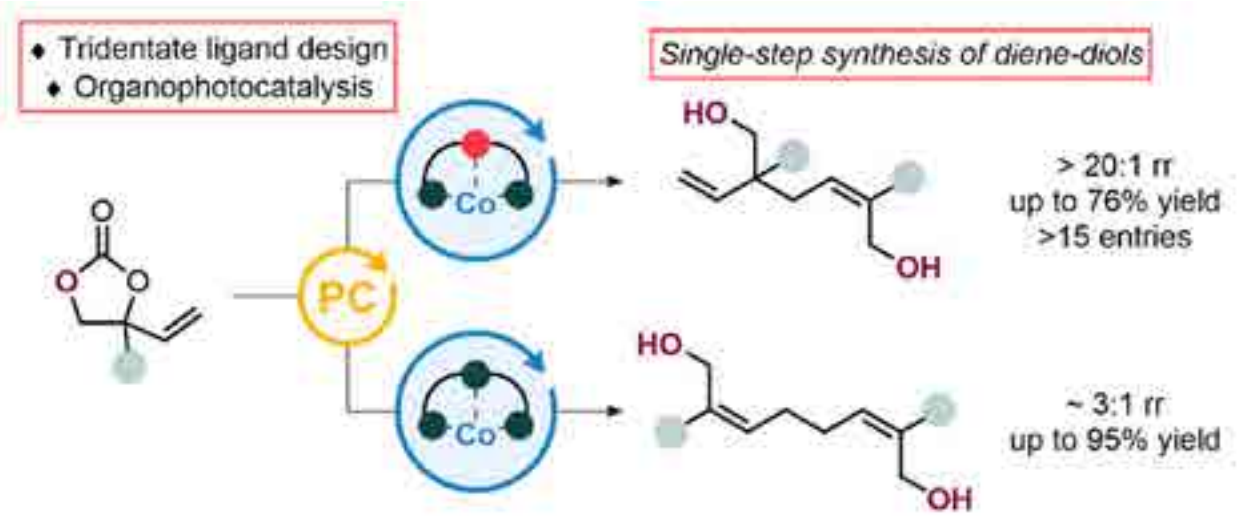

Figure 1. Co-mediated regio- and stereo-controlled decarboxylative synthesis of diene-diols.

References:

1. J. Twilton, C. Le, P. Zhang, M. H. Shaw, R. W. Evans, D. W. C. MacMillan, Nat. Chem. Rev. 2017, 1, 52.
2. B. Toth, S. G. E. Amos, A. W. Kleij, Org, Chem Front. 2025, 12, 1326–1339.
3. B. Limburg, À. Cristòfol, A. W. Kleij, J. Am. Chem. Soc. 2022, 144, 10912-10920.
4. À. Cristòfol, B. Limburg, A. W. Kleij, Angew. Chem. Int. Ed. 2021, 60, 15266-15270.
5. S. G. E. Amos, F. Gao, G. Armellin, A. W. Kleij, 2026, manuscript in preparation.

Chemoselective Hydrogenolysis of Formamides in the Presence of Esters by an Iridium Catalyst

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Chemoselective transformation of amides in the presence of esters remains one of the most challenging problems in synthetic chemistry because esters are generally more electrophilic and therefore more readily reduced than amides.1 As a result, selective reduction of amides without affecting ester functional groups is difficult to achieve. While several catalytic systems for amide hydrogenolysis using molecular hydrogen have been reported, achieving chemoselective amide hydrogenolysis in the presence of esters remains challenging.

In this study, we found that the combined use of an Ir complex bearing a phosphine–pyrrole bidentate ligand and LiOtBu as an additive enables chemoselective hydrogenolysis of formamides into amines and methanol over esters (Figure 1).2 Competitive experiments revealed that formamides were preferentially hydrogenated in the presence of esters, even though esters themselves were hydrogenated under the reaction conditions. This unusual chemoselectivity represents a reversal of the conventional reactivity order of carbonyl compounds. The catalytic system was applicable to formamides bearing various functional groups. Cyano, chloro, and silyl ether groups were well tolerated under the reaction conditions, and the corresponding amines were obtained without affecting these functional groups. Furthermore, substrates possessing both ester and formamide functional groups underwent selective cleavage of the formamide C–N bond, leaving the ester group intact.

A catalytic cycle is proposed involving metal–ligand–alkaline metal cooperation. Mechanistic studies were conducted to gain insight into the origin of the observed chemoselectivity. Hammett analysis of formanilide hydrogenolysis gave a positive ρ value, indicating that electron-withdrawing substituents accelerate the reaction. This result supports hydride transfer from the Ir center to the carbonyl carbon as the rate-determining step in a proposed cycle. Density functional theory calculations indicated that coordination of a formanilide to Li+ is thermodynamically more favorable than that of an ester. The calculated preference for formanilide coordination is consistent with the experimentally observed chemoselectivity and suggests that preferential recognition of formamides by Li+ contributes to the selective hydrogenolysis of formamides over esters.

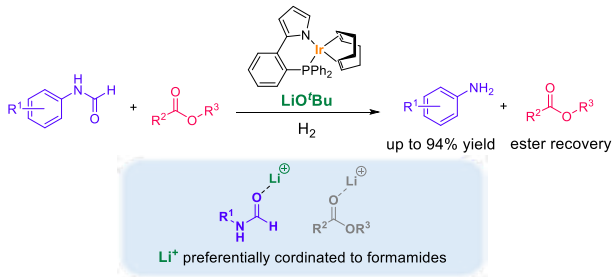

Figure 1. Chemoselective hydrogenolysis of formamides over esters

References:

1. T. Iwasaki, K. Nozaki, *Nat. Rev. Chem.* **2024**, *8,* 518–534.
2. S. Ajiro, T. Iwasaki, K. Nozaki, *ACS Catal. in press*. DOI: 10.1021/acscatal.6c01709

Investigating the Influence of the Symmetry of Self-Assembled Molecules on the Performance of Perovskite Solar Cell Devices

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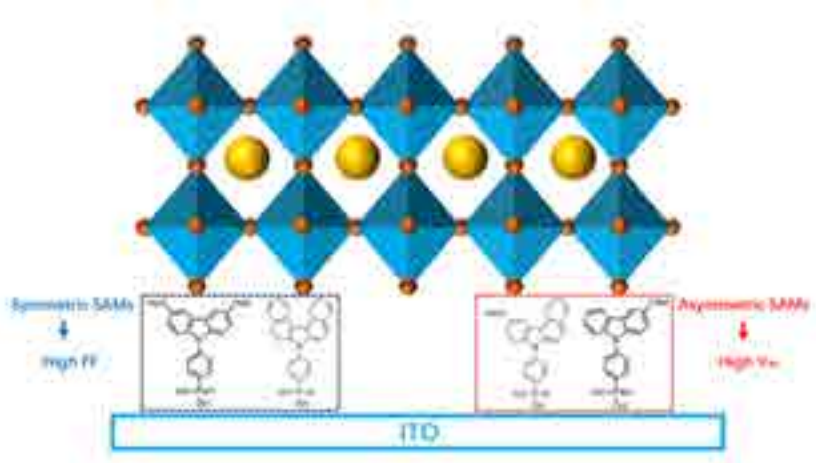
Since the concept of perovskite solar cells was first introduced in 2009, the device performance has improved dramatically.[1] In recent years, self-assembled monolayers (SAMs) have been introduced as hole selective contacts in perovskite solar cells, representing an important milestone in the development of this field.[2-3] To date, the certified power conversion efficiency (PCE) of single-junction perovskite solar cells has approached 28%, surpassing that of single-junction silicon solar cells for the first time.

However, systematic investigations on the influence of SAM molecular symmetry on device performance remain relatively limited. In this work, four SAM molecules with different structural symmetries (including symmetric and asymmetric configurations) were designed and synthesized. These molecules were employed as hole selective contacts in p–i–n structured perovskite solar cells for a systematic study.

Our results reveal that symmetric SAM molecules tend to form more ordered and compact assemblies on the ITO surface, which effectively reduces interfacial charge transport resistance and significantly improves the fill factor (FF). In contrast, asymmetric SAM molecules exhibit better energy level alignment with the perovskite layer and more effectively guide the conversion of PbI_2 into perovskite, thereby leading to a notable enhancement in the open-circuit voltage (V_{oc}).

These findings highlight the critical role of molecular symmetry in SAM-based interfaces and provide valuable insights for the rational design of next-generation SAM molecules for high-performance perovskite solar cells.



Schematic illustration of the mechanisms of symmetric and asymmetric SAMs.

References:

1. Lixiu Zhang et al., *Adv. Mater.* **2025**, e12221.
2. E. Yalcin et al., *Energy Environ. Sci.* **2019**, *12*, 230—237.
3. Ke Guo et al., *ACS Energy Lett.* **2025**, *10*, 4882–4910.

Deciphering Interfacial PCET Mechanisms Using Open-Circuit Potential Decay

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Electrochemical catalysis has emerged as a compelling route for energy production and the synthesis of value-added chemicals. Heterogeneous catalysts are promising candidates in this field, providing stable, active, and selective platforms for various reactions. However, elucidating the reaction mechanism of this type of catalyst is challenging due to surface heterogeneity, multiple (electro)chemical steps, and different reaction intermediates. Several approaches are available to decipher the reaction mechanism. Spectroelectrochemical techniques enable the identification of reaction intermediates, while electrochemical methods, such as Tafel plot or Foot-on-the-Wave analysis, are used to study reaction kinetics.

Recently, Open-Circuit Potential (OCP) measurements have proven to be a versatile tool for unravelling key aspects of electrochemical transformations. Mayer et. al. utilized OCP measurements to determine Proton-Coupled Electron Transfer (PCET) potentials and Bond Dissociation Free Energies (BDFE),[1] while Surendranath and co-workers quantified the interfacial hydricity.[2] Furthermore, the time-resolved OCP measurements can provide additional insights, such as the pH swing in the Hydrogen Evolution Reaction (HER).[3]

In this work, we present a methodology for determining interfacial PCET rate constants via OCP decay analysis. By establishing a robust quantification protocol and representative kinetic models, we explore the interfacial reaction mechanism of alcohol oxidation on doped spinel cobalt oxides deposited on a carbon Toray substrate. The integration of kinetic modelling, Kinetic Isotope Effects (KIE), and pH-dependency experiments provides detailed insights into the underlying reaction mechanism. This work demonstrates that OCP decay analysis serves as a powerful complement to traditional electrochemical techniques to elucidate complex interfacial mechanisms.

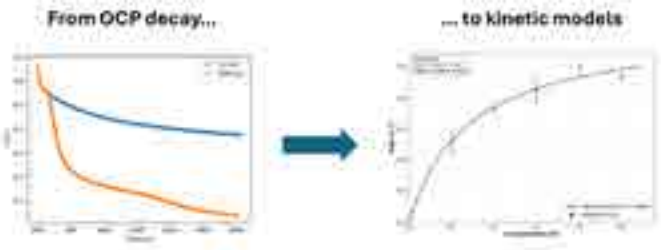

Figure 1. Illustrative representation of the proposed methodology.

References:

1. Wise, C.F., Agarwal, R. G., Mayer, J.M., *JACS* **2020** *142*(24), 10681-10691.
2. Chung, H. W., Wang, H., Desai, S. P., Müller, A. V., Sena, S., Glusac, K. D., Concepcion, J.J., Surendranath, Y., *JACS* **2025**, *147*(40), 36291-36300.
3. Sauvé, E. R., Tang, B. Y., Razdan, N. K., Toh, W. L., Wenig, S., Surendranath, Y., *Joule* **2024**, 8(3), 728-745.

Correcting the Overestimation of Dispersion Reproduces Supramolecular Host-Guest Equilibrium

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Accurate prediction of supramolecular host–guest equilibria remains a major challenge for computational chemistry, especially when several competing species coexist in solution. In this work, we combine experimental speciation data and DFT calculations to study the binding of 4-(azidomethyl)pyridine N-oxide and 4-ethynylpyridine N-oxide inside an octaimine biscalix[4]pyrrole cage[1]. Experimental measurements show the formation of different host–guest complexes and a clear selectivity between both N-oxide guests.

Conformational sampling was performed with xTB/CREST, followed by DFT optimization and higher-level single-point calculations. Standard B3LYP-D3BJ calculations overestimated the stability of the encapsulated species and failed to reproduce the experimental host occupancy distribution shown in Figure 1.

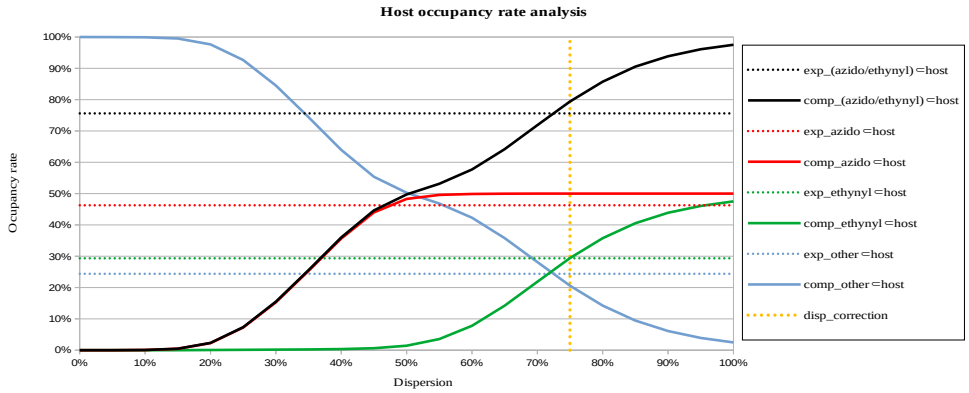

Figure 1. Predicted host occupancy as a function of the dispersion scaling factor. Solid lines: predicted host occupancies. Dotted lines: experimentally derived occupancies.

Explicit water clusters improved the description of the reference state by competing for the polar binding sites of the cage, but this effect alone was insufficient2. Therefore, the dispersion contribution was systematically scaled by interpolating between B3LYP and B3LYP-D3BJ free energies, and analysed using microkinetic modelling, following previous computational approaches3 (Figure 1).

The best agreement with the experimental speciation was obtained using 75% of the D3BJ dispersion contribution. These results indicate that standard dispersion-corrected DFT can over-stabilize π-stacking and van der Waals interactions in confined supramolecular cavities, and highlight experimental speciation as a stringent benchmark for computational models of host–guest chemistry.

References:

1. Y. Li, G. Aragay, P. Ballester, *Chem. Sci.* **2025**, *16*, 14534-14543.
2. H. Daver, A. G. Algarra, J. Rebek Jr., J. N. Harvey, F. Himo, *J. Am. Chem. Soc.* **2018**, *140*, 12527-12537.
3. C. Goehry, M. Besora, F. Maseras, *ACS Catal.* **2015**, *5*, 4, 2445–2451

PhotoScale : An Automated Continuous-Flow Photoreactor for Photocatalysis

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Photocatalysis offers a sustainable route to fuels, feedstocks, and fine chemicals, but optimising any new transformation requires sampling a high-dimensional parameter space (catalyst loading, photon flux, residence time, temperature, etc.). Manual screening limits throughput and reproducibility, motivating photoreactors in which sensing, control, and decision-making are embedded in the hardware. We present “PhotoScale”, an automated continuous flow-Photoreactor developed in ICIQ (Figure 1). The architecture of this Photoscale has been depicted in (Figure 2). The reagent solution is pumped from a reservoir via a peristaltic pump, an in-line ultrasonic flow meter, and a glass tubular reactor and returned to the reservoir. The photoexcitation is provided by eight 450 nm LUXEON high-power LED matrix plates (48 LEDs per plate) placed within the reactor and water cooled by an external chiller. The light intensity adjusted with four rotary dimmers (driving two plates each). All the dimmers, flow meter, and temperature sensors for each reactor plate wired to a Raspberry Pi, which logs the data and provides the user interface via a 7-inch touchscreen. This platform is envisioned as a hardware foundation for further autonomous photocatalytic research and for the data-driven optimization of reaction conditions.

Figure 1: PhotoScale **a)** front view **b)** Internal View

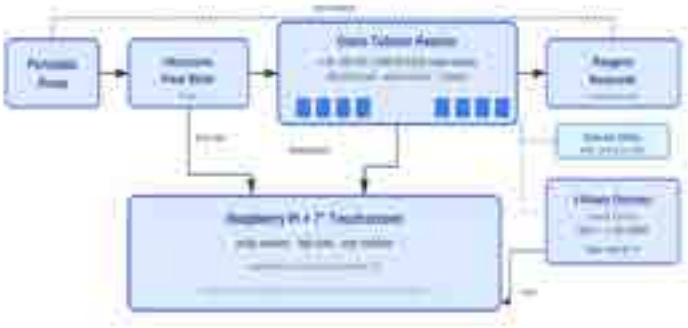

Figure 2: PhotoScale architecture.

References:

1. A. Slattery, Z. Wen, P. Tenblad, J. Sanjosé-Orduna, D. Pintossi, T. den Hartog, T. Noël, Science 2024, 383, eadj1817.

pH-Controlled Phospholipids Drives Active Self-Assembly of Vesicles for Programmed Release of Cargo

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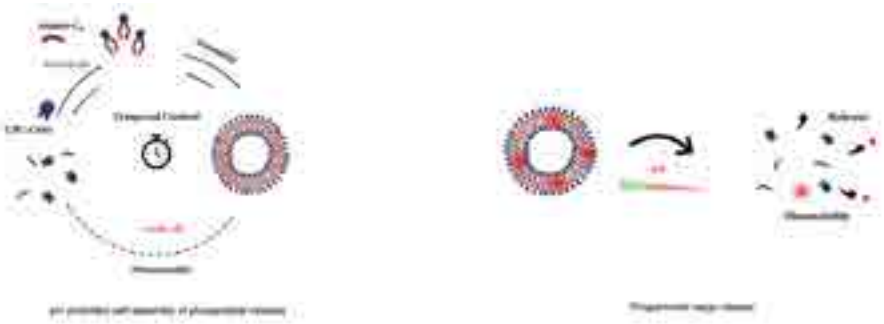
Reversible self-assembly of small molecules into dynamic higher order structures is ubiquitous in biology. In recent years, significant efforts have been devoted into developing active liposomes with precisely controllable structural properties1. These systems can be leveraged for the programmable transport and delivery of molecular cargoes, such as drugs, as well as for applications in synthetic biology. Among these, pH responsive vesicles are particularly attractive as they can respond to pH gradients that exist in biological environments2. pH variations trigger changes in the designed constituent molecular units, leading to vesicle disassembly and release of encapsulated cargo. Despite considerable progress, active self-assembly of liposomes are rarely reported and active liposomes that are capable of programmable assembly-disassembly in response to stimuli are scarce. In this study, active phospholipids are formed in-situ from simple molecular precursors. The activation of lipids is based on dynamic imine bond formation, makes the vesicular assemblies responsive to pH changes in the environment. Since imine bonds are stable at neutral pH but dissociates under acidic conditions, lowering the pH leads to breakdown of vesicles and release of encapsulated molecules into the surroundings. By employing Gluconolactone, which slowly hydrolyses to form gluconic acid, a temporally programmable vesicle disassembly and cargo release has been demonstrated. Notably, vesicle actively assemble and disassemble as the cycle can be repeated by switching the pH, establishing a key feature of dynamic systems. Furthermore, the vesicles exhibit diameters of approximately 200 nm, placing them within the optimal size range for drug delivery applications. Combined with its pH responsiveness, this feature gives the minimal chemical design strong potential to develop pH responsive active drug delivery systems. In addition, this dynamic system closely mimics the adaptive behaviour of biological structures, providing a platform to better understand the operation of such complex mechanisms.



References:

1. A.Venugopal, S.Ghosh, A.Calò, G. M.Tuveri, G.Battaglia, M.Kumar, Angew. Chem. Int. Ed.2025, 64, e2025008242.
2. FaezeShojaeinia, MostafaAmirinejad, AtoosaHaghighizadeh, OmidRajabi, ChemMedChem2026, 21, e202500709.

Exploring the Reactivity of Substituted Cycloheptatrienes via Gold Catalysis

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Cycloheptatriene (CHT) is a versatile and fascinating platform due to its unique electronic structure and propensity to undergo various cycloaddition pathways. Our group investigated the reaction between alkynes (**4a-b**) and cycloheptatriene (**5e**) mediated by a gold catalyst. Interestingly, the reaction outcome is highly dependent on the electronic nature of the alkyne partner. Electron-rich phenylacetylene (**4a**) delivers a bridged bicyclic framework (**6**), whereas electron-deficient methyl propiolate (**4b**) yields the functionalized CHT derivative (**7**).

Building upon these findings, this work explores the impact of steric and electronic perturbations on the cycloheptatriene core by employing substituted CHT derivatives. Specifically, we investigate the reactivity of phenyl- and cyclobutyl-substituted cycloheptatrienes in these gold-catalyzed transformations.

References:

1. M. Elena de Orbe, A. M. Echavarren, *Eur. J. Org. Chem.* **2018**, *22*, 2740-2752.

Generation of Digold(I) Carbenoid Complexes with Bidentate Phosphine Ligands

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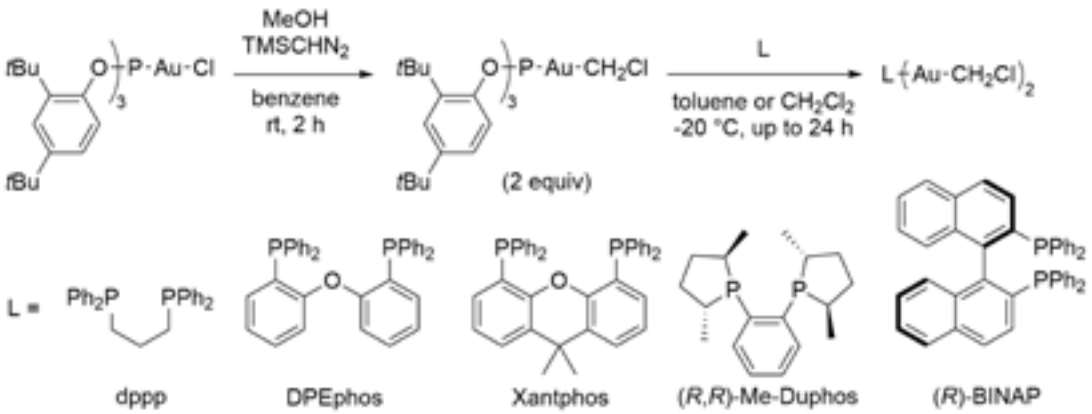
Gold(I) carbenoids are highly electrophilic intermediates that promote a variety of C-C bond formations like cyclopropanation, cycloaddition and C-H insertion reactions, making their preparation of high interest for organic chemists. Bourissou and coworkers have recently reported a “ligand exchange last” strategy employing the labile ancillary ligand tris(2,4-di-tert-butylphenyl) phosphite to generate a variety of gold(I) complexes with different ligands and organic groups [1].

We envisioned to implement this strategy for the preparation of highly reactive digold(I) carbenoid chloride complexes bearing bidentate phosphine ligands starting from tris(2,4-di-tert-butylphenyl) phosphite gold chloride (Scheme 1).

For the synthesis of the tris(2,4-di-tert-butylphenyl) phosphite gold carbenoid, we employed a strategy that has been developed by our group using the methanol promoted decomposition of trimethylsilyldiazomethane in the presence of the respective gold chloride [2]. The gold carbenoid was then subjected to reactions with the bidentate phosphine ligands DPEphos, dppp, Xantphos, (R,R)-Me-DuPhos and (R)-BINAP leading to phosphine ligand exchange due to the labile nature of the tris(2,4-di-tert-butylphenyl) phosphite ligand. The formed digold(I) carbenoid complexes were analyzed via NMR spectroscopy and X-Ray crystallography to confirm their structure.

Applications of the digold(I) carbenoid complexes in cyclopropanation reactions as well as computational results regarding the use of digold(I) carbene complexes in the activation of methane will also be discussed.



References:

1. D. Vesseur, S. Li, S. Mallet-Ladeira, D. Bourissou, *Chem. Commun.* **2025**, 61,18717-18720.
2. J. M. Sirria Toro, C. García-Morales, M. Raducan, E. S. Smirnova, A. M. Echavarren, *Angew. Chem. Int. Ed.* **2017**, 56, 1859-1863.

Towards Recyclable Thermosets: Tunable Polyether-Carbonate Networks

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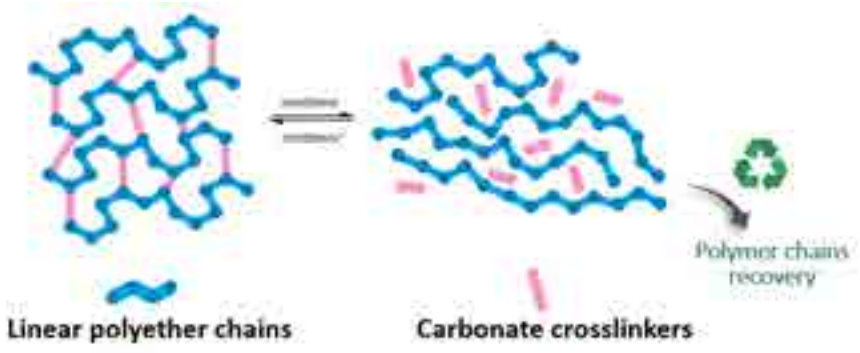
Thermoset materials are widely used in high-performance applications due to their excellent thermal and mechanical properties; however, their permanent crosslinked structure severely limits recyclability, as conventional melt-and-reshape strategies applicable to thermoplastics cannot be employed.1-2 In this work, we demonstrate the design of sustainable and chemically recyclable polyether-co-carbonate thermosets through the incorporation of selectively cleavable carbonate crosslinkers. The polymer precursors were synthesized via ring-opening polymerization (ROP) of potentially CO2-derived epoxide monomers (propylene oxide and glycidyl acetate) , providing access to polyether chains with tunable compositions.3-4 By varying the ratio between the epoxide monomers, polymers with different reactive sites were obtained, enabling control over the degree of crosslinking and, consequently, the thermal and mechanical properties of the resulting networks. Crosslinking was achieved through carbonate-based linkages that can be selectively cleaved under appropriate conditions while preserving the integrity of the polyether backbone, allowing recovery and reutilization of the polymer chains. This strategy combines the performance advantages of thermosets with an efficient end-of-life recycling pathway, offering a promising route toward more sustainable polymeric materials. The ability to tailor network properties through monomer composition while enabling chemical recycling highlights the potential of these polyether-co-carbonate thermosets for advanced and circular material applications.



References:

1. W. Post, et Al., *Polymer Reviews*, **2020**, 60(2), 359-388.
2. Y. Liu, et Al., *Green Chem.*, **2022**, 24, 5691-5708.
3. R. Klein, et Al., *Macromolecular Rapid Communications*, **2015**, 36, 1147–1165.
4. M. Gosecki, et Al., *Polymers*, **2016**, 8, 227

Regiodivergent sp^3-H Functionalization via Interrupted Nickel-Catalyzed Chain-Walking

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Interrupted nickel-catalyzed chain-walking provides a powerful approach for site-selective functionalization of aliphatic molecules. By controlling the interception of migrating nickel intermediates, regioselective C(sp^3)–C(sp^3) or C(sp^3)–X bond formation can be achieved at positions that are otherwise difficult to access.

We have developed strategies that enable both remote and regiodivergent C(sp^3)–H functionalization. Native amides directed deaminative C(sp^3)–C(sp^3) bond formation through Ni-catalyzed site-selective interrupted chain-walking, while a traceless directing-group approach allows ligand-controlled β- and γ-functionalization of alcohol-derived substrates. Mechanistic studies reveal how substrate coordination and ligand effects govern nickel migration and intermediate capture.

These studies demonstrate the potential of interrupted chain-walking as a general platform for programmable C(sp^3)–H functionalization.

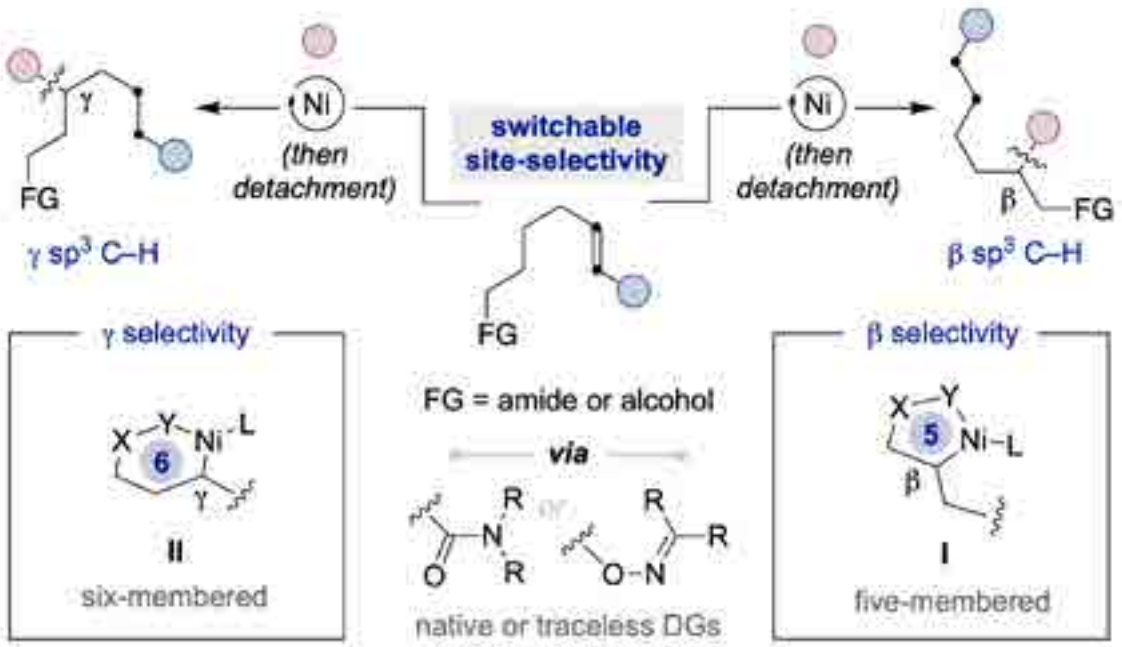

Fig.1 Regiodivergent sp^3-H Functionalization via Interrupted Nickel-Catalyzed Chain-Walking

References:

1. J. Rodrigalvarez, H. Wang, R. Martin, *J. Am. Chem. Soc.* **2023**, *145*, 3869–3874.
2. 2. H. Wang, H. Zhang, M. Martínez-Belmonte, J. Benet-Buchholz, R. Martin, *J. Am. Chem. Soc.* **2025**, *147*, 28610–28616.

Hammerhead Ribozymes Bearing Non-Canonical Nucleosides

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The RNA world is perhaps the most compelling hypothesis for how life can emerge in a prebiotic world.[1,2] RNA has the potential to serve the dual purposes essential for life; to not only store information but also to facilitate chemical reactions. The Hammerhead ribozyme is a prime example of this duality, being an RNA strand which binds to nucleotide substrates in a sequence-specific fashion before catalysing substrate cleavage. Herein, we report our modifications of a simple Hammerhead ribozyme using non-canonical nucleosides[3] such as the 'living fossils' found ubiquitously in tRNA. These modifications introduce greater functionality (viz. amides, amines, carboxylic acids) and in certain instances were found to dramatically increase ribozyme catalysis rates (**Fig 1.**). We propose that such hypermodified nucleosides could have served a critical role in the emergence of life on the early Earth, and today they may offer us the means for tuning ribozyme kinetics.

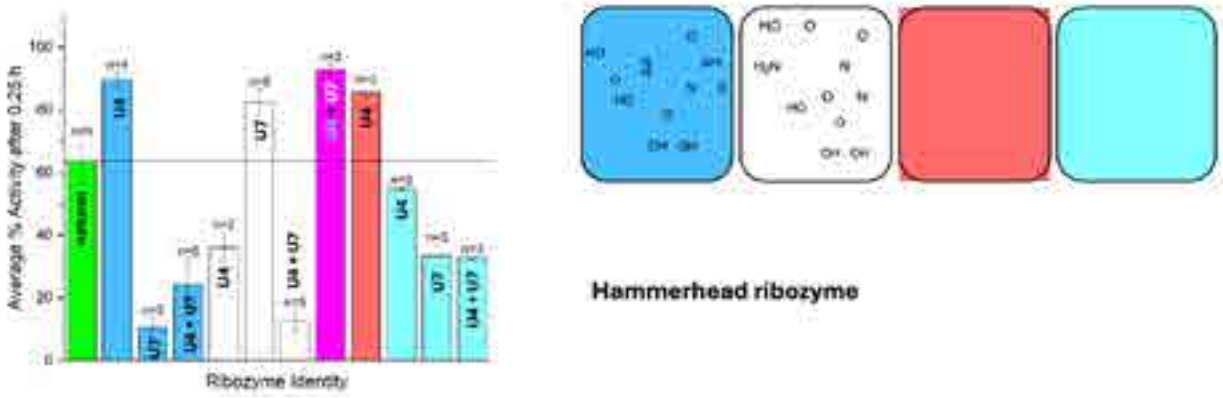

Figure 1. Non-canonical nucleoside modifications of the Hammerhead ribozyme at positions U4 and U7 allow for dramatic modulation of catalytic activity.

References:

1. Rich, A.* Horizons in Biochemistry, 1962, 103-126.
2. Demongeot, J.*, Thellier, M. Int. J. Mol. Sci., 2023, 24, 2274, 4, https://doi.org/10.3390/ijms24032274
3. Mejdr, E., Heinickel, L., Carell, T., Mejdr, I.* Chem. Eur. J., 2026, 32:e02848. https://doi.org/10.1002/chem.202502848

Aromatic decarbenation to access gold(I) carbenes

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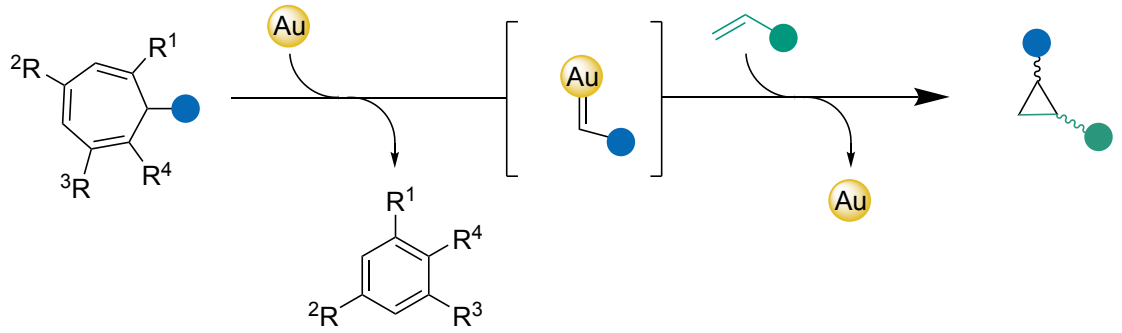
The gold(I)-catalyzed retro-Buchner transformation of 7-substituted cycloheptatrienes has emerged as a safe and powerful strategy for the generation of gold(I) carbene intermediates.[1,2] The exceptional reactivity of these highly energetic metal–carbene species enables a broad range of cascade transformations and cycloaddition processes. However, the relatively high temperatures required affect its synthetic applicability.[3]

A major advance was the development of substituted cycloheptatrienes capable of undergoing retro - Buchner reaction under gold(I) catalysis, at room temperature. In this context, a detailed understanding of the factors governing this transformation is essential for the rational design of new carbene precursors.[4] The aim of this work is to investigate, through kinetic studies and density functional theory (DFT) calculations, how different substitution patterns and electronic properties of cycloheptatriene carbene precursors influence the decarbenation process and the overall reactivity of the system.



References:

1. C. R. Solorio-Alvarado and A. M. Echavarren, *J. Am. Chem. Soc., 2010, 132* , 11881
2. Y. Wang , P. R. McGonigal , B. Herlé , M. Besora and A. M. Echavarren, *J. Am. Chem. Soc.,* **2014***, 136*, 801
3. H. Armengol-Relats, M. Mato, I. Escofet and A. M. Echavarren, *Synthesis,* **2021***, 53*, 3991–4003
4. M. Mato, C. García- Morales and A. M. Echavarren, *ChemCatChem,* **2019***, 11*, 53 – 72

Photo-induced dual-Nickel-catalyzed directly electrophile cross-coupling enables Csp3-Csp2 coupling of unactivated alkyl chlorides and aryl chlorides.

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Alkyl chlorides represent bench-stable and readily available chemical feedstocks; however, they remain one of the most underutilized electrophile classes in transition metal catalysis. their chemical inertness hinders their use as electrophilic partners in transition metal-catalyzed reactions, a limitation particularly evident in cross-electrophile couplings with aryl chlorides for C(sp^3)–C(sp^2) bond formation. To achieve this objective, prior strategies have relied on halogen-exchange protocols to convert unactivated alkyl chlorides into more readily activatable alkyl iodides or bromides[1, 2], or alternatively, the use of specialized alkyl silicon reagents to abstract the chlorine atom[3]. Collectively, these approaches underscore the inherent difficulty of directly activating unactivated alkyl chlorides using transition metals. If unactivated alkyl chlorides are to be established as practical synthetic building blocks, overcoming this challenge is imperative. In our previous work, we developed a photoinduced single-nickel catalytic system that enabled the cross-electrophile coupling of unactivated alkyl chlorides with para-dicyanobenzene. However, when this strategy was extended to the cross-electrophile coupling of unactivated alkyl chlorides with aryl chlorides, the reaction proved inefficient. Given that a single nickel catalyst is likely incapable of activating both electrophilic coupling partners, we introduced a second nickel catalyst with the aim of achieving cooperative catalysis[4]. The results demonstrate that the dual-nickel catalytic system is substantially more efficient, markedly reducing reaction times, lowering catalyst loadings, and significantly enhancing overall reactivity.

References:

1. Kim, S.; Goldfogel, M. J.; Gilbert, M. M.; Weix, D. J. Nickel-Catalyzed Cross-Electrophile Coupling of Aryl Chlorides with Primary Alkyl Chlorides. *Journal of the American Chemical Society* **2020**, *142* (22), 9902-9907.
2. Feng, X.; Li, X.; Zhang, N.; Zhwang, L.; Sun, F.; Liu, H.; Zhao, Z.; Li, X. Cross-Electrophile Coupling of Aryl Chlorides with Alkyl Chlorides Using Rotating Magnetic Field and Metal Rods. *Journal of the American Chemical Society* **2025**, *147* (15), 12664-12671.
3. Sakai, H. A.; Liu, W.; Le, C. C.; MacMillan, D. W. C. Cross-Electrophile Coupling of Unactivated Alkyl Chlorides. *Journal of the American Chemical Society* **2020**, *142* (27), 11691-11697.
4. Bucci, E. M.; Perea, M. A.; Lalisse, R. F.; Mukherjee, P.; Raab, T. J.; Kannadi Valloli, L.; Min, D. S.; Bird, M. J.; Gutierrez, O.; Doyle, A. G. Development, Application, and Mechanistic Interrogation of a Dual Ni Catalysis Approach to Photoredox-Based C(Sp3)–C(Sp3) Cross-Coupling. *Journal of the American Chemical Society* **2025**, *147* (46), 42311-42329.

Study of the Reactivity of Gold(I)-Catalyzed Pyridine Synthesis

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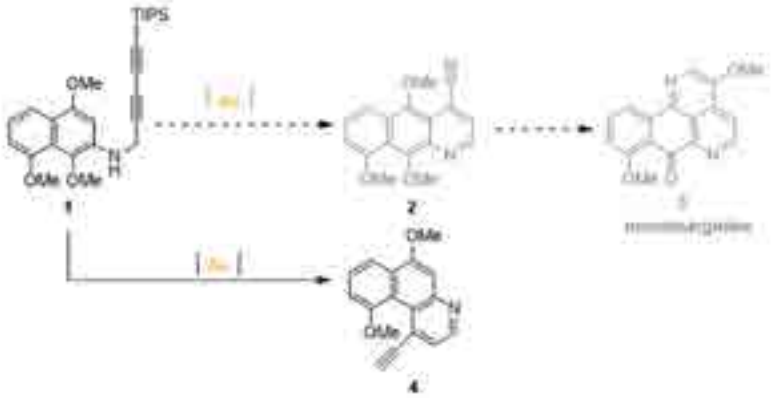
The activation of alkynes by gold(I) catalysts is one of the most effective manners to build carbon-carbon bonds, due to its selective activation of the π-bonds of alkynes. Moreover, gold(I)-catalyzed reactions offer the possibility to achieve diverse molecular structures, as the ones encountered in natural products.[1] The total synthesis of monomarginine, a tetracyclic alkaloid with pharmacological properties isolated from Monocarpia marginalis, has been a research objective in Echavarren´s group. Previously, we attempted a gold(I)-catalyzed cyclization of a juglone derivative, aiming to obtain the azaanthraquinone core by cyclization at the C2 position, following a reported methodology for anilines.[2] However, the cyclization took place at the C4 position, forming **4** (Scheme 1).[3]



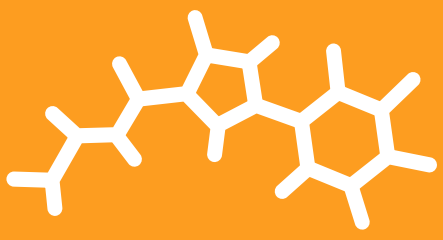
Scheme 1. Observed reactivity for the cyclization of **1**

This work focuses on the study of such gold(I)-catalyzed cyclization reactions performed in substrates with different substitution patterns, with the objective to explore the variations in the reaction outcomes by modifying the nature of aniline or naphtalene derivatives (Scheme **2**). The understanding of this reactivity will shed light on how the gold(I)-catalyzed cyclization works and will offer new possibilities to build N-heterocyclic skeletons.

Scheme 2. General scheme for the study of the gold(I)-cyclization reactivity

References:

1. (a) Lin, R.; Liu, T.; Luo, T. *Nat. Prod. Rep.* **2024**, *41*, 1091–1112
   (b) Dorel, R.; Echavarren, A. M. *Chem. Rev.* **2015**, *115* (17), 9028–9072.
2. Ogalla, G. Doctoral Thesis, 2025, URV-ICIQ.



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