DOCTORAL WORKSHOP

PhD in Chemistry

Scientific Programme and Book of Abstracts

May 20th-21st, 2026

Sala d'Actes

Faculty of Science

Organised by the Department of Chemistry

Sponsored by:

RSEQ Real Sociedad Española de Química

RSEQ Secció Territorial Catalana

SCQ Societat Catalana de Química

UAB Universitat Autònoma de Barcelona

Facultat de Ciències UAB

WELCOME TO THE XV DOCTORAL WORKSHOP OF THE PhD PROGRAMME IN CHEMISTRY

May 20-21, 2026

It is our great pleasure to welcome you to the new Edition of the Doctoral Workshop of the PhD programme in Chemistry that is organized by the UAB's Department of Chemistry.

This year's workshop continues its tradition of providing supportive environment for doctoral students to present and discuss their dissertation with peers, members of the program and other experienced reserchers, with the aim to strengthen the links and facilitating the exchange of research experiences and new ideas in the fields of entrepreneurship and small business.

During the event, 24 students, mostly on their third year will have an excellent opportunity to share their research. The Doctoral Workshop will also include an exciting series of plenary lectures given by international experts.

All the members of the PhD program in Chemistry and related programs, as well as other members of the research community are more than welcome.

We look forward to your participation in this event.

The Organizing Committee

ORGANIZING, SCIENTIFIC AND AWARDS COMMITTEE

Organizing and Scientific Committee:

Dr. Xavier Sala, Coordinator and president of the academic committee of the PhD in Chemistry
Dr. Rosario Núñez, Vocal of the academic committee of the PhD in Chemistry
Dr. Daniel Maspoch, Vocal of the academic committee of the PhD in Chemistry
Dr. Xavier Solans, Secretary of the academic committee of the PhD in Chemistry
Dr. Maria Jesús Sánchez, Vocal of the academic committee of the PhD in Chemistry
Dr. Carolina Gimbert, Vocal of the academic committee of the PhD in Chemistry

Awards Committee:

Dr. Xavier Sala, Coordinator and president of the academic committee of the PhD in Chemistry
Dr. Xavier Solans Monfort, Secretary of the academic committee of the PhD in Chemistry
Judit Prat Trunas, PhD Student
Mercè Alemany Chavarria, PhD Student

Contact

Prof. Xavier Sala Román
PhD Coordinator of PhD studies in Chemistry

Julia Nacarino
Administrative Assistant

Telf.: 935814434
E-mail: gestio.postgrau.quimica@uab.cat
More information: https://www.uab.cat/ca/quimica

Event sponsored by:

Real Sociedad Española de Química (RSEQ) – Secció Catalana de la RSEQ
Societat Catalana de Química (SCQ) – GEQO – Seminarios Itinerantes

INVITED SPEAKERS

Prof. Federico Bella
Politecnico di Torino

Federico Bella is Full Professor of Chemistry at Politecnico di Torino, where he leads research on materials chemistry for energy conversion and storage, with a focus on electrochemical nitrogen reduction, batteries, photovoltaics, and sustainable materials. He obtained his PhD in Electronic Devices from the Italian Institute of Technology and built his academic career at Politecnico di Torino, becoming Full Professor in 2022. His research combines electrochemistry, materials science, photochemistry, chemometrics, and green chemistry to develop more sustainable energy technologies. He has been the Principal Investigator of the ERC Starting Grant SuN2rise, devoted to solar-driven electrochemical nitrogen fixation for ammonia production. His group works on nitrogen and nitrate electroreduction, with particular attention to electrolyte design, interface control, analytical reliability, and process sustainability. He has authored more than 130 peer-reviewed papers, collecting over 12,500 citations and reaching an h-index of 81 according to Scopus. He serves on the editorial boards of leading journals including Energy Storage Materials, Chemical Engineering Journal, ChemSusChem, and ACS Sustainable Chemistry & Engineering. Among his recognitions are the ISE Prize for Electrochemical Materials Science, the ISE-Elsevier Prize for Applied Electrochemistry, the ACS Sustainable Chemistry & Engineering Lectureship, and the ChemComm Emerging Investigator Lectureship.

Prof. Jesús Campos
Instituto de Investigaciones Químicas (IIQ), Universidad de Sevilla and Consejo Superior de Investigaciones Científicas (CSIC)

Jesús Campos obtained his PhD (2012) in organometallic chemistry at the University of Sevilla (E. Carmona), including a visiting stay at the University of North Carolina (M. Brookhart). He developed his postdoctoral research at the universities of Yale (R. Crabtree) and Oxford (S. Aldridge). Since 2017 he is CSIC tenured scientist and group leader at the Institute for Chemical Research. During that time, he has been awarded with ERC Starting and Consolidator Grants to develop bimetallic cooperative systems from different perspectives. His work has been recognized with several distinctions, including the Premio a la Excelencia Investigadora from RSEQ or the Premio Nacional de Investigación Joven. His interests include all aspects of organometallic chemistry, particularly on the study of cooperative mechanisms for bond activation and catalysis.

Prof. Carme Rovira
Universitat de Barcelona

Carme Rovira is an ICREA Research Professor at the University of Barcelona. She obtained her PhD in Chemistry from the University of Barcelona and carried out research stays in Germany, at the Max Planck Institute for Solid State Research, and in the UK, at the University of York. Her research focuses on modelling enzyme catalytic mechanisms through computer simulations, with a special emphasis on carbohydrate-active enzymes. She has received several awards, including distinctions from the Generalitat de Catalunya, the Barcelona City Council, and the European Carbohydrate Organization (*Emil Fischer* award). In 2020, she was awarded an ERC Synergy Grant, and in 2025 she received the National Research Award “Enrique Moles” in Chemistry and Chemical Technology. She currently serves as President of the Computational Chemistry Group of the Spanish Royal Society of Chemistry and as Associate Editor of *ACS Omega*

SCIENTIFIC PROGRAM

May 20th

08:45—09:00 Welcome and opening

Prof. Ramon Alibés, Head of the Department of Chemistry
Mrs. Beatriz Ferrus Anton, Head of the Doctoral School

09:00—10:00 Plenary Lecture

Chair: Xavier Sala

Title: Ammonia by Electrons: Turning Nitrogen Feedstocks into Sustainable Fuels and Fertilizers
Prof. Federico Bella

10:00—12:00 Presentations I

Chair: Xavier Sala

10:00 - 10:15 DFT study on the electrocatalytic reduction of NO3 and N2 into ammonia. **Yanis Abid Charef. P1.1**

10:15 - 10:30 Synthesis of Organic Molecules via Spray-Drying. **Gerard Pena Pozo. P1.2**

10:30 - 10:45 Recovering Copper from vineyards: Phytoremediation as a circular strategy. **Camila Cazorla Ares. P1.3**

10:45 - 11:00 Sulfanilic Acid-capped Ruthenium Nanoparticles for Enhanced HER activity in neutral media. **Matilda Kraft. P1.4**

11:00—11:45 Poster session

11:45—12:45 Presentations II

Chair: Carolina Gimbert

11:45 - 12:00 Chitin - choline bio-sourced composites for CO2 electrolysis in atmospheric conditions. **Boya Wu. P2.1**

12:00 - 12:15 Beyond Isostructurality: Controlling Function and Scale in Zr and Hf Carborane MOFs. **Shuo Zhang. P2.2**

12:15 - 12:30 Giant Unilamellar Vesicles (GUVs) for Cell Membrane mimicry. Towards Artificial red bloods cells. **Carlos Cascales Guerrero. P2.3**

12:30 - 12:45 Development of 3D-printed sensing platforms applied to pH and hydrogen monitoring. **Mingyue Pan. P2.4**

12:45 - 13:00 Selective recovery of heavy metals from wine sludge using oxidizing agents: towards sustainable waste management in viticulture. **Mónica González Quintela. P2.5**

13:00—15:15 Break

15:15—16:15 Plenary Lecture

Chair: Daniel Maspoch

Title: Cooperation, Inhibition and other Bimetallic Synergies
Prof. Jesús Campos

16:15—17:30 Presentations III

Chair: Xavier Solans

16:15 - 16:30 Plant nano-biofortification selenium release in soil systems to produce functional foods. **Alejandro Fuentes García. P3.1**

16:30 - 16:45 Molecular electrocatalysts for RedOx reactions: water oxidation and CO2 reduction using carbanionic ruthenium. **Jake Tyler Kerkhof. P3.2**

16:45 - 17:00 Developing computational tools to explore reaction pathways for periodic systems. **Andreha Gelli. P3.3**

17:00 - 17:15 Rice Husk Ash-Derived Zeolite X Supported Mn-ZIF-67 for Visible-Light-Assisted PMS Activation: From Agro-Industrial Waste Valorisation to Organic Pollutant Remediation. **Hanwen Luan. P3.4**

17:15 - 17:30 Reversible colorless-to-colored thermochromic materials based on modified. **Noel Muñoz Pérez. P3.5**

May 21st

09:00—10:30 Presentations IV

Chair: Maria Jesús Sánchez

09:00- 09:15 TT-CF3+OTf-: a bench-stable trifluoromethylation reagent with formal CF3+, and CF3• reactivity. **Xiangyu Tan. P4.1**

09:15 - 09:30 Portable electrochemical biosensing platform for point-of-need. **Juan Carlos Porras. P4.2**

09:30 - 09:45 How Multi Component Reactions simplify the synthesis of Organic Radical Dendrimers as potential MRI contrast agents? **Ehsan Shirdel Tazehkand. P4.3**

09:45 - 10:00 Toward Cu Remediation of Vineyard Soils: A Sulfonated Amide COF and COF-Based Membrane Approach. **Di Cai. P4.4**

10:00 - 10:15 Making Mesocrystals with Colloidal MOF Particles. **Amir Mohammad Ghadiri Ghehi. P4.5**

10:15 - 10:30 Development of point-of-need potentiometric devices for the monitoring of rare inherited metabolic diseases. **Laia Garrido Carretero. P4.6**

10:30—11:15 Poster session

11:15—12:15 Presentations V

Chair: Rosario Núñez

11:15 - 11:30 Development of electrochemical sensors from revalorize biomass for emerging pollutant monitoring. **Yudong Bian. P5.1**

11:30 - 11:45 Electrocatalytic ammonia synthesis via iron-based nanoparticles: mechanistic insights from computational studies. **Adenilson Felipe Sousa Silva. P5.2**

11:45 - 12:00 Synergistic Enhancement of Cu (II) Adsorption by Tannic Acid and L-Cysteine Functionalized Magnetic Chitosan Beads: Role of Structure–Function Trade-Off. **Xiaojie Sun. P5.3**

12:00 - 12:15 Towards graphene functionalization with small organic molecules for neurotransmitters detection. **Aina Galceran Sabatés. P5.4**

12:15—13:15 Plenary Lecture

Chair: Mariona Sodupe

Title: Using Computer Simulations to Understand How Enzymes Work
Prof. Carme Rovira

13:15—13:30 Award and Closing Ceremony

Doctoral Workshop 2026 distinguished Diploma, along with a gift, will be given to the two best Poster & Presentation.

Venue:
Plenary Lectures and PhD students' presentations: in the Auditorium of the Faculty of Sciences (*Sala d'Actes*).
Posters' Exhibition: in the Hall on the ground floor of the Faculty of Sciences (in front of *Sala de Graus I*).

ABSTRACTS

INVITED SPEAKERS

Ammonia by Electrons: Turning Nitrogen Feedstocks into Sustainable Fuels and Fertilizers

Federico Bella

Department of Applied Science and Technology, Politecnico di Torino
Corso Duca degli Abruzzi 24, 10129 – Torino, Italy

federico.bella@polito.it

Electrochemical ammonia production is emerging as one of the most intriguing strategies to rethink the nitrogen cycle at the interface between chemistry, energy and sustainability. Ammonia is not only a cornerstone of global fertilizer production, but also a potential energy carrier and hydrogen vector. Yet, its current industrial synthesis through the Haber-Bosch process remains energy-intensive, centralized and largely dependent on fossil-derived hydrogen. In this context, the possibility of producing ammonia under mild conditions, using renewable electricity and alternative nitrogen sources, offers a fascinating scientific and technological challenge.

This lecture will focus on two complementary electrochemical routes to ammonia: nitrogen reduction and nitrate reduction. The direct reduction of molecular nitrogen represents an ambitious frontier in electrocatalysis, where the activation of the exceptionally stable N≡N bond competes with parasitic hydrogen evolution and requires rigorous analytical validation. Nitrate reduction, by contrast, starts from a more reactive nitrogen feedstock and opens the possibility of coupling ammonia production with wastewater treatment, pollutant valorization and circular nitrogen management. Together, these pathways highlight how the choice of feedstock reshapes the chemistry, thermodynamics, kinetics and practical relevance of ammonia electrosynthesis.

Beyond individual catalysts or performance metrics, electrochemical ammonia production should be viewed as a multidisciplinary problem involving materials chemistry, interfacial catalysis, electrolyte design, reactor engineering and analytical chemistry. Progress in the field depends not only on achieving high Faradaic efficiency or ammonia yield, but also on understanding selectivity, avoiding false positives, ensuring long-term stability and defining realistic benchmarks for scalability. By connecting fundamental electrochemical concepts with global sustainability challenges, ammonia electrosynthesis provides a powerful case study of how chemistry can contribute to redesigning essential industrial processes and closing the nitrogen cycle [1-3].

References

[1] Our group, *Angew. Chem. Int. Ed*. 64 (2025) art. no. e202416027.

[2] Our group, *Adv. Energy Mater.* 14 (2024) art. no. 2400076.

[3] Our group, *J. Energy Chem.* 107 (2025) 599-611.

Acknowledgements

This project has received funding from the ERC under the ERC-2024-POC call (grant agreement No. 101213773, project title: GINNY).

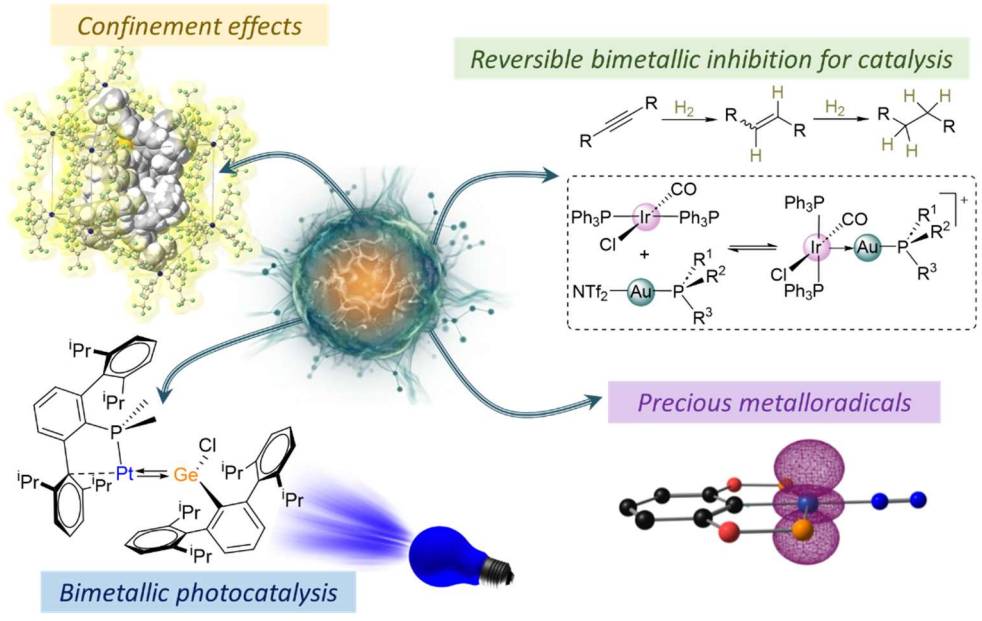
Cooperation, Inhibition and other Bimetallic Synergies

Jesús Campos

[a] *Instituto de Investigaciones Químicas (IIQ), Universidad de Sevilla and Consejo Superior de Investigaciones Científicas (CSIC). Avenida Américo Vespucio 49, 41092 Sevilla (Spain).*

E-mail: jesus.campos@iiq.csic.es

Cooperative chemistry has become a broad area of intensive research with many prospects for catalysis. Cooperative approaches capitalize on the fact that synergistic effects between a variety of chemical entities may surpass more traditional catalytic strategies in fundamental aspects as activity, selectivity or substrate scope. Among the many cooperative approaches applied to catalysis, the use of bimetallic structures that rely on the existence of two metals in close proximity, paralleling what is often found in metalloenzymes, has gained considerable attention.[1] This is partly because bimetallic compounds offer a manifold of tunable features that are just not available for mononuclear analogues, as the M–M bond order and polarity, the distance between the metals and the facility to enable multi-site bond activation mechanisms. In this context, our group has explored a wide variety of bimetallic approaches that go from multiply bonded bimetallic complexes to single and polarized bonds, reaching the extreme case of bimetallic pairs hold together by weak or even no interactions in bimetallic Frustrated Lewis Pairs (FLPs).[2] In this journey, we have analysed how ligand properties, bimetallic combinations, confinement effects or external stimuli affect reactivity and selectivity during bond activation and catalysis, disclosing unexpected reactivity or rather unconventional mechanisms.[3] In this contribution, I will discuss our last results on cooperative bimetallic activation, reversible bimetallic inhibition and other bimetallic synergies.



References

1. a) Buchwalter, P.; Rosé, J.; Braunstein, P. *Chem. Rev.* **2015**, *115*, 28; b) Farley, C. M.; Uyeda, C. *Trends Chem.* **2019**, *1*, 497; c) Campos, J. *Nat. Rev. Chem.* **2020**, *4*, 696.

2. Navarro, M.; Moreno, J. J.; Pérez-Jiménez, M.; Campos, J. *Chem. Commun.* **2022**, *58*, 11220.

3. See for example: (a) Serrano-Díez, E.; Pita-Milleiro, A.; Rangel-García, J.; Moreno, J. J.; Roselló-Merino, M.; Campos, J. *J. Am. Chem. Soc.* **2025**, *147*, 1271; (b) Pita-Milleiro, A.; Hidalgo, N,; Moreno, J. J.; Fernández, I.; Campos, J. *Nat. Chem.* **2025**, *17*, 606; (c) Bajo, S.; Soto, E.; Fernández-Buenestado, M.; López-Serrano, J.; Campos, J. *Nat. Commun.* **2024**, *15*, 9656.

Using Computer Simulations to Understand How Enzymes Work

Carme Rovira[1]

1. Facultat de Química & Institut de Química Teòrica i Computacional, Universitat de Barcelona, Marti i Franquès 1, 08028 Barcelona, Spain.
2. Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluís Companys 23, 08010 Barcelona, Spain.

c.rovira@ub.edu

Enzymes are among nature's most remarkable catalysts, capable of accelerating complex chemical reactions with exquisite selectivity and efficiency. Among them, carbohydrate-active enzymes (CAZymes), including glycoside hydrolases and glycosyltransferases, are the primary molecular machinery responsible for the degradation, synthesis, and modification of carbohydrates in nature. They underpin a wide range of industrial and biotechnological applications, from biomass conversion and biofuel production to the development of biotherapeutics. To use these enzymes in a controlled way and improve them for practical purposes, we need a detailed understanding of how they recognize carbohydrates and how sugar units "move" through the catalytic cycle. Such mechanistic insight can guide the design of new drugs and chemical probes for glycobiology and immunology. In this talk, I will illustrate how modern computer simulations can reveal enzyme mechanisms at atomic resolution, and I will highlight computational approaches that are expanding what we can learn about CAZyme catalysis.

ABSTRACTS

PhD STUDENTS

(In order of presentation)

DFT study on the electrocatalytic reduction of NO3 and N2 into ammonia

Y. Abid Charef*, M. Sodupe,L. Rodriguez-Santiago,X. Solans-Monfort
Departament de Química, Universitat Autònoma de Barcelona, 08193 - Bellaterra, Spain
yanis.abid-charef@outlook.com

Ammonia has become in the 21st century the main component in most chemical fertilizers in particular urea for which 40% of the global food yield relies on. By 2020, the global demand had already reached 183 Mt with an expected increase of 20% by 2030[1]. It is essentially produced through the Haber-Bosch process which is very demanding in energy (2% of the global energy consumption) and polluting (emission of 1% of the total CO2 greenhouse gas)[1]. Moreover, the increase of nitrate concentration in aqueous environments due to excessive use of industrial fertilizers in a context of intensive agriculture has led to the contamination of ground and surface waters which poses significant public health concerns[2]. Thus the need in finding newer and greener ways to not only produce ammonia but also to denitrify polluted waters. In this context, electrocatalysis has become in the past few years a ground breaking technique.

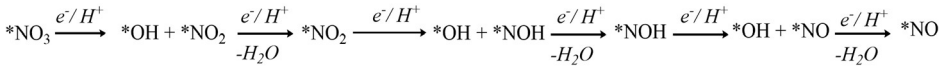


Figure 1 : Reduction mechanism of NO3 into NO leading to ammonia.

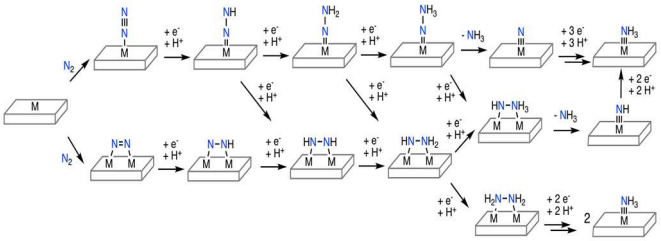


Figure 2 : Possible reduction mechanism of N2 into NH3.

In this contribution, we analyze the different behaviour of Cu, Ag and PdCu as electrocatalysts for both NO3- and N2 reduction to urea by means of DFT calculations. For that, we performed a comprehensive mechanistic exploration of both reductions. In addition, several metal surfaces are considered to understand the role of surface morphology and different modelling approaches are explored to include the effect of counter-ions and solvation. Results show that while the different computational strategies predict slightly different relative Gibbs energies for the key steps, the main conclusions are independent on the modelling approach. Simulations suggest that very reductive potentials should be applied for the initial reduction of N2 for both PdCu FCC and BCC surfaces with the initial reduction being potential limiting. For NO3- was showcased a small effect of surface morphology suggesting that flatter surfaces favour the NO3RR reaction by decreasing the NO2 adsorption. Moreover, subtle differences also arise from the catalyst composition and results suggest that Ag requires lower overpotentials to undergo the electrocatalytic reduction of NO3- to ammonia.

References:

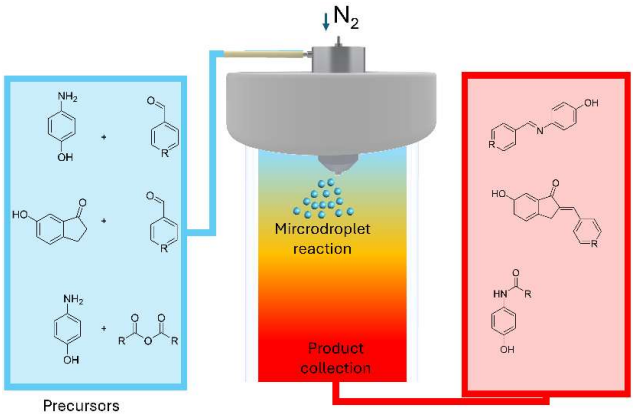
[1] Wang, Y., Wang, S., Fu, Y., Sang, J., Wei, P., Li, R., Gao, D., Wang, G., & Bao, X. (2025). Ammonia electrosynthesis from nitrate using a stable amorphous/crystalline dual-phase Cu catalyst. Nature Communications, 16, Article 897.
[2] Wei, J., Li, Y., Lin, H., Lu, X., Zhou, C., & Li, Y.-Y. (2023). Copper-based electro-catalytic nitrate reduction to ammonia from water: Mechanism, preparation, and research directions. Environmental Science & Ecotechnology, 20, Article 100383.

Keywords: DFT, Electrocatalysis, N2RR, nanosurfaces, NO3RR

Synthesis of Organic Molecules via Spray-Drying

G. Pena,[1,2] J. Albalad[1,2], I. Imaz[1,2*] and D. Maspoch[1,2,3*]
[1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and the Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193, Barcelona, Spain.
[2]Departament de Química, Facultat de Ciències, Universitat Autònoma de Barcelona (UAB), Cerdanyola del Vallès, 08193, Barcelona, Spain.
[3]ICREA, Pg. Lluís Companys 23, Barcelona, 08010, Spain.
e-mail: gerard.pena@icn2.cat
Keywords: *Spray-drying, Organic synthesis, Aerosol technologies.*

Synthetic organic chemistry has long played a crucial role in the design and preparation of new molecules that benefit society.[1] Beyond the discovery of new reactions, progress in this field has been driven by the development of innovative methodologies that ensure efficient and sustainable synthesis, such as continuous flow chemistry, mechanochemistry, and the use of robotic tools.
Among recent innovations, microdroplet reactions are emerging as a particularly promising approach. Microdroplets provide unique conditions at the solution–air interface, where partial solvation of the reactants reduces the activation energy of the reaction.[2,3] Recent works have demonstrated that several reactions such as epoxy ring-opening,[4] amination of benzylic sp^3 carbon atoms,[5] and aza-Michael additions,[6] could be accelerated by employing electrospray ionization coupled to mass spectrometry.



Building on these pioneering efforts, the next step is to make aerosol technologies more universally accessible for synthetic organic chemistry, both in academia and industry. This means developing and utilizing systems that are readily available, user-friendly, scalable, and ideally, commercially viable. Spray-drying (SD) technologies, consisting on the atomization of a liquid feed with a hot gas stream and its posterior evaporation,[7] fulfil these criteria.
In this work, we investigate and optimize three distinct families of reactions under spray-drying conditions, with the aim of achieving high reaction yields while minimizing solvent use and avoiding time-consuming purification steps.[8] Specifically, we explored Schiff base condensations, Claisen-Schmidt condensations, and amide synthesis. By optimizing experimental conditions, we successfully obtained highly pure products, eliminating the need for additional purification steps. Encouraged by these results, we applied this approach to the synthesis of paracetamol, a widely used analgesic, achieving high yield and purity without the use of auxiliary bases. Furthermore, we successfully scaled up this reaction, demonstrating that spray-drying is a viable method for the continuous and efficient synthesis of organic compounds. We are currently exploring the extension of this methodology to Knoevenagel condensation reactions and anticipate its application to Friedel–Crafts acylations catalyzed by magnetite (Fe_3O_4) nanoparticles.

Bibliography:

1. Nicolaou K. C., *Proc R. Soc. A.*, **2014**, 470, 20130690
2. M. Girod, E. Moyano, D.I. Campbell and R. G. Cooks, *Angew. Chem. Sci.*, **2011**, 2, 501-510.
3. X. Yan, R.M. Bain and R. G. Cooks, *Angew. Chem. Int. Ed.*, **2016**, 55, 12930-12972.
4. Y. H. lai, S. Sathyamoorthi, R.M. Bain and R. N. Zare, *J. Am. Soc. Mass Spectrom.*, **2018**, 29, 1036-1043
5. Y. Meng, E. Gnanamani and R. N. Zare, *J. Am. Chem. Soc.*, **2022**, 144, 19709-19713.
6. J. Gosh, J. Mendoza and R. G. Cooks, *Angew. Chem. Int. Ed.*, **2022**, 61, e202214090.
7. Z. Song, C. Liang, K. Gong, S. Zhao, X. Yua, X. Zhang and J. Xie, *J. Am. Chem. Soc.*, **2023**, 145, 26003-26008.
8. G Pena, J. Albalad, I. Imaz and D. Maspoch, *Chem. Sci.*, **2025**, 16,5770-5775.

Recovering Copper from vineyards: Phytoremediation and Biomass valorization as a circular strategy

C.Cazorla-Ares [a)*]; E.Cardo-Reyes [a)]; J.Leiva [a)]; I.H.Valido[a)]; M.Valiente [a)]; M.Llugany [b)]; M.López-Mesas [a)]

a) GTS Research Group, Department of Chemistry, Faculty of Science, Universitat Autònoma de Barcelona, Cerdanyola del Vallès, 08193 Barcelona, Spain.

b) Plant Physiology Group (BABVE), Faculty of Biosciences, Universitat Autònoma de Barcelona, Cerdanyola del Vallès, 08193 Barcelona, Spain

* camila.cazorla@uab.cat

Viticulture plays a key role in grape and wine production, contributing significantly to the economic sustainability of the wine sector. One of the main threats affecting grapevine cultivation is downy mildew, a disease caused by *Plasmopara viticola* that primarily affects vine leaves. To control this pathogen, copper-based fungicides such as the Bordeaux mixture (copper sulphate and calcium hydroxide) and copper oxychloride have been widely used across Europe. However, the long-term application of these fungicides has led to increasing Cu accumulation in vineyard soils. Although Cu is an essential micronutrient, high concentrations become phytotoxic, inhibiting root growth, disrupting photosynthesis, and reducing plant biomass, among other detrimental effects[1].

To mitigate Cu accumulation while avoiding more aggressive remediation techniques (e.g., excavation or chemical treatments), phytoremediation has been proposed as a sustainable alternative. This approach takes advantage of the ability of certain plants species to tolerate and accumulate Cu in their tissues, thereby progressively reducing soil contamination.

Recent studies have shown that *Plantago lanceolata* can accumulate more than 100 µg/g Cu in leaf tissues, whereas typical concentrations in plants range between 5–20 µg/g. This property, along with the fact that it is a native Mediterranean species frequently found in vineyards, makes *Plantago lanceolata* a promising candidate for phytoremediation[2].

This study was structured into three main parts aimed at evaluating Cu behavior in different contexts, within the framework of a circular economy strategy. First, the phytoremediation potential of *Plantago lanceolata* was assessed under controlled laboratory conditions by exposing plants to different Cu concentrations in both hydroponic nutrient solutions and universal substrate, the latter to simulate more realistic growth conditions as a preliminary step prior to experiments using vineyard soils.

In parallel, a screening study involving 5 weed species commonly present in vineyards from Banyeres de Penedès was conducted to compare Cu accumulation patterns in native plants from ecological and conventional vineyards.

Finally, an incineration method for plant biomass was developed as a strategy for Cu recovery from harvested weeds. BCR and Tessier sequential extractions were conducted to the resulting ashes as an indirect speciation approach to support future Cu recovery and valorization strategies. In all cases, total Cu concentrations were analyzed by Inductively Coupled Plasma Mass Spectrometry (ICP-MS).

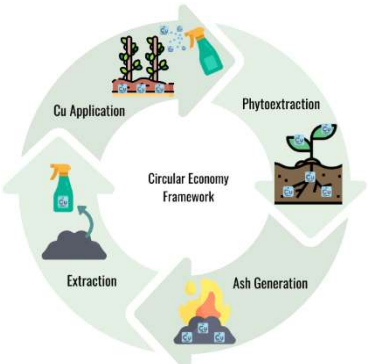


Figure 1. Cu circular strategy

Keywords: Copper, Phytoremediation, plant tissue analysis, circular economy, soil contamination

References:[1] V. Kumar et.al, Copper Bioavailability, Uptake, Toxicity and Tolerance in Plants: A Comprehensive Review, *Chemosphere* 2021, 262, 127810. [2] J. Widmer, L. Norgrove, Identifying Candidates for the Phytoremediation of Copper in Viticultural Soils: A Systematic Review. *Environ. Res.* 2023, 216, 114518. [3] A. Mattiello et.al, Copper Accumulation in Five Weed Species Commonly Found in the Understory Vegetation of Mediterranean Vineyards. Environ. Pollut. 2023, 329, 121675.

Sulfanilic Acid-capped Ruthenium Nanoparticles for Enhanced HER activity in neutral media

M. Kraft[1]*
Supervisors: M. Gil-Sepulcre[2]; J. García-Antón[1]; X. Sala[1]
[1]Department de Química, Universitat Autònoma de Barcelona, Barcelona, [2]Department de Química, Universitat Valencia, Valencia, Spain.
matilda.kraft@uab.cat

Metal-based nanoparticles (NPs) have experienced rising popularity due to their unique properties compared to their corresponding bulk metals or molecular metal complexes. They are now utilized in a broad range of applications, such as electrocatalysis, photo(electro)catalysis, and medicine. The advantage of NPs lies in their high surface-to-volume ratio, due to their small size. As a result, the availability of potential active sites on the surface is increased, which can lead to higher activity in catalytic reactions.[1] In our group, nanoparticles are synthesized via the organometallic approach, which allows for a clean modification of the surface and a narrow size distribution of the particles. The organometallic approach is based on the decomposition of an organometallic precursor with hydrogen under mild conditions in the presence of the ligand of interest and it yields nanoparticles whose surface only contains the chosen ligand plus hydrides, with no contaminants or by-products that could alter the activity.[2] In particular, the hydrogen evolution reaction (HER) requires new materials that can act as catalysts and maintain high activity in neutral media.[3] To work towards this objective, in this contribution we report sulphonate-capped Ru-based NPs where the negatively charged ligand is intended to increase activity by creating a proton-attracting negatively charged environment near the surface. They have been tested at pH 0 and pH 7, outperforming unsulfonated nanoparticles in both media (**Fig. 1**).

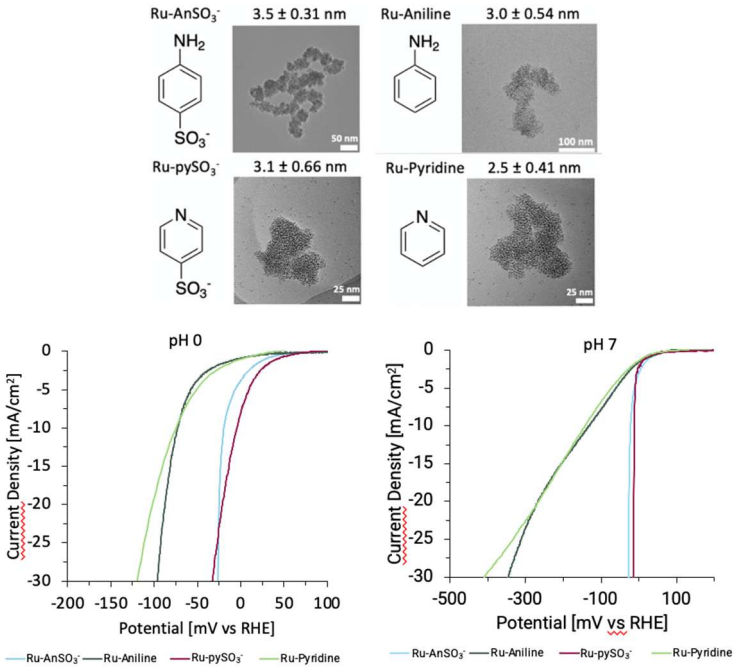


Figure 1. top: Nanoparticles with their corresponding ligand functionalization. Bottom: Electrocatalytic activity in HER in acidic (0.5M H_2SO_4) and neutral (0.1M PBS) pH.

Keywords: Renewable Energy, Electrochemistry, Green Chemistry, Nanoparticles

References

[1] G. Martí, L. Mallón, N. Romero, J. García-Antón, X. Sala, *Adv. Energy Mater.* **2023**, *13*, 2300282.
[2] C. Amiens, B. Chaudret, K. Philippot, *New J. Chem.* **2013**, *37*, 3374-3401.
[3] H. Jin, J. Xu, H. Liu, H. Shen, H. Yu, M. Jaroniec, Y. Zheng, S.-Z. Qiao, *Sci. Adv.* **2023**, *9*, eadi7755.

Chitin - choline bio-sourced composites for CO_2 electrolysis in atmospheric conditions

B. Wu[1,3], C. Coudret[1]*, M. Vedrenne[2], G. Guirado[3]*, J. Fitremann[1]*

[1] Université de Toulouse, CNRS UMR 5623, Laboratoire Softmat, Toulouse, France

[2] Plateforme scientifique et technique Institut de Chimie de Toulouse : Université de Toulouse, CNRS UAR 2599, ICT, Toulouse, France

[3] Departament de Química, Universitat Autònoma de Barcelona, Cerdanyola del Vallès 08193, Spain
Corresponding authors:
juliette.fitremann@cnrs.fr
christophe.coudret1@utoulouse.fr
gonzalo.guirado@uab.cat

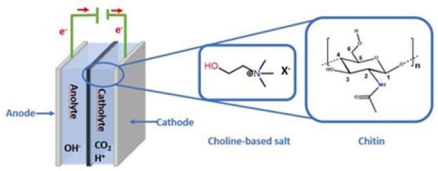
Global warming, driven by increasing CO_2 emissions, requires effective climate mitigation strategies. One promising approach is CO_2 electrolysis, which converts CO_2 into valuable chemicals like carbon monoxide, formic acid, and in the presence of nitrogenous species, into urea, through electrochemical reduction. Current designs for CO_2 electrolyzers can build on advances in water electrolysis, but challenges remain, particularly the competition between CO_2 and water during reduction, as well as electrolyte stability [1]. Our research aims to develop a new electrolyte based on bio-sourced, biodegradable and non-toxic materials to produce urea specifically for agricultural use. This would ensure sustainability and safety in crop science. We propose a bio-based electrolyte using chitin coming from shrimp shells and choline salts for capturing and reducing simultaneously CO_2.

In a first strategy, we evaluated choline salts for both CO_2 capture in atmospheric conditions and electrolyte functions. CO_2's low atmospheric concentration presents challenges, including low reaction efficiency at ambient CO_2 levels and the need for high-sensitivity measurement techniques. CO_2 and bicarbonate concentrations in choline salts and their aqueous solutions was measured using ^{13}C NMR in different conditions. We compared detection sensitivities between natural CO_2 (containing around 1% of ^{13}C CO_2) and CO_2 enriched in ^{13}C at 99%. We also measured the conductivity of choline salts, and we evaluated their long-term behavior focusing on their hygroscopic nature and resistance to crystallization, which is important for electrolyte stability. Then, chitin–choline composites were prepared and analyzed for CO_2 capture and conductivity. In a second strategy, cationic or anionic chitin derivatives were synthesized and investigated as water-soluble polyelectrolytes and gel-state electrolytes. Their gel properties and conductivity have been characterized in different conditions. These modified chitin polymers and composites will be then integrated to a flow electrolyzer as electrolyte for CO_2 conversion to urea.

Acknowledgement

The authors thank the European Union's Horizon Europe programme under the grant agreement no. 101115182 (CONFETI-HORIZON-EIC-2022-PATHFINDERCHALLENGES-01) for financial support.

[1] O'Brien, C. P.; Miao, R. K.; Shayesteh Zeraati, A.; Lee, G.; Sargent, E. H.; Sinton, D. *Chem. Rev.* **2024**, *124* (7), 3648–3693.



Beyond Isostructurality: Controlling Function and Scale in Zr and Hf Carborane MOFs

S. Zhang,[a] J. De Tovar,[a] O. I. Tovar Arredondo,[b] M. Sendra Garcia,[c] L. Francàs,[c] J. Silvestre-Albero,[b] J. G. Planas[a]*

[a]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193, Bellaterra, Spain.

[b]Laboratorio de Materiales Avanzados, Departamento de Química Inorgánica-Instituto Universitario de Materiales, Universidad de Alicante, Ap. 99, E-03080 Alicante, Spain.

[c]Departament de Química, Universitat Autònoma de Barcelona, Campus UAB, 08193 Bellaterra, Spain.

E-mail: jginerplanas@icmab.es

Keywords: Metal–Organic Frameworks (MOFs), Carborane linkers, Zirconium / Hafnium, Electrocatalysis (glycerol oxidation).

Metal–organic frameworks (MOFs) are a pivotal class of crystalline porous materials composed of metal ions or clusters coordinated to organic linkers. Their exceptional chemical and structural tunability, ultrahigh porosity, large surface area, and remarkable stability make them highly versatile platforms for diverse applications,[1] including gas storage and separation, catalysis, drug delivery, magnetism and emerging quantum technologies.[2, 3] However, their long-term stability under practical conditions remains a key challenge.

In this context, the incorporation of hydrophobic carborane-based linkers has emerged as an effective strategy to enhance the hydrolytic stability and functional performance of MOFs.[4-6] Building on this concept, we report two isostructural MOFs based on Zr^{IV} and Hf^{IV} metal–oxo clusters, constructed from meta-carborane-functionalized linkers. These systems provide a well-defined platform to isolate the role of the inorganic node while preserving identical topology, pore architecture, and boron-rich hydrophobic environments. Although Zr and Hf share closely related coordination chemistry, subtle differences in their electronic structure, arising from variations in atomic mass, Lewis acidity, polarizability, and metal–ligand bonding, can lead to distinct physicochemical behavior. In particular, differences in bond strength, hydrolytic robustness, and activation of coordinated species may translate into variations in adsorption properties and catalytic response.

In this contribution, we will present recent results highlighting these differences through a comparative study of gas sorption properties and electrocatalytic performance toward glycerol oxidation. Furthermore, we will discuss the controlled miniaturization of these MOFs to the nanoscale, as an initial step toward their integration in bio-related applications.

References

[1] Christian S. Diercks, Stefan Wuttke. *et al. Angew. Chem. Int. Ed.* **2021**, *60*, 2.

[2] Huang, Z. *et al. Small Sci*. **2024**, 4, 2400161.

[3] Bartolomé, E. *et al. Adv. Appl. Mat. Inter.* **2025**, 17, 29, 42082.

[4] Lei, G. *et al. J Am Chem Soc*, **2023**, *145*, 13730.

[5] Lei, G. *et al. ACS Appl Mater Interfaces*, **2023**, 15, 5309.

[6] Li, Z. *et al. Chemistry of Materials*, **2022**, 34, 4795.

Giant Unilamellar Vesicles (GUVs) for Cell Membrane Mimicry. Towards Artificial Red Blood Cells

C. Cascales-Guerrero[1]; S. Battista[1]; J. Waeterschoot[2]; J. Gan[2]; H. Alizadeh-Zeinabad[2]; X. Casadevall i Solvas[2] and A. González-Campo[1*]

[1]Functional Nanomaterials and Surfaces Group, Instituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC) - Bellaterra, Barcelona (Spain)

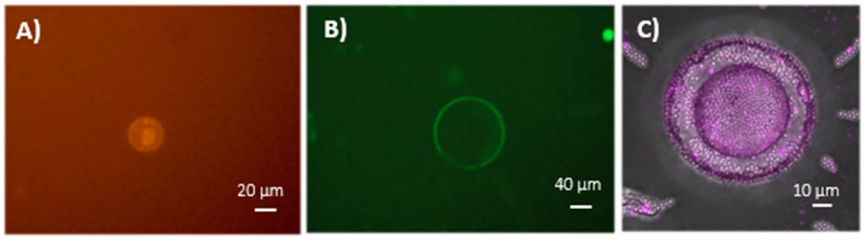
[2]Biomimetics Group, Department of Biosystems, KU Leuven, Willem de Croylaan, 42, 3001 (Belgium)

ccascales@icmab.es

Biological membranes are dynamic systems that regulate essential cellular processes. In this context, giant unilamellar vesicles (GUVs) are widely used as biomimetic models[1,2], including as simplified analogues of erythrocyte membranes for biomedical applications[1,2].

In this work, we develop a nanoparticle-based method for GUVs formation using boronic acid (BA)-functionalized particles, which can establish reversible interactions with carbohydrates[3,4]. Therefore, artificial glicolipids were first employed as simplified systems to investigate BA–carbohydrate interactions and their contribution in GUVs formation. This strategy is then extended to more complex systems using nanoerythrosomes (NERs), which provide a more realistic membrane model due to the presence of glycosylated proteins[5,6]. These models allow the formation of GUVs with features closer to erythrocyte membranes. Finally, membrane organization is modulated through the formation of domains using micro- (MPs) and nanoparticles (NPs), where the MPs/NPs ratio enables control over spatial organization and biomolecular interactions[7].

Overall, this work demonstrates a progressive approach to constructing GUV systems of increasing complexity—from simple artificial lipid membranes to NERs models while enabling control over membrane assembly and domain organization through particle composition and ratio.



Fluorescence microscope images of GUVs formed from: A) Artificial lipids; B) NERs. Confocal image of: C) Droplet showing the organization of SiO_2 MPs and NPs.

Acknowledges: This work was supported by the SynEry project, which has received funding from the Horizon Europe programme under grant agreement No 101046894.

References

[1] Waeterschoot J et al., *Nature Communications*. **2024**, 15, 2504.
[2] Nair, K et al., *Adv. Colloid Interface Sci*. **2023**, 318, 102935.
[3] Waeterschoot et al., *Adv. Sci.* **2023**, 10, 2302461.
[4] Delidovich I et al., *Green Chem*. **2024**, 26, 720–738.
[5] Hsu K et al., *Frontiers in Physiology*. **2018**, 9, 733.
[6] Burzyńska P et al., *Biomolecules*. **2022**, 12(11), 1669.
[7] Schroën K et al., *Advances in Colloid and Interface Science*. **2024**, 334, 103321.

Keywords: Giant unilamellar vesicles (GUVs), Boronic acids (BA), Nanoerythrosomes (NERs), Biomimetic models and Functionalized particles

Development of 3D-printed sensing platforms applied to pH and hydrogen monitoring

M. Pan*; F. Paré; M. Baeza
* Corresponding author
GENOCOV Research Group, Department of Chemistry, Faculty of Science, Edifici C- Nord, Universitat Autònoma de Barcelona, Carrer dels Til·lers, 08193 Bellaterra, Barcelona, Spain
E-mail of corresponding author: Mingyue.Pan@uab.cat

In numerous chemical, biological and environmental processes, it is crucial to have an accurate real-time monitoring of key parameters. The conventional sensors are facing multiple limitations when taken out of the laboratory and applied to real reactors, boosting the growth of the interest in customized sensors. For this purpose, 3D printing, also known as additive manufacturing, stands out due to its ability turn computer-aided designs into 3-dimensional objects. In this study, two types of 3D-printed sensing platforms have been developed to monitor two distinct reactors.

The first investigated reactor is an ammonia recovery biochemical reactor, where changes in pH indicate the recovery efficiency, while the reactor shape restricts the use of conventional pH sensors. To address this issue, a customized 3D-printed sensing platform (Figure 1A), consisting of five working electrodes (WEs) of varying lengths and two Ag/AgCl reference electrodes (REs), was integrated into the reactor. In the individual sensor tests, the IrOx modified WEs showed a super-Nernstian response around -77.0 mV/pH in a pH measurement range of 2-12. Small sensitivity variations resulting from differences in the electrode length were observed, ensuring reliable pH monitoring at different depths of the reactor. Furthermore, the WEs also exhibited excellent repeatability across repeated measurements and good long-term stability. In the real-time reactor monitoring, the sensing platform remained operatable for 28 days, immersed in the recovery solution (Figure 1B). During the monitoring period, the platform was able to detect pH changes during the ammonia recovery process, despite the observed signal variability.

Beyond pH monitoring, 3D-printing has also been used for the fabrication of hydrogen sensors designed for a sulfide production reactor, which is based on hydrogenotrophic bacteria. In this approach, Nafion, a proton-exchange polymer membrane, was drop-casted on the 3D-printed sensors to facilitate the sensing mechanism. To achieve a well-adhered Nafion membrane with an optimal thickness, various sensor designs have been evaluated during the initial phase of the study.

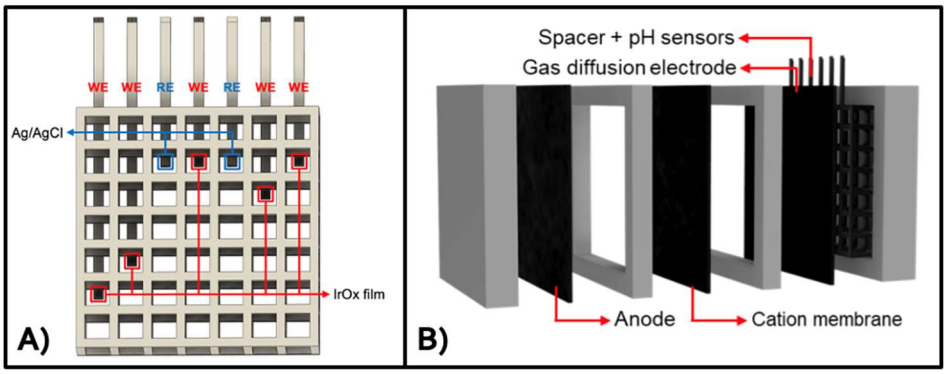


Figure 1. A) Schematic illustration of the 3D-printed integrated sensing platform for pH monitoring (WE: working electrode; RE: reference electrode). B) Scheme of the ammonia-recovery biochemical reactor with the 3D-printed sensing platform integrated.

Keywords: Environmental monitoring; 3D printing; pH sensor; Hydrogen monitoring

Selective recovery of heavy metals from wine sludge using oxidizing agents: towards sustainable waste management in viticulture

M. González Quintela*, I. H.Valido, M. Valiente and M. López-Mesas
GTS-UAB Research Group, Department of Chemistry, Faculty of Science, Universitat Autónoma de Barcelona, Bellaterra, (Cerdanyola del Vallés), 08193 Barcelona, Spain.
Monica.Gonzalez.Quintela@uab.cat

Vine mildew is one of the main fungal diseases affecting viticulture, causing significant economic losses. In this context, the European Union, as the world's leading wine producer, faces a growing challenge in the sustainable management of vineyards. Traditionally, the control of fungal infections has been based on the intensive application of phytosanitary compounds based on copper (Cu) which has generated a progressive accumulation of these metals in agricultural soils, vegetation and wine residues, representing a serious environmental and agro-industrial problem [1].
On the other hand, one of the most relevant current challenges in sustainable agriculture is the utilization of byproducts generated during winemaking, especially winery sludge. These residues are rich in organic matter and nutrients, making them potentially valuable for use as organic amendments in agricultural soils [2]. However, their heavy metal content, particularly copper, makes direct application in the field difficult. To mitigate this impact and close the resource cycle, the selective extraction of these metals is proposed to recover copper as a fungicide and reintroduce the sludge as fertilizer, transforming it back into a useful resource for other processes or applications, rather than allowing it to pollute the environment
Here, we report a sequential extraction approach for the selective recovery of Cu from vineyard sludge. Conventional acid leaching achieved high extraction efficiencies but lacked selectivity. Sequential extraction analysis BCR [3] revealed distinct metal partitioning, guiding the use of ligand-specific organic acids. Zn, Mn, Fe and Cu, were extracted differentially between oxalic acid and citric acid, allowing a selective extraction of Cu. In this sense, a two-step.
In this sense, a two-step process was developed combining an initial citric acid extraction followed by oxalic acid treatment. Optimization through Design of Experiments (DoE) and kinetic studies demonstrated that efficient and selective metal separation can be achieved under mild conditions within short extraction times (1h).
This strategy overcomes intrinsic selectivity limitations in multi-metal systems and provides a sustainable pathway for the valorization of winery sludge, enabling Cu recovery and supporting circular economy approaches in the viticultural sector.

Keywords: copper, recovery, sludge, extraction

References:
[1] R. Vázquez, J. C. Nóvoa, M. Arias, D. Fernández, P. Pérez, *Elsevier Agriculture, Ecosystems & Environment*, **2022**, 339 (108146), 1-9.
[2] G. D. Gabur, C. Teodosiu, D. Fighir, V. V. Cotea, I. Gabur, *Agriculture* **2024**, 14(9), 1-20.
[3] K. Nemati, N. K. A. Bakar, M. R. Abas, E. Sobhanzadeh, Elsevier Journal of Hazardous Materials, 2011, 192 (1), 402-410.

Plant nano-biofortification mediated by controlled selenium release in soil systems to produce functional foods

A. Fuentes García*, M. J. Sánchez Martín

GTS-UAB Research Group, Department of Chemistry, Faculty of Science, Universitat Autónoma de Barcelona, Bellaterra, (Cerdanyola del Vallés), 08193 Barcelona, Spain.
Alejandro.Fuentes@uab.cat

Selenium (Se) deficiency is a global nutritional concern due to its biological importance in the human body. More than 25 selenoproteins participate in key physiological processes, including hormonal regulation, immune response, fertility, and antioxidant defense mechanisms [1,2]. The World Health Organization states that intake below 55 µg Se/day in adults impairs their functionality, while levels above 400 µg Se/day may be toxic. Despite its essential role, nearly one billion people have insufficient Se intake, mainly due to low soil concentrations, limited bioavailability, and depletion from intensive agriculture [1,3].

Agricultural biofortification has emerged as a promising strategy to sustainably increase Se in the human diet. Soil-based controlled-release systems are particularly effective due to efficient root uptake of inorganic Se and its conversion into bioactive plant compounds. Nanostructured systems that modulate micronutrient release therefore offer an innovative approach to improve Se stability, availability, and agronomic efficiency while reducing environmental impact [3].

In this work, chitosan-coated liposomal nanocapsules were developed for controlled Se release in agricultural soils. Synthesis was performed via lipid film hydration followed by electrostatic polymer coating, generating stable core–shell nanostructures with improved encapsulation. A Design of Experiments (DoE) approach was used to optimize preparation conditions and particle size, systematically assessing formulation and process variables.

The resulting formulations were characterized by hydrodynamic size, polydispersity index, zeta potential, morphology, and encapsulation efficiency, confirming nanoscale formation with good colloidal stability and reproducibility. Finally, the nanocapsules were applied to soil to evaluate Se release behavior and interactions with the soil matrix. Results showed enhanced stability and a gradual, sustained release profile, improving Se availability and reducing losses by leaching or immobilization. These findings support the potential of nanostructured systems as effective tools for sustainable agricultural biofortification and improved micronutrient delivery.

Keywords: Selenium, biofortification, nanocapsules, controlled-release systems

References

[1] Bai, S., Zhang, M., Tang, S., et al. (2025). *Effects and Impact of Selenium on Human Health: A Review*. Molecules, 30(1), 50. https://doi.org/10.3390/molecules30010050

[2] Sadler, R. A., Mallard, B. A., Shandilya, U. K., et al. (2024). *The Immunomodulatory Effects of Selenium: A Journey from the Environment to the Human Immune System*. Nutrients, 16(19), 3324. https://doi.org/10.3390/nu16193324

[3] Xu, Z. N., Lin, Z. Q., Zhao, G. S., & Guo, Y. B. (2024). *Biogeochemical behavior of selenium in soil-air-water environment and its effects on human health*. International Journal of Environmental Science and Technology, 21, 1159–1180. https://doi.org/10.1007/s13762-023-05169-0

Molecular electrocatalysts for RedOx reactions: water oxidation and CO_2 reduction using carbanionic ruthenium complexes and heterogenized cobalt complexes

J. T. Kerkhof[1,2], L. De Biasi[3], A. Tessier[3], X. Sala[2], A. Llobet[1,*]
[1]Institut Català d'Investigació Química, Av. Països Catalans 16, 43007 Tarragona, Spain
[2]Universitat Autònoma de Barcelona, Campus de la UAB, 08193 Bellaterra (Cerdanyola del Vallès), Barcelona, Spain
[3]Nantes Université, Chem. de la Censive du Tertre, 44300 Nantes, France
allobet@iciq.cat

The storage of energy in chemical bonds is a promising way of harnessing intermittent energy sources such as sunlight and furthermore allows energy to be more efficiently transported.[1] Improving the performance and viability of these technologies requires the mastery of different types of RedOx reactions and their catalysis. In this work we have investigated the RedOx reactions of water oxidation and CO_2 reduction using molecular electrocatalysts through the tuning of their ligand scaffold and their immobilization onto electrode surfaces.

To improve the catalyzed water oxidation reaction, we have introduced a carbon-metal bond into a ruthenium complex. The strong σ-donating nature of the carbon donor was expected to stabilize high oxidation states at the metal center and reduce the oxidation potential of the catalyst, thus reducing the onset potential of water oxidation. While the synthesized complex did not produce results exactly as hypothesized, mechanistic insights and structure–activity relationships were identified that may guide the future development of improved catalytic systems.

Homogeneous molecular cobalt catalysts have been cited in the literature to have high activity and selectivity for the electrochemical conversion of CO_2 into CO. These catalysts have been modified such that they can be covalently attached onto graphitic electrode surfaces. By immobilizing this molecular catalyst onto an electrode surface, turnover number can be improved and in addition, the catalyst can be confined to a specific environment using polymeric compounds and tuned to convert CO_2 into higher value compounds.

The synthesis, electrochemical characterization, and catalytic performance of these systems will be discussed.

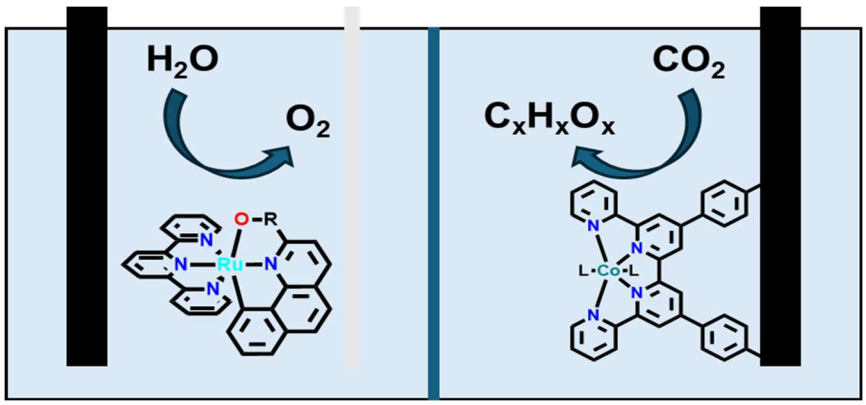


Figure 1. Artistic representation of the catalytic systems in study.

Keywords: catalysis, water oxidation, CO_2 reduction, molecular catalysts, carbanions

(1) Berardi, S.; Drouet, S.; Francàs, L.; Gimbert-Suriñach, C.; Guttentag, M.; Richmond, C.; Stoll, T.; Llobet, A. *Chem. Soc. Rev.*, **2014,** *43*, 7501-7519.

Developing computational tools to explore reaction pathways for periodic systems

A. Gelli[1,2] *; S. Casassa[2]; A. Rimola[1]
* Corresponding author
[1]Department de Química, Universitat Autònoma de Barcelona, 08193 Catalonia, Spain
[2]Dipartimento di Chimica, University of Torino, 10125 Torino, Italy
andreha.gelli@uab.cat

The identification of transition states and the calculation of energy barriers are central problems in theoretical chemistry, particularly for the description of reactive, diffusive, and adsorption processes in molecular and condensed-phase systems. Among Transition State Search methods, the Nudged Elastic Band (NEB) approach allows the determination of the Minimum Energy Path (MEP) between initial and final states through the optimization of a set of intermediate configurations (images), relying only on first derivatives of the energy. This makes it particularly suitable for integration with accurate electronic structure methods.

In this work, a complete implementation of the NEB method has been developed within the periodic electronic structure CRYSTAL code, taking the advantage of its high accuracy in the description of forces due to the use of Gaussian basis sets and hybrid functionals. In addition to the standard formulation, several advanced variants have been implemented, including Climbing Image NEB (CI-NEB), Variable Spring Constant NEB (VARK-NEB), as well as dynamic approaches such as Dynamic and Scaled optimization NEB. The generation of the initial path was improved through the implementation of Image Dependent Pair Potential (IDPP) and IDPP-NEB methods.

The implementation has been also extended by introducing multithread parallelization and variable cell approaches such as the Generalized Solid-State NEB (GSSNEB), which explicitly includes cell degrees of freedom via the stress tensor, enabling the study of structural transformations in solids. These developments significantly broaden the applicability of the method, allowing the investigation of not only reactive processes but also cooperative phenomena and phase transitions.

To address the challenge of describing phase transitions, a protocol was developed to extrapolate realistic transition temperatures and pressures from 0 K calculations by combining Equation of State analysis with vibrational properties at finite temperature. Its effectiveness was demonstrated for the molecular-to-covalent transition in solid nitrogen, with results in good agreement with experimental data.

While complementary to these approaches, ab initio molecular dynamics is often limited by its high computational cost. In this context, the use of Grassmann extrapolation has been explored as a possible strategy to accelerate the electronic dynamics; however, the results show that this approach is not effective within the CRYSTAL framework. This outcome motivated the exploration of alternative strategies to reduce computational cost. In particular, current efforts are focused on the development of Machine Learning Interatomic Potentials, with the aim of achieving an accuracy comparable to quantum mechanical methods while significantly reducing computational time. The integration of active learning and enhanced sampling techniques enables the study of complex dynamical processes in condensed-phase systems, allowing for realistic applications.

Keywords: Computational Chemistry / Reaction Mechanisms / Energy Barriers / Molecular Dynamics

Rice Husk Ash-Derived Zeolite X Supported Mn-ZIF-67 for Visible-Light-Assisted PMS Activation: From Agro-Industrial Waste Valorisation to Organic Pollutant Remediation

Hanwen Luan[1] and Roberto Boada[1,*]
GTS-UAB Research Group, Department of Chemistry, Faculty of Science, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Spain
Corresponding author: roberto.boada@uab.cat

Our project seeks to valorise agro-industrial residues by converting rice husk ash, an abundant silica-rich by-product, into zeolite-based composite materials for environmental remediation. In this work, rice husk ashes obtained from different combustion routes and geographic origins were employed as alternative silicon sources for the synthesis of Zeolite X, thereby linking waste-derived silica extraction with the construction of functional porous supports. The resulting FAU-type zeolite offers a high-surface-area, ion-exchangeable and chemically robust framework, which can favour pollutant preconcentration, improve the dispersion of active phases and alleviate the aggregation commonly observed in powder metal-organic frameworks [1]. On this basis, Mn-modified ZIF-67 was integrated with rice husk ash-derived Zeolite X to construct Mn-ZIF-67@Zeolite X composites for visible-light-assisted peroxymonosulfate activation and organic dye degradation.

Structural and physicochemical characterisation confirmed the successful formation of the hybrid composite while preserving the main features of the zeolite support. X-ray diffraction revealed the coexistence of FAU-type Zeolite X and ZIF-67-related crystalline domains, indicating that the zeolite framework remained largely intact after MOF growth. Electron microscopy further showed that the Zeolite X support promoted a more dispersed ZIF-derived morphology, limiting particle aggregation and exposing accessible interfacial regions. Nitrogen sorption analysis demonstrated that the composite retained substantial porosity, although partial micropore filling and interfacial blocking occurred after the introduction of the MOF phase [2]. The Mn-ZIF-67@Zeolite X composite displayed rapid methylene blue degradation under visible light in the presence of PMS, clearly outperforming single-component and control systems. This enhanced activity arises from the synergistic interaction between the waste-derived zeolite support and the Mn-modified ZIF-67 phase. Zeolite X contributes to pollutant enrichment, structural stabilisation and active-phase dispersion, whereas Mn incorporation modulates the local electronic environment of Co-based sites and facilitates reactive oxygen species generation [3]. Radical quenching experiments and electron paramagnetic resonance analysis suggest that sulfate radicals and singlet oxygen dominate the oxidation process, while hydroxyl radicals and superoxide species participate as secondary pathways. Although the degradation efficiency decreased in complex water matrices due to the presence of competing ions and natural organic matter, the composite still maintained considerable catalytic performance, indicating its potential for practical water treatment applications.

Overall, this study connects the upstream valorisation of rice husk ash with a downstream catalytic application in advanced oxidation processes. By transforming agricultural waste into a functional zeolite support for MOF-derived catalytic phases, the work demonstrates a sustainable route from biomass-derived silica to high-value environmental remediation materials. The proposed strategy provides both resource-recovery significance and catalytic functionality, highlighting the potential of waste-derived zeolite-supported MOF composites for water pollutant treatment.

Keywords: Rice husk ash; Zeolite X; Mn-ZIF-67; Peroxymonosulfate; Dye degradation

References

[1] R. Wu, B. Hong, et al. Environmental Science and Technology. 2024, 58, 9612-9623

[2] D. Chen, Q. Bai, et al. Chemical Engineering Journal. 2022, 435, 1385-8947

[3] L. Xing, J. Liu, et al. Applied Catalysis B: Environmental. 2020, 275, 0926-3373

Reversible colorless-to-colored thermochromic materials based on modified spiropyrans

*Noel Muñoz Pérez, Diptiman Dinda, Daniel Ruiz-Molina, *and Claudio Roscini**
E-mail: noel.munoz@icn2.cat

Abstract:

Photo- and thermochromic materials with tunable absorption over the visible and near-infrared regions are essential for cutting-edge applications, including solar light-energy management, optical sensors, smart windows and rewritable devices. In these applications, both photochromic and thermochromic colorless-to-colored transitions are particularly valuable, as they provide important functionalities (such as solar light filtration during high irradiance or temperature) and much higher contrast than other transitions (e.g. color[1]-to-color[2] or colored-to-colorless). However, while current photochromic materials already offer fast and high-contrast colorless-to-colored transitions, achieving the same in thermochromic materials is still a challenge.

Recently our group reported novel strategies to accomplish colorless-to-colored transitions, based on three-component mixtures (color developer (CD), phase change material (PCM) and organic dyes) [1,2] . The possibility of using different dye families (lactams, lactons, fluorans, ketocyanines) allowed for a highly tunable hot state color palette. In this respect, spiropyrans, are very interesting dyes which, besides exhibiting inherent multicolored photochromism due to the medium-dependent coloration of the photogenerated merocyanines, can be potentially exploited for colorless-to-colored thermochromism, though previous attempts carried out by our group revealed lack of reversibility.

To overcome these limitations, we designed and synthesized new spiropyrans bearing a long alkyl chains attached in the indole *N*-position. The steric hindrance provided by the alkyl chain prevents molecular aggregation in the dye open form ensuring full reversibility. Furthermore, the implementation of the modified spiropyrans into the 3-component mixtures exhibited sharp colorless-to-colored tunable transitions where the type of the PCM (paraffin, alcohol/ester, acid) dictates the hot liquid state color, spanning from reddish tones, to purple or orange-like. Finally, both photochromic and thermochromic behaviors were preserved upon miniaturization into micro- and nanoparticle sized suspensions, which could be used as inks or coating for future applications.

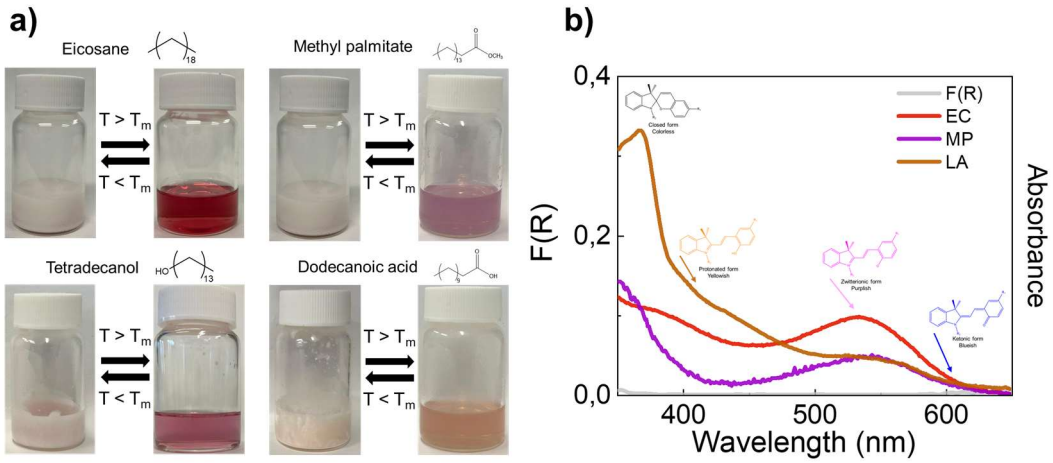


Figure 1: a) Solid-liquid transition images of the modified spiropyran and color developer combined with different PCMs (eicosane (20 C), methyl palmitate (16 C), tetradecanol (14 C) and dodecanoic acid (12 C). b) solid F(R) and liquid absorbance measurements

(1) Dinda, D.; **Pérez, N. M.**; Faraudo, J.; Ruiz-Molina, D.; Roscini, C. High-Contrast Colorless-to-Colored Thermochromic Materials. *Small* **2025**, *21* (51), e11454. https://doi.org/10.1002/smll.202511454.

(2) López, A. J.; **Pérez, N. M.**; Magerramov, R.; Puyol, M.; Crugeira, F.; Miltsov, S.; Ruiz-Molina, D.; Roscini, C. Ketocyanine-Based Materials for Near Infrared-to-Visible Thermochromism. *Adv. Opt. Mater.* **2025**, *13* (9), 2401411. https://doi.org/10.1002/adom.202401411.

Keywords: Photochromsim, Thermochromism, Spiropyran, Emulsion.

TT-$CF_3^+OTf^-$: a bench-stable trifluoromethylation reagent with formal CF_3^+, and $CF_3^\bullet$ reactivity

Xiangyu Tan, Roser, Pleixats, Carolina Gimbert-Suriñach, Adelina Vallribera*, and Albert Granados*
Departament de Química y Centro de Innovación y Química Avanzada (ORFEO-CINQA), Universitat Autònoma de Barcelona, Cerdanyola del Vallès, 08193, Spain
xiangyu.tan@uab.cat

Thianthrenium (TT) salts have emerged as versatile reagents with utility across transition-metal (TM) catalysis, photochemistry, biocatalysis, electrochemistry, and polar transformations.[1] Fluorinated molecules, particularly those containing trifluoromethyl (-CF_3) groups, are highly valuable in medicinal chemistry, agrochemicals, and materials science due to their enhanced metabolic stability, lipophilicity, and bioavailability.[2-3] Our strategies provide access to fluorinated scaffolds with high structural diversity, offering new opportunities in drug discovery and functional material design.

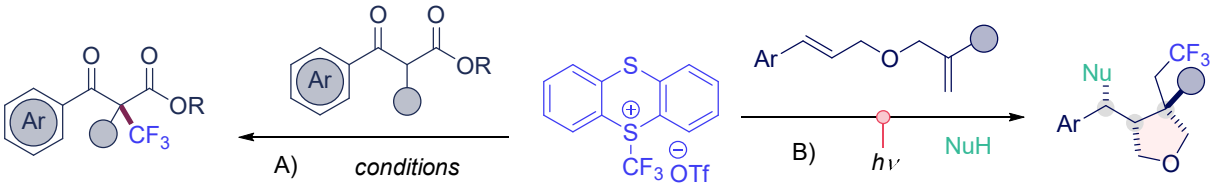


Figure A) Synthesis of acyclic quaternary α-CF_3-β-oxo carbonyls via nucleophilic substitution induced by single-electron transfer. B) Visible-light-induced diastereoselective synthesis of fluorinated tetrahydrofurans.

The development of efficient methods for the formation of quaternary centers in organic compounds has been a constant challenge in synthetic chemistry. Quaternary *β*-oxo esters are fundamental structures in the synthesis of natural products, pharmaceutical compounds, and other bioactive molecules. A direct and versatile approach to quaternary acyclic *β*-oxo esters was reported using trifluoromethyl thianthrenium salt as highly reactive and selective reagent under mild conditions (**Figure** A). Mechanistic investigations supported the operation via single-electron transfer induced nucleophilic substitution. [4] In addition, the stereocontrolled construction of molecules bearing three contiguous stereocenters is a formidable challenge in synthetic organic chemistry.[5-7] We have developed a visible-light-driven, three-component radical cascade that enables the efficient and regioselective formation of fluorinated frameworks containing three consecutive stereocenters (**Figure** B). Using trifluoromethyl thianthrenium triflate as a dual-function reagent, the reaction proceeds via in situ generation of $CF_3^\bullet$·and thianthrene radical cation species under photochemical control. The CF_3 radical selectively engages addition to 1,6-dienes to initiate a cascade cyclization/trapping/nucleophilic substitution sequence, forming highly functionalized tetrahydrofuran derivatives in up to 87% yield. This operationally simple protocol exhibits broad nucleophile and substrate scope, including primary, secondary, and tertiary alcohols, as well as water, azide and acetamide sources. Single-crystal X-ray diffraction and NMR analyses confirmed the structures and relative configurations of the products. The observed diastereomeric ratios are attributed to the occurrence of hydrogen bonding interactions as suggested by Density Functional Theory (DFT) calculations.

Keywords: acyclic *β*-dicarbonyls; trifluoromethylation; thianthrenium salts; tetrahydrofurans; electron transfer mechanism

Bibliography: [1] *Acc. Chem. Res.* **2026**, *59*, 915−931. [2] *J. Chem. Inf. Model.* **2020**, *60*, 6242–6250. [3] *J. Med. Chem.* **2018**, *61*, 10602–10618. [4] *J. Org. Chem.* **2025**, *90*, 15956−15964. [5] *Nat. Commun.* **2020**, *11*, 792. [6] *Chem. Commun.* **2023**, *59*, 8424–8427. [7] *Molecules* **2024**, *29*, 3677.

Portable electrochemical biosensing platform for point-of-need diagnostics.

J.C. Porras[1,2], J. Ferrer-Dalmau[1] *, M.I. Pividori[1,2,3].*
* Isabel.Pividori@uab.cat / Jofre.ferrerdalmau@bioeclosion.com
[1]BioEclosion S.L., Parc de Recerca, Universitat Autònoma de Barcelona, Bellaterra, Spain.
[2]Grup de Sensors i Biosensors, Departament de Química, Universitat Autònoma de Barcelona, Bellaterra, Spain.
[3]Biosensing and Bioanalysis Group, Institute of Biotechnology and Biomedicine, Universitat Autònoma de Barcelona, Bellaterra, Spain.

Development of rapid, portable, and reliable in vitro diagnosis (IVD) devices is essential to improve early detection of diseases and enable decentralized analysis in clinical, environmental, and veterinary settings. However, conventional diagnostic methods frequently require centralized laboratory infrastructure, trained personnel, and multi-step workflows that limit their implementation in point-of-care settings.

To address these limitations, this work presents a hand-held modular IVD platform based on immunomagnetic separation coupled to electrochemical biosensing designed to provide rapid, sensitive, and quantitative detection in a portable format. The system integrates two main components (Figure 1): A) a disposable cartridge, including a sample holder containing reagents (functionalized magnetic particles and labelled antibody which binds specifically to the analyte), and the cartridge containing the electrode where the magnetic actuation is performed, while excess of sample and reagents are removed. B) A portable digital reader, which allows the electrochemical readout in less than a minute. The output of the device is a quantitative response if needed.

A critical aspect for the implementation of this technology is the optimization of sample preparation workflows and reagent stabilization strategies to ensure analytical robustness and compatibility with decentralized use. Indeed, different sampling approaches are being evaluated according to sample matrix and target application to optimize analytical performance while ensuring compatibility with real-world workflows. In parallel, reagent storage strategies for horseradish peroxidase based detection systems including ready-to-use formulations and lyophilized formats, are being evaluated to improve shelf-life and facilitate deployment outside laboratory environments.

The versatility of the platform has been demonstrated in distinct proof-of-concept applications (Figure 1), including the detection of celiac disease through antibodies against deamidated gliadin peptides, and the detection of *Escherichia coli* for water quality control. Overall, this work contributes to the development of a scalable biosensing platform for rapid, portable, and versatile diagnostics, bridging laboratory analytical performance with decentralized implementation and aligning with the One Health framework.

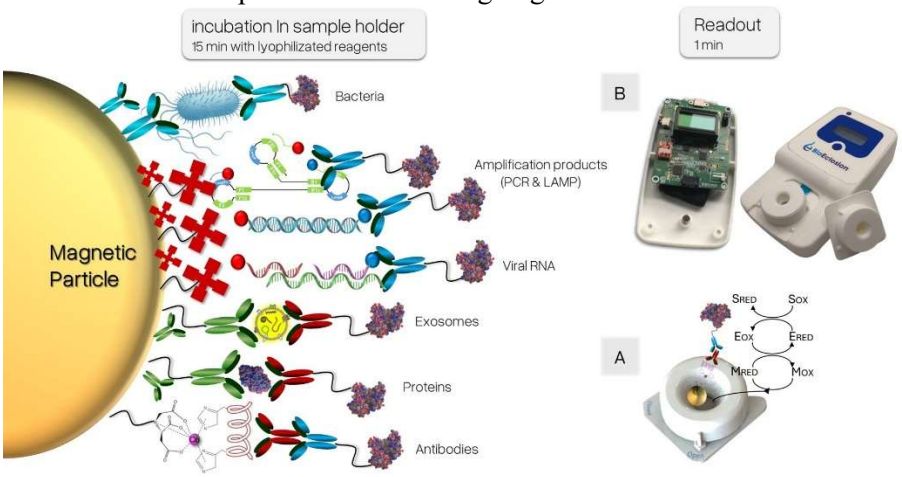


Figure 2. *Schematic representation of the immunomagnetic assay for different proof-of-concept applications integrated into the modular IVD platform. Target analytes are selectively captured from the sample using magnetic particles, followed by binding labelled antibodies to form a sandwich complex. After incubation, the magnetic complexes are transferred to the disposable cartridge (A), where magnetic actuation enables separation and concentration of the target while excess reagents are removed. The signal is generated through an enzymatic reaction and detected by electrochemical readout using a portable digital reader (B), providing quantitative response.*

Keywords: Immunomagnetic separation, point-of-care diagnostics, rapid diagnostic tests, electrochemical iosensing, decentralized diagnostics.

How Multi Component Reactions simplify the synthesis of Organic Radical Dendrimers as potential MRI contrast agents?

E. Shirdel[1], X. Wang[1], D. Abdulin[2], O. Schiemann[2], J. Vidal Gancedo[1], V. Lloveras[1]*

[1] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Spain

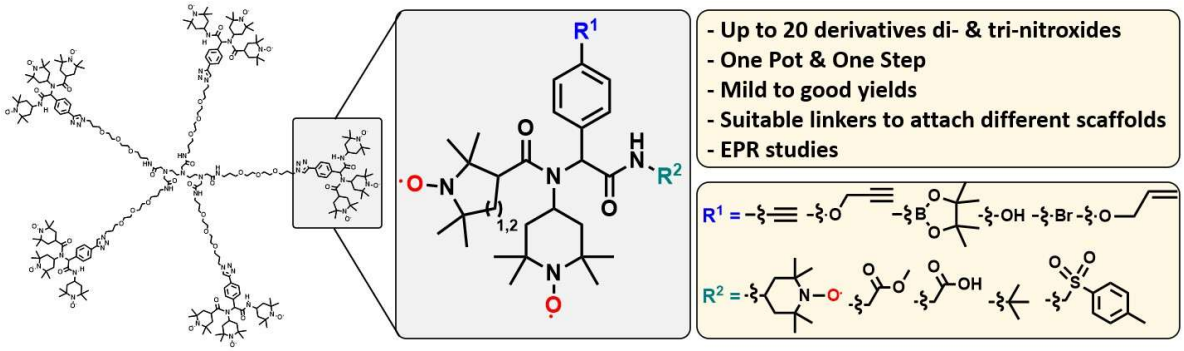
[2] Clausius-Institute of Physical and Theoretical Chemistry, University of Bonn, Germany

eshirdel@icmab.es

Although application of commercial Gadolinium (Gd^{3+})-based contrast agents (CAs) are indispensable in magnetic resonance imaging (MRI) for improving image contrast and its resolution, recent reports caution against their use either due to the severe side effects or Gd^{3+} ions accumulations in vital organs such as the brain [1]. As a safer alternative, organic nitroxyl radicals have been studied due to the magnetic property stem from unpaired electrons. However, nitroxyl radicals suffer from weak contrast property in MRI application and rapid bioreduction. To improve their performance as CAs, dendrimers-monodisperse macromolecules including significant number of branches-were applied to carry individual nitroxyl radicals [2]. Nevertheless, the stepwise synthesis and tedious purification process of such macromolecules remained as challenges.

Herein, we present a strategy to circumvent the synthesis of larger (i.e., higher generation) dendrimers by attaching di- and trinitroxyl radicals to lower generation of dendrimers as opposed to the up-to-date method of anchoring one nitroxyl radical per each branch in the higher-generation dendrimers. To achieve that, Multi Component Reactions (MCRs), in particular Ugi reaction [3], were exploited to synthesize up to 20 derivatives of dinitroxides and trinitroxides, including appropriate functional groups as linkers and water-soluble tag, in one pot and one step (Scheme1). Ultimately, we demonstrate the feasible attachment of a trinitroxide per each branch of a dendrimer through click reaction.

The intrinsic magnetic properties of such spin-active systems were studied by using electron paramagnetic resonance (EPR) spectroscopy. This technique was applied both to characterize the all 20 derivatives and to study electron-electron spin interactions. So, continuous wave (CW) X-band measurements were conducted at different temperature to extract isotropic parameters. Q-band pulsed measurements were conducted at low temperature to quantify relaxation times (T_1, T_m) and spin state distributions. Furthermore, The EPR results revealed that diradicals and triradicals mainly exhibit strong exchange coupling between the two closer radicals.



Scheme 1: General structure of nitroxyl-radical adducts including different functional groups

Keywords: Nitroxide, Dendrimers, MRI, Ugi, EPR

[1] L. Blomqvist et al., *Biomolecules* **2022,** 12, 742.

[2] S. Zhang et al., *Biomacromolecules* **2022,** *23*, 2767-2777.

[3] I. Ugi et al., *Angewandte Chemie* **1959,** *71*, 373-388.

Toward Cu Remediation of Vineyard Soils: A Sulfonated Amide COF and COF-Based Membrane Approach

Di Cai[1*], Heber E. Andrada[1,2], María-Jesús Sánchez-Martín[1]

[1]GTS Research Group, Department of Chemistry, Faculty of Science, Universitat Autnòma de Barcelona, 08193 Bellaterra, Spain

[2]Universidade de Franca, Av. Dr. Armando Salles Oliveira 201, Franca, SP, 14404-600, Brazil

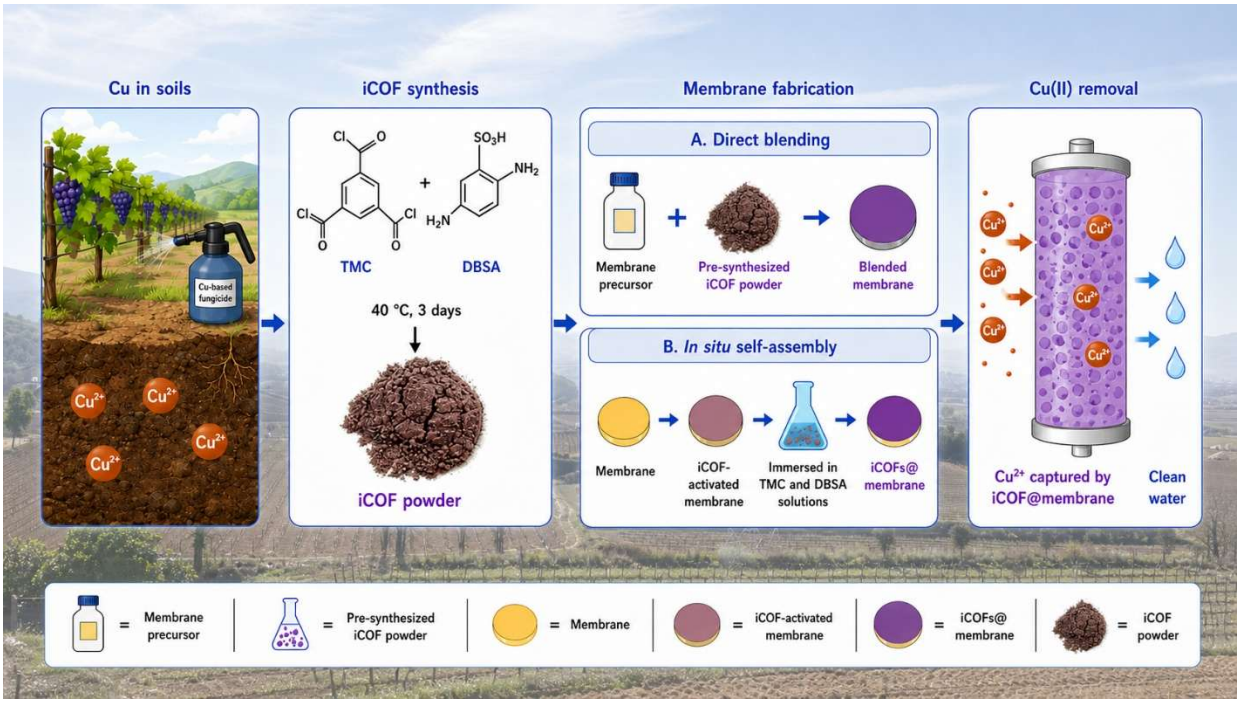
E-mail: Di.Cai@uab.cat

The extensive use of copper-based fungicides in agriculture has resulted in copper accumulation in soils, raising concerns regarding soil sustainability and potential risks to the food chain. Ionic covalent organic frameworks (iCOFs) have attracted increasing attention as adsorbent materials due to their high chemical stability, tunable structures, and ionic functionality. In this work, a sulfonic acid-functionalized amide-based iCOF was synthesized under low-temperature solvothermal conditions.

To overcome the processing limitations associated with the powdered material, a Jeffamine®-epoxy interlocked membrane was fabricated through an epoxide ring-opening reaction and employed as a support platform for iCOF immobilization. Two different strategies were explored to integrate the iCOF with the membrane: (i) direct blending of the pre-synthesized iCOF into the membrane matrix, and (ii) *in situ* self-assembly of the iCOF on the membrane surface.

The resulting materials were characterized and their Cu(II) adsorption performance was evaluated under different experimental conditions through adsorption isotherm and kinetic studies. The results suggest that membrane-supported iCOF systems provide a feasible approach for Cu(II) capture, while highlighting the important role of the immobilization route, membrane structure, and interfacial assembly on the overall removal efficiency.

This work provides preliminary insights into the development of supported iCOF-based materials for copper remediation in agricultural environments.



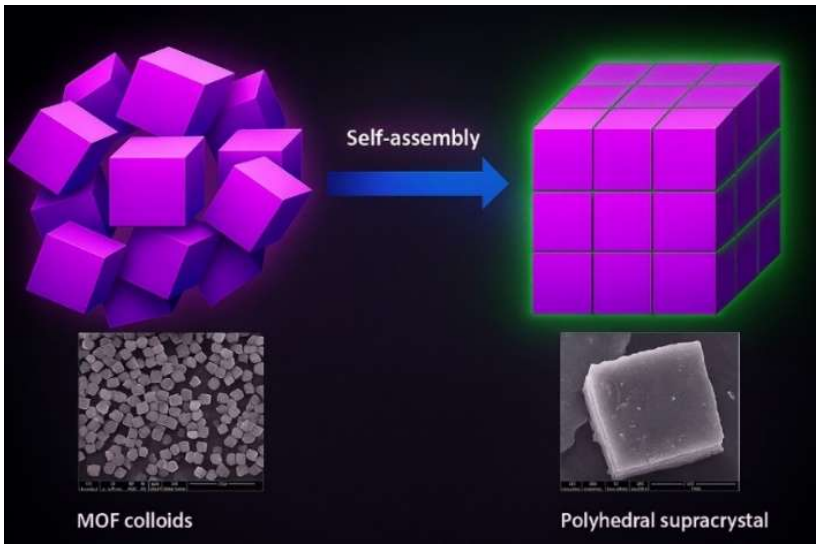
Keywords: ionic covalent organic frameworks; composite membrane; direct blending; in situ self-assembly; Cu(II) adsorption.

Making Mesocrystals with Colloidal MOF Particles

Amir Mohammad Ghadiri[1,2], Sahel Fajal[1,2], Lingxin Meng[1], Inhar Imaz[1,2*], Daniel Maspoch[1,2,3*]

[1] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC, and Barcelona Institute of Science and Technology, 08193 Bellaterra, Barcelona, Spain
[2] Departament de Química, Facultat de Ciències, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain.
[3]ICREA, Barcelona
*Corresponding authors. E-mails: inhar.imaz@icn2.cat and daniel.maspoch@icn2.cat

The self-assembly of colloidal particles into ordered superstructures enables the creation of advanced materials with applications in photonics, sensing and electronics. Metal–organic framework (MOF) colloids have recently emerged as promising building blocks for such architectures due to their colloidal stability, tunable size, diverse polyhedral morphologies, intrinsic porosity and chemical functionalization. Yet, achieving highly ordered, well-defined 3D superstructures at large scales remains a significant challenge. In this work, we demonstrate the spontaneous self-assembly of polyhedral MOF colloids into sub-centimeter three-dimensional mesocrystals with precisely defined shapes. These supracrystals exhibit cubic and trigonal morphologies arising from the periodic superlattice arrangement of individual MOF particles. Using well-dispersed ZIF-8 polyhedral colloids, we obtain mesocrystals that behave as single crystals, displaying both atomic-level coherence and long-range periodicity. Beyond their structural perfection, these 3D architectures also show emergent photonic responses that are not present in the isolated particles. This combination of structural order and functional properties highlights the potential of MOF colloids as versatile building blocks for next-generation photonic and porous materials.



Keywords: Colloidal self-assembly, Superstructure, Mesocrystals, Metal-organic frameworks, ZIF-8.

Development of point-of-need potentiometric devices for the monitoring of rare inherited metabolic diseases

L. Garrido; A. Calvo; J. Alonso; M. Puyol*

Group of Sensors and Biosensors, Department of Chemistry, Autonomous University of Barcelona, Edifici Cn, 08193, Bellaterra, Barcelona, Spain

MariaDelMar.Puyol@uab.cat

Hereditary metabolic diseases (HMDs) are genetic disorders that can severely affect patients' health and quality of life, particularly due to complications involving the nervous system. To prevent these outcomes, close biochemical monitoring is essential.

Currently, monitoring of these diseases is carried out in laboratories of reference centres. This requires patients to travel to the hospital, preventing continuous monitoring of the disease. To address this problem, it is necessary to develop point-of-need (PON) analytical devices that are affordable, reliable, and easy to use, allowing patients to self-monitor their disease from home, similar to what is done today for diabetes.

This investigation is framed within a translational project that begins with the design of potentiometric sensing strips and aims to progress towards hospital validation using real clinical samples. For this purpose, the project is being developed in collaboration with Hospital Sant Joan de Déu, Universitat Politècnica de Catalunya, and Fundación PKU-OTM (PKU Y OTROS TRASTORNOS METABÓLICOS).

In this 15th Doctoral Workshop, I present cyclic olefin copolymer (COC)-based detection strips designed for the potentiometric determination of ammonium in blood, enabling the direct or indirect quantification of biomarkers associated with several HMDs, depending on the specific enzymes immobilized in the device. These enzymes catalyse specific reactions that convert the corresponding biomarkers into ammonium, which is subsequently detected by ion-selective electrodes (ISEs). These (bio)sensing strips integrate two identical ammonium ISEs and a gas diffusion membrane, which allows the target ion to be isolated from the complex sample matrix. Owing to their versatility, these strips offer a promising platform for monitoring different metabolic diseases.

The theoretical basis used for the measurement in this research is the autocalibration concept. Autocalibration means that the device automatically performs a calibration step just before the sample measurement, without any conscious intervention from the user. This increases reliability, reduces errors, and makes the system easier to use, which is particularly important for its future implementation as a PON device operated by patients and non-specialized end-users at home. This methodology has been validated for measurements of chloride in sweat [1]. It is an innovative procedure that can be applied to potentiometric measurements in general; in this case, its applicability to the measurement of different concentrations of NH_4^+ is verified.

Additionally, with the aim of ensuring proper storage and long-term stability of the reagents required for patient monitoring, as well as assessing the feasibility of bringing these devices to market, the encapsulation of reagents, including enzymes into different embedded substrates of the strips is being studied. This requires lyophilization, which is being optimized on three key enzymes associated with different HMDs: phenylalanine ammonia-lyase (PAL), leucine dehydrogenase (LeuDH), and alanine dehydrogenase (AlaDH). Evaluating their performance after the lyophilization process not only provides insight into their stability and retained activity during extended storage, but also supports the optimization of formulations and processing conditions.

Overall, my work demonstrates the feasibility of using enzymatic potentiometric sensing strips to quantify multiple HMDs biomarkers within clinically relevant ranges. These advances have led to the filing of a patent, confirming that point-of-need devices for HMDs monitoring are no longer only a concept, but an achievable and tangible reality.

Keywords: Point-of-need, Ion selective electrodes, Hereditary metabolic diseases, Biomarkers, Enzyme.

[1] Calvo-López, A., Garrido-Carretero, L., Alonso-Chamarro, J., Puyol, M., 2025. Novel autocalibration strategy for disposable potentiometric test strips. Journal of Electroanalytical Chemistry 977, 118829.

Development of electrochemical sensors from revalorized biomass for emerging pollutant monitoring

Y. Bian[1,2,*], J. Bastos-Arrieta[3] , C. Palet[1], M. Baeza[2]

[1]GTS, Department of Chemistry, Carrer dels Til·lers, Universitat Autònoma de Barcelona, 08193 Bellaterra (Cerdanyola del Vallès), Barcelona, Spain

[2]GENOCOV, Department of Chemistry, Carrer dels Til·lers, Universitat Autònoma de Barcelona, 08193 Bellaterra (Cerdanyola del Vallès), Barcelona,Spain

[3]Grup d'Electroanàlisi Departament Enginyeria Química i Química Analítica, Universitat de Barcelona, 08028 Barcelona, Spain

*e-mail: Yudong.Bian@uab.cat

The development of efficient analytical methods for pharmaceutical quality control is essential to ensure drug safety and efficacy. While traditional HPLC-UV, chromatography, and spectroscopy techniques can accurately quantify multi-component formulations [1], their high cost, operational complexity, and limited portability restrict their application in rapid screening. In response to these limitations, this work aims to develop a low-cost and portable electrochemical sensing strategy based on biochar-modified electrodes for the sensitive and reliable detection of ibuprofen and paracetamol.

In this study a comparison between conventional screen-printed electrodes (SPEs) and composite electrodes (Figure 1) in the detection of ibuprofen and paracetamol [2], is presented. Composite electrodes based on graphite are also modified with some amount of biochar, to combine the inherent advantages of electrochemical sensors with the sustainable, low-cost, and surface-functional properties of biochar. The modified composite electrodes showed promising analytical responses toward paracetamol, demonstrating the potential of biochar modification to sensing approach by enhancing surface reactivity and interfacial charge-transfer properties. With the advantages of simplicity, sustainability, low cost, and compatibility with portable electrochemical devices, the proposed composite biochar-carbon based sensor offers a promising alternative for rapid on-site emerging pollutant screening.

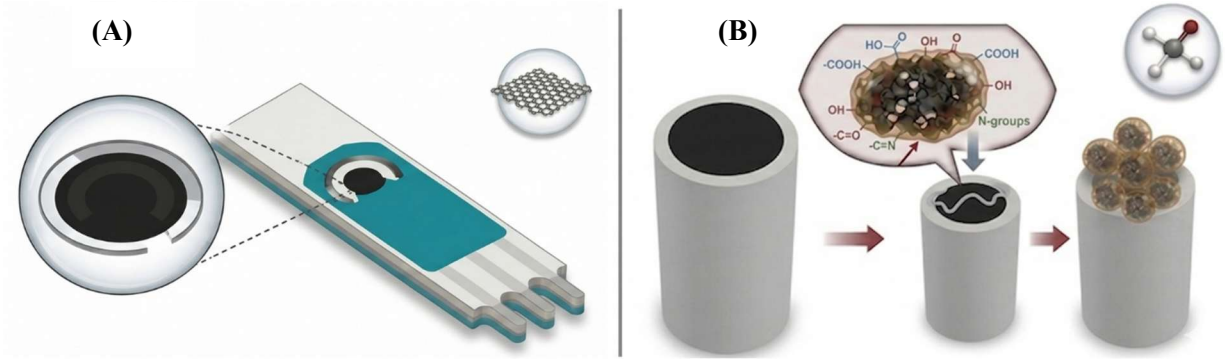


Figure 1: (A) SPE and (B) composite graphite and biochar electrode

Keywords: biochar; composite electrodes; electrochemical sensor; paracetamol; ibuprofen

References:

[1] Dubey, N.; Jain, D. K.; Jadhawani, S.; JPC-J. Planar Chromat. 2012, 25, 162. https://doi.org/10.1556/JPC.25.2012.2.13

[2] Serrano, N., Castilla, Ò., Ariño, C., Diaz-Cruz, M., & Díaz-Cruz, J. (2019). Commercial Screen-Printed Electrodes Based on Carbon Nanomaterials for a Fast and Cost-Effective Voltammetric Determination of Paracetamol, Ibuprofen and Caffeine in Water Samples. Sensors, 19(18), 4039. https://doi.org/10.3390/s19184039

Electrocatalytic ammonia synthesis via iron-based nanoparticles: mechanistic insights from computational studies

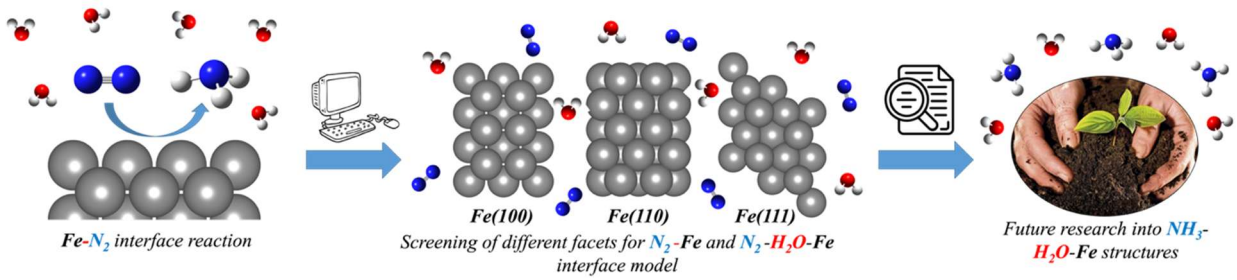
A. F. Sousa-Silva[1*], X. Solans-Monfort[1], L. Rodriguez[1], M. Sodupe[1]
[1]Universitat Autònoma de Barcelona – Bellaterra – Barcelona – Spain

*felipetruu@hotmail.com

Ammonia is essential for modern society, serving as a key raw material in the production of fertilizers, pharmaceuticals, explosives, and other industrial products. It has also attracted attention as a hydrogen carrier due to its high hydrogen content and advantages for storage and transport. Currently, large-scale ammonia production relies mainly on the Haber–Bosch process, which uses iron-based catalysts to promote the reaction between nitrogen and hydrogen. However, this process requires high temperatures and pressures and is associated with significant greenhouse gas emissions, motivating the search for more sustainable routes for NH_3 synthesis.

Electrochemical nitrogen reduction reaction (NRR) has emerged as a promising alternative because it can operate under mild conditions, using water as a hydrogen source and electrical energy as the driving force. Despite these advantages, its application remains limited by low faradaic efficiency, low N_2 solubility in aqueous media, and competition with the hydrogen evolution reaction. Therefore, understanding the mechanisms and interfacial phenomena governing N_2 activation is essential for designing more efficient electrocatalytic systems.

In this work, density functional theory calculations were used to investigate N_2 activation and water interaction on different crystalline facets of body-centered cubic iron, namely Fe(100), Fe(110), and Fe(111), under distinct electrochemical conditions. Clean, partially hydrogen-covered, and fully hydrogen-covered surfaces were considered to evaluate the effect of surface passivation. Water adsorption was also analyzed from isolated molecules to full monolayer coverage to describe the structure of the electrochemical interface.



The results show that nitrogen adsorption strongly depends on the exposed Fe facet and the availability of highly coordinated sites. Nitrogen atoms and molecules preferentially occupy sites that allow stronger coordination, resulting in lower adsorption energies. N_2 activation was evaluated through distal associative, alternating associative, and dissociative pathways, whose intermediates are governed by proton-coupled electron transfer steps. Water simulations revealed that, at low coverage, water dissociates on all three surfaces, whereas higher coverage reduces the energetic favorability of dissociation due to site saturation. Under reducing potentials, Fe(110) and Fe(111) are predicted to be covered by a full hydrogen monolayer, while Fe(100) presents lower hydrogen coverage. Overall, potential energy surfaces and Pourbaix diagrams provide valuable insight into the role of surface morphology, water coverage, and electrochemical conditions in Fe-catalyzed NRR, contributing to the development of more sustainable strategies for ammonia synthesis.

Keywords: ammonia synthesis; nitrogen reduction reaction; iron electrocatalysts; density functional theory; electrochemical interface.

Synergistic Enhancement of Cu (II) Adsorption by Tannic Acid and L-Cysteine

Functionalized Magnetic Chitosan Beads: Role of Structure–Function Trade-Off

Xiaojie Sun, Montserrat López-Mesas, María-Jesús Sánchez-Martín
GTS Research Group, Department of Chemistry, Faculty of Science, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain
Xiaojie.Sun@uab.cat

Grapes represent one of the most economically significant fruit crops in Europe, with Spain consistently ranking among the leading countries in vineyard area and wine production [1]. The growth of the wine industry has led to the generation of large quantities of by-products. Recently, increasing attention has been paid to the environmental and food safety risks associated with heavy metals in winery residues. Grape pomace and related by-products often contain detectable amounts of heavy metals, which can vary significantly depending on the type of residue, thereby raising environmental and agricultural safety issues [2]. The long-term use of copper-based fungicides, such as Bordeaux mixture, has contributed to copper accumulation in vineyard soils. Although micronutrient metal ions are essential for plant growth at appropriate levels, excessive heavy metal accumulation, especially Cu, poses significant environmental risks.

Adsorption is considered one of the most promising technologies for heavy metal removal due to its simplicity, high efficiency, and broad applicability. Among numerous functional groups, thiol groups (-SH) exhibit strong and selective adsorption capacity for Cu^{2+} ions [3]. In this study, chitosan, an environmentally friendly biopolymer, was modified with L-cysteine to introduce the -SH groups [4]. In addition, tannic acid was incorporated due to its ability to form multidentate coordination complexes with Cu^{2+} and to create a dense cross-linked network with chitosan, enhancing both the mechanical stability of the beads and their adsorption capacity, particularly at low pH [5]. SPIONs were also incorporated to impart magnetic properties, enabling rapid and non-destructive recovery of the beads under a magnetic field [6].

Based on this approach, novel chitosan-tannic acid-SPIONs magnetic adsorption beads were successfully developed (Fig. 1). Cu^{2+} adsorption experiments showed that these beads exhibit high adsorption capacity for Cu^{2+} and maintain their performance even at low pH values (Fig. 2).

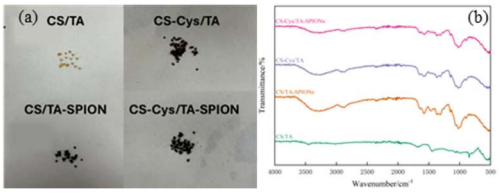


Fig. 1 Adsorption beads (a) and FTIR spectra (b).

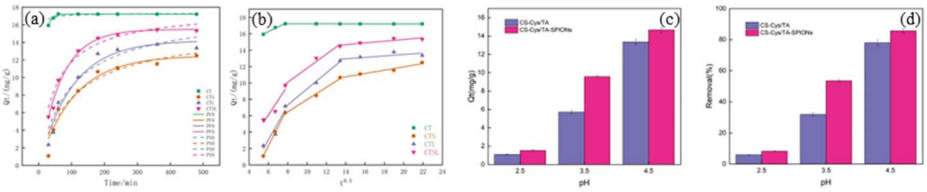


Fig. 2 Adsorption kinetics of the beads (a,b) and effect of pH on adsorption capacity (c,d).

Keywords: Copper accumulation; Vineyard soils; Chitosan-based magnetic beads; Thiol functionalization.

References:

[1] Homet, P., et al. (2024). Viticulture and the European Union's Common Agricultural Policy (CAP): Historical overview, current situation and future perspective. J. *Sustain. Agric. Environ*.
[2] Herrero-Hernández, E., et al. (2012). Long-term variability of metals from fungicides applied in amended young vineyard fields of La Rioja (Spain). *Environ. Monit. Assess.*, 184, 3359–3371.
[3] Wang, J., et al. (2014). Chitosan-based biosorbents: Modification and application for biosorption of heavy metals and radionuclides. *Bioresour. Technol.*, 160, 129–141.
[4] Federer, C., et al. (2021). Thiolated Chitosans: A Multi-talented Class of Polymers for Various Applications. *Biomacromolecules*, 22,24−56.
[5] Haslam, E., et al. (1996). Natural polyphenols (vegetable tannins) as drugs: Possible modes of action. *J. Nat. Prod.*, 59(2), 205–215.
[6] Pu, S., et al. (2017). Novel highly porous magnetic hydrogel beads composed of chitosan and sodium citrate: an effective adsorbent for the removal of heavy metals from aqueous solutions. *Environ Sci Pollut Res.*, 24:16520–16530.