ARCANE SCIENTIFIC DAY

May 19, 2026

La galerie des amphis
Amphithéâtre 7
Bâtiment Pierre-Mendès-France
180 allée des amphis
38400 Saint-Martin d'Hères

PROGRAM

9h00	**Welcome**
9h05	**KN1 – Anna Szarpak** *Rational Design of Hyaluronic Acid Hydrogels for Wound Dressing*
9h30	**OC1 – Shirley Ooi** *Glycoconjugate microarrays: synthesis to analysis*
9h45	**OC2 – Eve Le Dauphin** *Plasma copolymer coating to overcome bacteriophages adsorption: Atmospheric pressure plasma for nanocoating development*
10h00	**KN2 – Adrien Quintard** *Catalytic processes initiated by hydrogen transfer: greener tool for molecule activation*
10h25	**Coffee break**
10h45	**OC3 – Matteo Favre** *Solving the challenge of oxa-Michael addition through borrowing hydrogen*
11h00	**Luca Dell' Amico** *Mechanistic investigations in light-driven synthetic chemistry. From direct photochemistry to organophotoredox catalysis*
12h00	**Poster Session**
12h30	**Lunch**
13h45	**KN3 – Giulia Veronesi** *Tracking metals in cells with synchrotron X-rays: from nanoparticle transformation to the mechanism of action of anticancer compounds*
14h10	**OC4 – Cécile Dupont** *Development of a novel fluorescence anisotropy assay to study polyphenolic inhibitors of Tau Protein fibrillation*
14h25	**OC5 – Tom Di Santo** *Design of molecular imaging probe for Zinc (II) detection in-vivo*
14h40	**OC6 – Ankan Nath** *Determining Surface Chemistry of Perovskite Nanocrystals with DNP-Enhanced Solid-State NMR at 30 K*
14h55	**OC7 – Céline Naddour** *Understanding the Role of Proton Donors in Metal-Catalyzed N-O Bond Reduction*
15h10	**Coffee break**
15h30	**KN4 – Elisa Migliorini** *Biomimetic adaptable materials for in vitro studies*
15h55	**Raphaël Lévy** *Questioning the reproducibility and integrity of scientific publications*
16h55	**Conclusions & prizes**
17h00	**Beer session**

PLENARY LECTURE

Mechanistic investigations in light-driven synthetic chemistry From direct photochemistry to organophotoredox catalysis

Luca Dell'Amico

Department of Chemical Sciences, University of Padova
luca.dellamico@unipd.it

In this presentation, I will focus on two different topics from my research group, moving from the design of new photosensitizers to the development of powerful redox catalysts

1. Based on experimental evidence and mechanistic information, we have identified and structurally optimized a new family of photosensitiser.[1] This class of molecules is characterized by a short S1-T1 gap. We observed and increased selectivity in the strain-release functionalization of azabyclic scaffolds. This new reaction manifold grants access to highly functionalized azetidine scaffolds.

2. We have designed and developed two new classes of photoredox catalysts (PCs) capable of activating diverse types of redox inert substrates. To do so, we have used i) a catalytic proton-coupled electron-transfer (PCET) manifold;[2] and ii) an unconventional regenerative photocatalytic mechanism.[3]

Acknowledgements: *The authors are grateful to the European Research Council for the ERC-St. Grant SYNPHOCAT.*

References

[1] Rodríguez, R. I., Corti, V., Rizzo, L., Visentini, S., Bortolus, M., Amati, A. Natali, M., Pelosi, G., Costa, P., Dell'Amico, L. *Nat. Catal.*, **2024**, *7*, 1223–1231.
[2] Bortolato, T.; Simionato, G.; Vayer, M.; Rosso, C.; Paoloni, L.; Benetti, E. M.; Sartorel, A.; Lebœuf, D.; Dell'Amico, L. *J. Am. Chem. Soc.* **2023**, *145*, 1835–1846.
[3] Rosso, C.; Barison, G.; Droghetti, F.; Michelazzo, N.; Sartorel, A.; Pelosi, G.; Bortolus, M.; Costa, P.; Natali, M.; Dell'Amico, L. *ChemRxiv Preprint*, **2024**. https://doi.org/10.26434/chemrxiv-2024-dgxlp

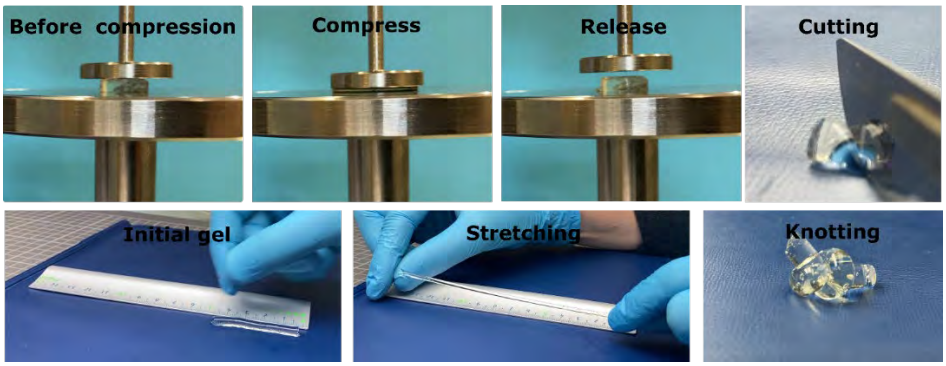
KEYNOTE LECTURES

Rational Design of Hyaluronic Acid Hydrogels for Wound Dressing

Szarpak Anna[1]

[1] Univ. Grenoble Alpes, CNRS, CERMAV, 38000 Grenoble
anna.szarpak@cermav.cnrs.fr

Hyaluronic acid (HA), a biopolymer naturally present in the extracellular matrix of the human body, is particularly suitable for clinical applications such as joint fluid supplementation, tissue engineering, and drug delivery. To be used as wound dressings, HA-based hydrogels must meet several requirements. Their mechanical properties must be precisely tailored to the targeted application, particularly in terms of stiffness, viscoelasticity, and deformation behavior, in order to match the characteristics of the target tissue. Moreover, tissues or organs subjected to constant motion, such as the heart, bladder, or joints, require highly stretchable hydrogels with good elastic properties to withstand repetitive movements. While many HA hydrogels exhibit brittle behavior and rupture under low deformation, we demonstrate how different parameters can be varied to obtain highly stretchable and elastic HA hydrogels with excellent recovery properties. The uniqueness of this material relies on:
i) A simple and green preparation method – pure HA hydrogels are obtained through a one-step process under physiological conditions.
ii) Tunability of stretchability – the extent of hydrogel elongation can be adjusted by varying parameters such as HA molar mass, cross-linking density, and HA concentration.
iii) Elasticity with excellent recovery properties – repeated loading–unloading cycles show negligible hysteresis, and the hydrogels recover their initial shape after deformation.
The strengthening of biopolymer hydrogels through the incorporation of different types of nanoparticles will also be demonstrated.



Acknowledgements: This work was partially supported by Arcane et CBH-EUR-GS (ANR-17-EURE-0003).

References

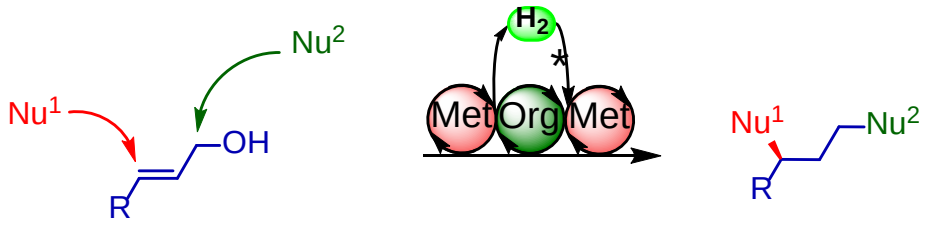
[1] A. Szarpak* et al., Carbohydrate Polymers, Vol 320, 2023, 121212

Catalytic processes initiated by hydrogen transfer: greener tools for organic synthesis

Adrien Quintard

[1] Université Grenoble Alpes, Département de Chimie Moléculaire, 38000 Grenoble
adrien.quintard@univ-grenoble-alpes.fr

During this talk, we will focus on the latest discoveries of our group on borrowing hydrogen catalyzed reactions. Borrowing hydrogen where alcohols are activated into reactive carbonyls in a reversible manner, are processes of choice in order to limit steps and waste. In this context, we pioneered the development of enantioselective versions, notably by taking advantage of multicatalytic processes, where a chiral organocatalyst activates the transient carbonyl. Such strategies can enable the direct functionalization of simple allylic alcohols to generate complex chiral aliphatic ones.[1] During this talk, we will focus on the latest discoveries of our group on borrowing hydrogen-catalyzed reactions involving allylic alcohols, notably enabling reactivities unprecedented at the carbonyl level.



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References

[1] For a recent review from our group: M. Vaglio-Pret, M. Favre, M. Odgen, A. Kochem, A. Quintard, Allylic alcohols in borrowing hydrogen catalysis: from simple substrates to complex molecules. *Org. Chem. Front.* **2026**, 10.1039/D6QO00148C.

Tracking metals in cells with synchrotron X-rays: from nanoparticle transformation to the mechanism of action of anticancer compounds

Giulia Veronesi[1]

[1] Univ. Grenoble Alpes, CNRS, CEA, IRIG, Laboratoire de Chimie et Biologie des Métaux, 17 Rue des Martyrs, 38000 Grenoble, France
giulia.veronesi@cea.fr

At the forefront of inorganic chemistry research for health applications, metal-based and metal-targeting materials offer innovative strategies for imaging and therapy. Bioconjugated metal-based nanomaterials, for instance, can serve as platforms for integrated imaging, drug delivery, and treatment.[1] In cancer therapy, metallodrugs are already used as therapeutic agents, and novel strategies targeting cellular copper are emerging.[2]

The *in vivo* behavior of these materials is a crucial parameter determining their performance: imaging agents are expected to be stable to ensure non-toxicity and preserve their optical properties, whereas drugs must interact with cells to exert their desired effects. Thus, these research areas share a common concern regarding the fate of the materials in biological systems, *i.e.* their biodistribution and chemical transformations.

Synchrotron-based techniques such as X-ray fluorescence (XRF) imaging and X-ray absorption spectroscopy (XAS) can provide information on the subcellular distribution of elements, including trace metals, and on the chemistry of a selected metal, respectively. Therefore, they are ideal tools for interrogating metal-based and metal-targeting materials in cellular models and for elucidating their transformation, in order to assess whether they perform the functions they were designed for. In this context, we will present two research projects making use of XAS and XRF imaging to assess the fate of materials in cellular models.

In the first example, we developed biocompatible Ag_2S-based nanocrystals for NIR bioimaging, investigated their structural properties as a function of reaction parameters, and demonstrated their stability in hepatic cells.[3] In the second example, we elucidate the mechanism of action of Cu(I)-ionophores, *i.e.* molecules that can bind and mobilize intracellular Cu(I) and thus induce cancer cell death, thus being regarded as a promising anticancer strategy.[4]

In both examples, synchrotron-based techniques reveal the properties of the materials in cells, enabling the optimization of formulations to tailor their *in vivo* performance.

Acknowledgements

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References

[1] Q. Peng et al. *Front. Chem.* **2022**, 10:899321.

[2] R. Kong et al. *Front. Pharmacol.* **2023**, 14:1203447.

[3] O. El-Dahshan, A. Deniaud, W. L. Ling, K. D. Wegner, O. Proux, G. Veronesi and P. Reiss, *Nanoscale*, **2025**, 17, 14637–14646.

[4] N. Renier, G. Weyckmans Mele, …, G. Veronesi, I. Jabin, A. Deniaud, H. Valkenier, *J. Am. Chem. Soc.* **2026**, 148, 1, 593–604.

Biomimetic adaptable materials for *in vitro* studies

Nathan Thibieroz[1], Alima Chali[1], Carlos Neri-Cruz[1], Paul Machillot[1], Catherine Picart[1] and Elisa Migliorini[1]

[1] Université Grenoble Alpes, BRM team (EMR 5000), Biosanté laboratory U1292 INSERM, IRIG, CEA Grenoble
Elisa.migliorini@cea.fr

Streptavidin-based supports are widely used in molecular studies and biosensing because they enable robust and versatile immobilisation of biotinylated molecules. Building on this concept, we and others have developed streptavidin-based glycosaminoglycan (GAG) biomaterials for investigating growth factor interactions and cellular responses[1-2]. A major advantage of these systems is the possibility to quantitatively characterise the surface presentation of each molecular component using complementary surface-sensitive and fluorescence-based techniques[1,5]. Using these biomaterials, we have investigated the role of GAGs and adhesion ligands in growth factor signalling and cell adhesion[3,6].

More recently, we developed Biomimetic Adaptable Microenvironments (BAM) (Figure 1), a modular biomaterial platform combining tunable mechanical properties, controllable biochemical functionalisation, and 3D scaffold integration. BAM enables the automated fabrication of reproducible 2D and 3D biomimetic environments while preserving quantitative control over molecular functionalisation. By introducing mechanically tunable and chemically defined 3D architectures, BAM provides new opportunities for studying extracellular matrix functions in physiologically relevant conditions and for developing advanced platforms for drug screening and predictive *in vitro* models.

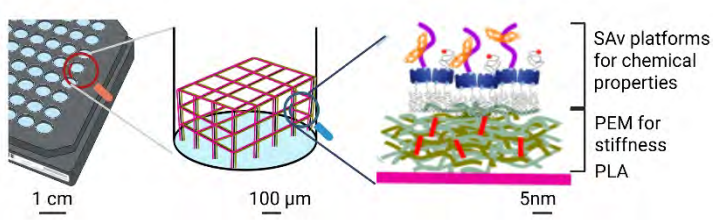

Figure 1: Schematic representation of the biomimetic adaptable materials 2D and 3D composition. The 3D printed scaffolds can enter inside 96 well plates. They are deep-coated by a biomaterial which provide a specific stiffness and chemical composition

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References

[1] E Migliorini et al., Well-defined biomimetic surfaces to characterize glycosaminoglycan-mediated interactions on the molecular, supramolecular and cellular levels Biomaterials 35,(2014).
[2] F Gude et al., Hedgehog is relayed through dynamic heparan sulfate interactions to shape its gradient Nature communications 14,(2023).
[3] J Sefkow-Werner et al., Heparan sulfate co-immobilized with cRGD ligands and BMP2 on biomimetic platforms promotes BMP2-mediated osteogenic differentiation Acta biomaterialia 114,(2020).
[4] D Thakar et al., Binding of the chemokine CXCL12alpha to its natural extracellular matrix ligand heparan sulfate enables myoblast adhesion and facilitates cell motility Biomaterials 123,(2017).
[5] J Sefkow-Werner et al., Combining Fluorescence Fluctuations and Photobleaching to Quantify Surface Density Analytical chemistry 94,(2022).
[6] J Le Pennec et al., Glycosaminoglycans exhibit distinct interactions and signaling with BMP2 according to their nature and localization Carbohydrate polymers,(2024)

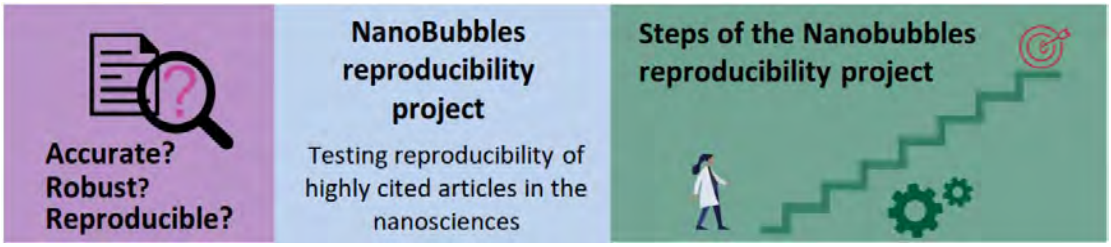
TOPIC OF THE YEAR

Questioning the reproducibility and integrity of scientific publications

Maha Said,[1] Mustafa Gharib[1] and Raphaël Lévy[1]

[1] Université Sorbonne Paris Nord and Université Paris Cité, INSERM, LVTS, Paris, France
raphael.levy@univ-paris13.fr

The NanoBubbles Reproducibility Initiative investigates the robustness of highly cited articles in nanobioscience. It starts from a paradox: hundreds of articles report the use of nanoparticles as efficient intracellular sensors of various cytosolic target (ions, mRNAs, etc). Yet, nanoparticles enter cells by endocytosis, a process that results in their confinement within intracellular vesicles, the endosomes, where they do not have access to the targets they are supposed to detect. As an attempt to solve that paradox, our replication initiative focuses on the most cited articles reporting intracellular sensing with nanoparticle probes. The presentation will introduce the NanoBubbles replication initiative [1], the open science approach that was adopted, the results and conclusions of the first replication [2] and present an open call [3] for contributions to this replication effort. The presentation will conclude with a general discussion on the (lack of?) reliability of the scientific literature and of the various approaches that could be used to improve it.



Acknowledgements: The NanoBubbles project is supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme – Grant agreement number ID:951393

References

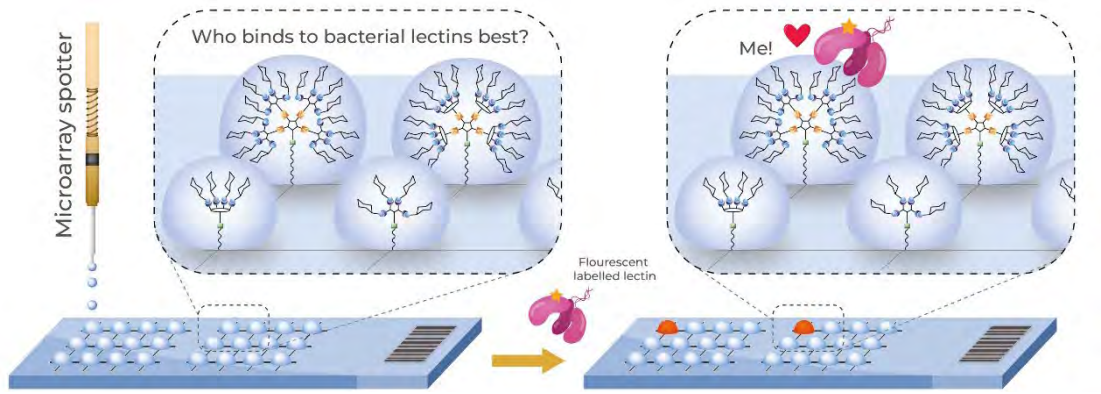
[1] Said, M., Gharib, M., & Lévy, R. (2026) Towards More Robust Nanobioscience: Launching the NanoBubbles Replication Initiative, Angew. Chemie Intern Edition; DOI: https://dx.doi.org/10.1002/anie.202511631/
[2] Gharib, M., Said, M., Pons, T., Hondow, N., Zrig, S., & Lévy, R. (2025). Failed, Aborted Replication of "Carbon-Dot-Based Dual-Emission Nanohybrid Produces a Ratiometric Fluorescent Sensor for In Vivo Imaging of Cellular Copper Ions". https://doi.org/10.31219/osf.io/2x3hv_v2
[3] Call for participation: Independent Replication of Carbon Quantum Dots Fluorescence and Cu^{2+} Sensing; https://nanobubbles.hypotheses.org/replication-initiative/call-for-participation-replication-in-bionanoscience/

ORAL COMMUNICATIONS

Glycoconjugate microarrays: synthesis to analysis

Shirley Y. Ooi[1], Eugénie Laigre[1], David Goyard[1], Olivier Renaudet[1]
[1] Univ. Grenoble Alpes, CNRS, DCM UMR 5250, F-38000 Grenoble, France
olivier.renaudet@univ-grenoble-alpes.fr

Carbohydrate-protein interactions between glycans and glycan-binding proteins (GBPs) play crucial roles in biological processes and are potential therapeutic targets. While multivalent interactions are necessary for high affinity and selectivity with target GBPs, designing effective multivalent glycan ligands involves complex structural parameters. Traditional methods requiring individual synthesis and study of various structures are time-consuming and expensive due to extensive purification steps. This project developed a microarray-based tool using glycoconjugate arrays to rapidly evaluate multivalent architectures against carbohydrate-binding proteins using minimal material. The approach involves synthesizing glycoconjugates directly on surfaces using functionalized synthons through stepwise chemical ligations, reducing purification steps. These glycoconjugates can then be simultaneously screened for bioactivity against GBPs. Interaction assays were developed using fluorescent-labelled lectins for direct testing to identify anti-adhesive compounds, while indirect tests used human serum and secondary fluorescent antibodies to find high-affinity antibody-binding molecules. Our team successfully synthesized various glycoconjugates on surface using different chemo-selective ligation reactions. Using surface MALDI-ToF MS, the compounds synthesized were successfully characterized. Several structures demonstrated promising bioactivity, with results comparable to classical physicochemical tests. This success enables exploration of more potential structures and ligation reactions using the microarray platform.



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References

[1] D. Goyard, A. M. S. Ortiz, D. Boturyn, O. Renaudet, *Chem. Soc. Rev.*, 2022, 51, 8756–8783.
[2] E. Laigre, C. Tiertant, D. Goyard and O. Renaudet, *ACS Omega*, 2018, 3, 14013–14020.
[3] A. Hoang, E. Laigre, D. Goyard, E. Defrancq, F. Vinet, P. Dumy and O. Renaudet, *Org. Biomol. Chem.*, 2017, 15, 5135.
[4] A. Cioce, M. Thépaut, F. Fieschi, N. Reichardt, *Chem. Eur. J.* 2020, 26, 56. 12809-12817

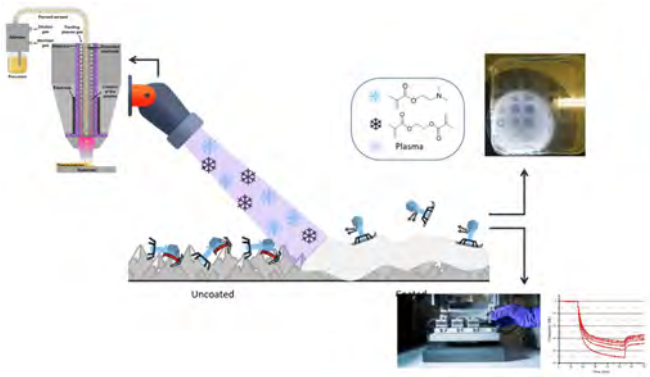
Plasma copolymer coating to overcome bacteriophages adsorption: Atmospheric pressure plasma for nanocoating development

Le Dauphin Eve[1], Durand Hippolyte[1] and Marcoux Pierre[1]

[1] Université Grenoble Alpes, CEA-Leti, F-38000 Grenoble, France
eve.ledauphin@cea.fr

The global burden of antibioresistance has been recently estimated at 10 million lives per year at the horizon 2050. In response to this alarming situation, phage therapy relies on the use of specific bacterial viruses called bacteriophages (phages) which are therefore natural antibacterial agents.
However, some studies [1,2] have recently highlighted difficulties associated with bacteriophage storage, notably due to vials material composition impacting suspension stability.

The aim of the study was to develop antibiofouling thin films that prevent bacteriophages, and other amphiphilic biomolecules such as proteins, from adsorbing onto the inner-walls of vials.
PEG-like and zwitterionic compounds are generally cited as having a good antibiofouling potential [3,4]. Atmospheric pressure plasma-assisted deposition equipment (figure 1) was used to coat with plasma copolymer ppEGDMA-co-DMAEMA (Ethylene glycol dimethacrylate -co- (dimethylamino)ethyl methacrylate) on silicon substrate. This thin film was deposited from a mixture of EGDMA and DMAEMA monomers. The plasma copolymer zwitterion was formed by Propanesultone vaporization. Its antibiofouling ability was tested with proteins and bacteriophages.
In addition to thickness, wettability, FTIR and XPS measurements, Quartz Cristal Microbalance with Dissipation monitoring (QCM-D) was used to investigate the adsorption kinetics of bacteriophages or amphiphilic protein (BSA) on raw and functionalized substrates.



References

[1] Ł. Richter "Adsorption of bacteriophages on polypropylene labware affects the reproducibility of phage research" Scientific Reports **11 pp.** 7387 (2021).

[2] L. O'Connell "Container material dictates stability of bacteriophage suspensions" Journal of Applief Microbiology (2022).

[3] T. Hartig "iCVD Polymer Thin Film Bio-Interface-Performance for Fibroblasts, Cancer-Cells, and Viruses Connected to Their Functional Groups and In Silico Studies" Advanced Materials Interfaces **11pp.** 2300587 (2024).

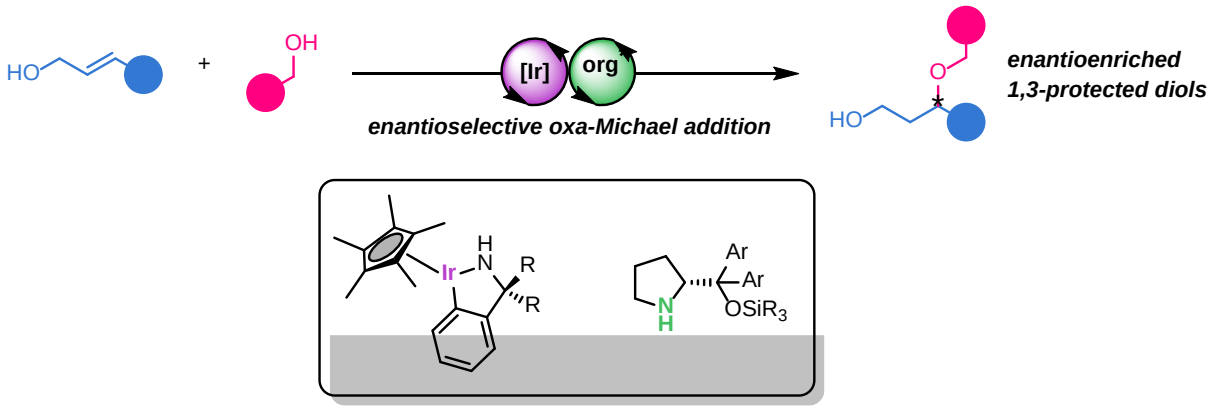
[4] R. Yang "Ultrathin Antifouling Coatings with Stable Surface Zwitterionic Functionality by Initiated Chemical Vapor Deposition (iCVD)" Langmuir **28pp.** 12266–12274 (2012).

Solving the challenge of oxa-Michael addition through borrowing hydrogen catalysis

Matteo Favre[1,2], Amélie Kochem[1] and Adrien Quintard[2]

[1] Université Grenoble Alpes, Département de Chimie Moléculaire, 38000 Grenoble
[2] CEA, LCBM, F-38000 Grenoble
matteo.favre@univ-grenoble-alpes.fr

Enantioselective intermolecular oxa-Michael reactions are notoriously difficult to achieve due to the low reactivity of alcohol nucleophiles and the high reversibility results in low yield and poor enantioselectivity. Despite the long-going efforts, the examples achieving high enantioselectivity in intermolecular additions remain scarce and are based on the use of oximes as nucleophiles [1], while reports using alcohols are practically nonexistent [2]. We are presenting the first multicatalytic enantioselective intermolecular oxa-Michael addition methodology involving borrowing hydrogen catalysis and chiral iminium organocatalysis, allowing to start from oximes or readily available alcohols as nucleophiles and allylic alcohols as pro-electrophiles. Using a cooperative catalytic system involving an iridium complex and a proline-derived organocatalyst under mild conditions, this efficient reaction affords enantioenriched protected 1,3 diols with high levels of enantioselectivity. This new methodology provides a green, atom economical synthetic route for important building blocks and opens the way for cascade reactions and applications in the synthesis of complex molecules.



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References

[1] a) Bertelsen, S.; Dinér, P.; Johansen, R. L.; Jørgensen, K. A. *J. Am. Chem. Soc.* **2007**, *129* (6), 1536–1537; b) Nising, C. F.; Bräse, S. *Chem. Soc. Rev.* **2012**, *41* (3), 988–999.
[2] Kano, T.; Tanaka, Y.; Maruoka, K. *Tetrahedron* **2007**, *63* (35), 8658–8664.

Development of a novel fluorescence anisotropy assay to study polyphenolic inhibitors of Tau Protein fibrillation

Dupont Cécile[1,2], Benjamin Boucherle[1], Marine Peuchmaur[1], Sabine Chierici[2]

[1] Département de Pharmacochimie Moléculaire, UMR 5063, Université Grenoble Alpes, CNRS, 38041, Grenoble, France
[2] Département de Chimie Moléculaire, UMR 5250, Université Grenoble Alpes, CNRS, 38041, Grenoble, France
cecile.dupont@univ-grenoble-alpes.fr

Neurofibrillary tangles, which are intracellular fibrillar aggregates of the Tau protein, are one of the pathophysiological markers identified in Alzheimer's disease, alongside amyloid plaques. In a therapeutic context, the search for inhibitors of Tau aggregation is therefore of great interest. As part of our previous research, polyphenolic derivatives have been identified as *in vitro* inhibitors of Tau aggregation. The standard assay using Thioflavin T (ThT) has been employed to detect the fibrillation process, as the ThT fluorescence signal increases upon presence of fibrils. However, a major limitation of this assay is the occurrence of false positives due to the displacement of ThT by inhibitors. These observations have prompted the development of a novel *in vitro* assay based on fluorescence anisotropy.

In this framework, short peptide fragments, AcR3 and AcPHF6, derived from the R3 repeat region of the Tau protein involved in fibrillation process, are employed as models. The evaluation of inhibitors is performed in the presence of fluorescently labeled analogues of AcR3 or AcPHF6, which serve as reporters. Upon incorporation into fibrillar assemblies, the rotational mobility of these fluorescent probes is strongly restricted, resulting in a FA signal. Preliminary experiments performed using AcPHF6 model and its fluorescein-labeled analogue as probe revealed a significant FA signal. In addition, a decrease in this signal in the presence of myricetin, as well as the appearance of a lag phase in the presence of tlkivw peptide, two known fibrillation inhibitors, were observed. In order to minimize potential spectral interference between inhibitors and fluorescent probes, peptides labeled with BODIPY and rhodamine B, which exhibit absorption wavelengths distinct from that of fluorescein, are also under investigation. This novel assay will enable an in-depth study of polyphenolic derivatives and facilitate the screening of other compound series.

Acknowledgements

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References

[1] Wegmann, S. and al. *Current Opinion in Neurobiology* **2021**, *69*, 131.
[2] Lunven, L. and al. *ACS Chemical Neuroscience* **2016**, *7*, 995.
[3] Boukherrouba, E. and al. *European Journal of Medicinal Chemistry* **2022**, *231*, 114139.
[4] Levine III, H. *Protein Science*, **1993**, *2*, 404.
[5] Goux, Warren J. and al. *Journal of Biological Chemistry* **2004**, *279*, 26868.

Design of molecular imaging bimodal MRI/PET probe for Zinc(II) detection *in-vivo*

Tom Di Santo[1], Luke Marchetti[2],Kyangwi P. Malikidogo[1], Célia Bonnet[2], Mylène Richard[3], Bertrand Kuhnast[3], Olivier Sénèque[1]

[1]Univ. Grenoble Alpes – CEA – CNRS – LCBM (UMR 5249), Grenoble (France) ; [2]CNRS – CBM (UPR 4301), Orléans (France) ; [3]Univ. Paris-Saclay – CEA – CNRS – BIOMAPS (UMR 9011)
tom.disanto@cea.fr

Zn^{2+} levels is highly regulated in living organisms, and an imbalance in Zn^{2+} regulation can be associated with many different diseases, such as cancer, diabetes and neurodegenerative diseases even if its role is not always fully understood. In this context, the development of non-invasive probes for early diagnosis of zinc-related diseases are highly desired. Medical technologies provide capability to non-invasive detection, localization and visualization of this kind of biomarkers. In the recent years, combination of Magnetic Resonance Imaging (MRI) and Positron Emission Tomography (PET) represent a big advance in medical imaging; combining the quantitative precision and high sensitivity of PET radionuclide detection with the unparalleled temporal and spatial resolution of MRI[1,2]. For efficient detection, MRI often requires a contrast agent and Gadolinium(III)-based contrast agents are among the most efficient and popular. Several Zn^{2+}-responsive MRI probes have been reported in the literature. There are based on small molecular complexes.[3–6] In a different approach, we have recently proposed a family of bioinspired contrast agent based on (i) a zinc finger peptide for selective Zn^{2+} recognition and (ii) a Gd^{3+} complex for MRI detection,[7,8] that proved to be efficient for Zn^{2+} detection in the pancreas of mice, provided that the local concentration of probe is known. Peptide-based contrast agents offer plenty of possibility to optimize the MRI response by fine tuning of the molecular structure, by playing with keys parameters of the contrast agent: the rotational correlation time τ_r and affinity k_d can be influenced by the amino acid composing the zinc finger, while the water exchange rate k_{ex} depends on the Gd^{3+} macrocycle chelator. In this communication, we will present our efforts to optimize the MRI properties of these probes as well as to develop a bimodal PET/MRI probe allowing the biodistribution of the contrast agent for quantitative Zn^{2+} detection.

References

[1] Jadvar, H. et Colletti, P.M. (2014). Competitive advantage of PET/MRI. European Journal of Radiology.

[2] Kretschmer, J. et al. (2024). A Macrocyclic Hybrid PET/MRI Probe for Quantitative Perfusion Imaging In Vivo. Angewandte Chemie International Edition.

[3] Bonnet, C.S. et Tóth, É. (2016). Smart Contrast Agents for Magnetic Resonance Imaging. CHIMIA.

[4] Bonnet, C.S. (2018). Zn2+ detection by MRI using Ln 3+ -based complexes: The central role of coordination chemistry. Coordination Chemistry Reviews.

[5] Lux, J. et Sherry, A.D. (2018). Advances in gadolinium-based MRI contrast agent designs for monitoring biological processes in vivo. Current Opinion in Chemical Biology.

[6] Malikidogo, K.P. et al. (2020). From Zn(II) to Cu(II) Detection by MRI Using Metal-Based Probes: Current Progress and Challenges. Pharmaceuticals.

[7] Isaac, M. et al. (2018). MRI and luminescence detection of Zn 2+ with a lanthanide complex–zinc finger peptide conjugate. Chemical Communications.

[8] Malikidogo, K.P. et al. (2023). Zinc-sensitive MRI contrast agents: importance of local probe accumulation in zinc-rich tissues. Chemical Communications.

Determining Surface Chemistry of Perovskite Nanocrystals with DNP-Enhanced Solid-State NMR at 30 K

Ankan Nath[1,2], Shadi Alarab[1,2], Subhradip Paul[1], Dmitry Aldakov[2], Gaël De Paëpe[1]

[1] Univ. Grenoble Alpes, CEA, CNRS, IRIG, MEM, RM, 38000 Grenoble (France)
[2] Univ. Grenoble Alpes, CEA, CNRS, IRIG, SyMMES, STEP, 38000 Grenoble (France)
ankan.nath@cea.fr

$CsPbBr_3$ and other halide perovskite nanocrystals have sparked significant interest due to their exceptional optical properties. However, their seemingly simple colloidal synthesis has proven challenging, primarily due to the soft ionic nature of their core and the lack of stability. Precise determination of the surface chemistry is essential for optimal ligand design to render these nanocrystals more stable. Solid-state NMR can be the ideal technique for this purpose as highly specific and detailed information about the interface can be obtained by selectively probing ligand and perovskite nuclei.

The primary limitation of the solid-state NMR is low sensitivity, which can be alleviated through hyperpolarization techniques such as Dynamic Nuclear Polarization (DNP). However, polarizing halide perovskite nanocrystals is extremely challenging, especially on commercially available systems that operate at 100 K. The sensitivity limitations can be drastically overcome by optimizing sample preparation for DNP, together with operation at 20-30 K using home-built instrumentation that sustainably employs cryogenic helium [1]. As a result, experimental times for high quality NMR spectra can be significantly reduced, by 2 to 3 orders of magnitude compared with previous studies. Enabled by this considerable improvement in sensitivity, I will demonstrate a versatile solid-state NMR toolbox comprised of intricate experiments which are essential for unambiguous determination of the surface chemistry of $CsPbBr_3$ nanocrystals, and have been previously impossible. In conjunction with DFT simulations and TEM studies, these experiments provide critical information allowing to elucidate the nanocrystal stabilization mechanism, such as (1) nanocrystal surface terminations, (2) dual mechanism of ligand binding involving substitution and adsorption, and (3) cooperative ligand binding. The techniques discussed can be used to study a wide variety of other inorganic as well as biological materials.

Figure 1: (Left) Our He MAS-DNP System, (Right) The ligand-binding scheme

References

[1] Paul, S. *et al.*, Sustainable and cost-effective MAS DNP-NMR at 30K with cryogenic sample exchange, *J. Magn. Reson.*, 2023, 356, 1090.

Understanding the Role of Proton Donors in Metal-Catalyzed N–O Bond Reduction

Céline Naddour[1], Cyrille Costentin[1] and Sylvie Chardon-Noblat[1]

[1] Univ Grenoble Alpes, DCM, CNRS, 38000 Grenoble, France

Celine.naddour@univ-grenoble-alpes.fr

Proton donors play a central yet often ambiguous role in metal-catalyzed N–O bond reduction, where proton transfer, hydrogen bonding, and electron transfer can be intimately coupled. Rather than acting solely as sources of protons, these species can influence catalytic reactions in different ways, including stabilization of key intermediates, modulation of activation barriers, facilitation of catalyst regeneration,[1] and control of reaction selectivity.[2]

In this presentation, we outline the different mechanistic roles that proton donors can adopt in N–O bond reduction. We further discuss how electrochemical methods, especially cyclic voltammetry, provide insight into these roles through observable traits such as shifts in redox potentials, changes in catalytic current, and kinetic dependencies on proton donor concentration. Complementary approaches, including isotopic substitution and variation of acid strength,[3] enable deeper identification of rate-limiting steps and proton involvement.

Overall, this work highlights how electrochemical methods can provide detailed mechanistic insight into catalytic N–O bond reduction and offers an insight into the role of proton donors, beyond simple proton transfer.

References

[1] Naddour, C., Deeba, R., Kjellberg, M., Chardon-Noblat, S., & Costentin, C. (**2025**). H-Bond Assistance and Electronic Effects Accelerate the Cleavage of the N–O Bond in the Electrochemical Reduction of N_2O Catalyzed by Rhenium Bipyridine Tricarbonyl Complexes. *Inorganic Chemistry, 64* (29), 15217

[2] Naddour, C., Durin, G., Chardon-Noblat, S., Costentin, C. (**2025**). Proton-Coupled Electron Transfer Deoxygenation of Pyridine N-Oxide: A Mechanistic Study. *ChemPhysChem, 0*, e202500292.

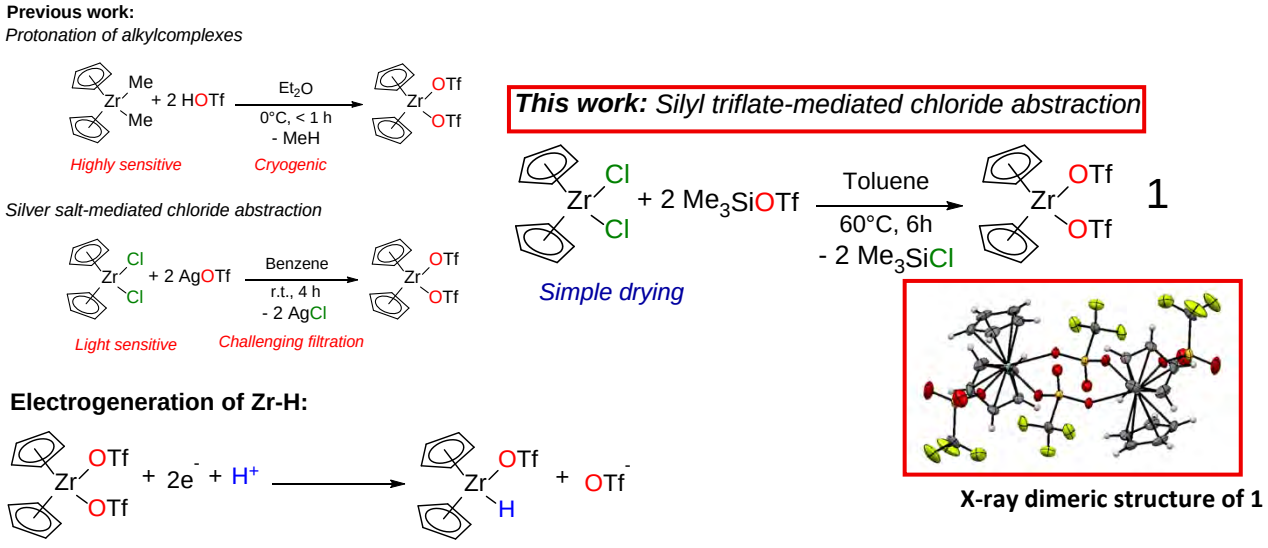
[3] Naddour, C., Deeba, R., Chartier, C., Nicolas, E., Chardon-Noblat, S., & Costentin, C. (**2025**). H-Bond-Assisted cleavage of N–O bond in the electrochemical reduction of N2O catalyzed by iron tetraphenylporphyrin. *ACS Catalysis, 15* (11), 9393

POSTERS

Straightforward Synthesis of Cyclopentadienyl Zirconium Triflate Complexes: Solvent Effects and Electrochemical Properties

Karim Akar* [(1)], Cyrille Costentin [(1)], Sylvie Chardon [(1)], Gabriel Durin [(1)]
[1] *Univ Grenoble Alpes, DCM, CNRS, 38000 Grenoble, France.*
Email: karim.akar@univ-grenoble-alpes.fr

The transition toward sustainable chemical processes motivates the development of electrocatalytic strategies that directly use electrons and protons as reducing equivalents.[1] In this context, well-defined organometallic complexes offer unique opportunities to control reactivity and elucidate mechanisms.[2] Here, we present our recent work on cyclopentadienyl zirconium triflate complexes as promising candidates for Zr-H molecular electrocatalysis. We report a straightforward and efficient synthesis of these complexes via silyl triflate-mediated chloride abstraction, providing a practical alternative to conventional methods based on silver salt. Particular attention is given to the role of solvent coordination in controlling the structure and speciation of the complexes, which directly impacts their reactivity. Their electrochemical behaviour is also investigated, highlighting the importance of electrolyte choice to preserve catalyst integrity and access reversible redox processes. Building on these findings, this work contributes to the broader objective of developing zirconium hydride electrogeneration, along with all the potential perspectives in electrocatalysis that could result from this.



References:

[1] M. Kobylarski, L.J. Donnelly, J-C. Berthet, T. Cantat, Zirconium-catalysed hydrosilylation of esters and depolymerisation of polyester plastic waste. *Green Chem.*, ***2022***, *24, 6810-6815.* **https://doi.org/10.1039/D2GC02186B**

[2] N. W. Kinzel, C. Werle, W. Leitner, Transition Metal Complexes as Catalysts for the Electroconversion of CO_2: An Organometallic Perspective. *Angew. Chem. Int. Ed.* ***2021***, *60, 11628-11686.* **https://doi.org/10.1002/anie.202006988**

De novo antimicrobial peptides for drug and diagnostic method development

Lucie BASTIEN[1, 2, 3], Emna BEN EL-HADJ SALEM[1], Quang-Thinh DON-NGUYEN[2], Mehavi MEHAVARNAN[3], Eric PARDOUX[1, 2], Didier BOTURYN[2], Sandrine BOISSET[3] & Yoann ROUPIOZ[1]

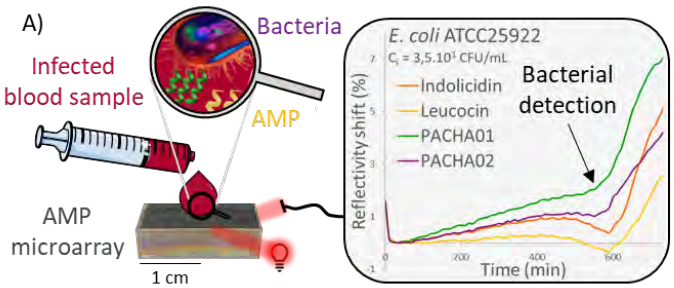
[1]Univ. Grenoble Alpes, CEA, CNRS, Grenoble INP, IRIG, UMR 5819, SyMMES
[2]Univ. Grenoble Alpes, CNRS, UMR 5250, DCM
[3]Univ. Grenoble Alpes, CHU Grenoble Alpes, CNRS, CEA, UMR5075, IBS
lucie.bastien@univ-grenoble-alpes.fr

The fight against drug-resistant bacterial strains requires multiple complementary approaches including the development of novel therapeutic options and faster diagnostic methods. Antimicrobial peptides (AMP) are promising candidates to address this health crisis thanks to their unique mechanisms of action, broad-spectrum activity and versatility.

We designed two *de novo* peptides, PACHA01 and PACHA02, with the same amino acids but featuring different primary sequences. The antimicrobial activity of both peptides against different bacterial strains as well as their toxicity toward B lymphocyte was assed. They were also added to an AMP microarray integrated to a surface plasmon resonance imaging (SPRi) platform that proved to enable bacterial detection and identification.[1,2] Interestingly, while PACHA01 demonstrated good affinity with bacteria when immobilised on surface, highlighting its potential as molecular probe, PACHA02, with activity against both Gram-negative and Gram-positive bacteria and limited toxicity, showed promises for antibiotic development (Figure 1).

Overall, PACHAs have strong potentials for drugs and diagnostic tools design.

A)



B)

Peptide	MIC against *S. aureus*	MIC against *E. coli*	Toxicity (% of B lymphocyte death at the higher MIC value determined)
PàCHA01	64 mg/L	64 mg/L	80%
PàCHA02	4 to 8 mg/L	4 to 32 mg/L	0%
Indolicidin	8 mg/L	8 mg/L	20%

Figure 1 – PACHA01 and PACHA02 applications. A) AMPs functionalised SPRi-prism for bacterial detection of infected blood sample models. B) B lymphocyte toxicity and minimal inhibitory concentration (CMI) of PACHA01 and PACHA02 compared to Indolicidin a well-known AMP

References:

1. É. Pardoux, A. Roux, R. Mathey, D. Boturyn, Y. Roupioz. Antimicrobial peptide arrays for wide spectrum sensing of pathogenic bacteria. *Talanta*, *203*, 322–327 **(2019)**.
2. É. Pardoux, L. Bastien, R. Mathey, S. Boisset, D. Boturyn, Y. Roupioz. Rapid one-step detection of live bacteria in blood using antimicrobial peptides micro-arrays. (under review).

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Computational Study of CO_2 Capture Mechanisms in Liquid Media: From Aqueous Amines to Complex Solvents

Louis Biancon, Rolf David and Anne Milet

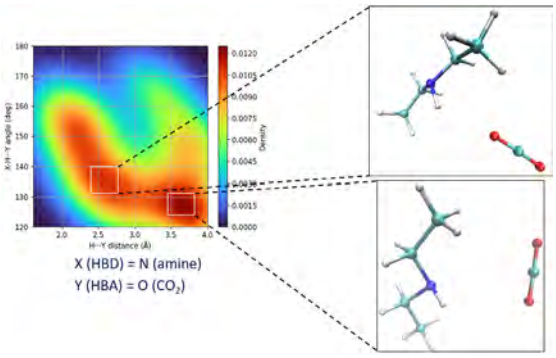
DCM, Université Grenoble Alpes, CNRS, 38000 Grenoble, France
louis.biancon@univ-grenoble-alpes.fr

Direct air capture and recycling of CO_2 offer a promising route toward closing the carbon cycle and reducing reliance on fossil resources. However, this strategy faces a major challenge: CO_2 is thermodynamically stable and highly diluted in the atmosphere, making its conversion into value-added molecules difficult.

This work investigates, through molecular simulations, the mechanisms governing CO_2 capture in liquid solvents, with the objective of developing a theoretical framework for carbon capture applications. Although the broader project focuses on deep eutectic solvents (DES)[1], the present study concentrates on aqueous amines[2] in collaboration with an experimental team, in order to rationalize experimentally observed trends and ultimately design new amines for efficient CO_2 capture, storage, and reuse.

Classical molecular mechanics (MM) and density functional theory (DFT) simulations are employed to characterize the solvation environment and reactivity of CO_2 in these systems. Model systems composed of an amine and a CO_2 molecule solvated in water are first constructed with careful attention to reactive species (carbamates, carbonates) and acid–base equilibria. Long molecular dynamics simulations are performed to identify preferential CO_2 interaction sites, while enhanced sampling methods such as umbrella sampling are used to compute free-energy profiles associated with CO_2–amine interactions.

This initial work provides a foundation for future investigations of DES and ionic liquids. In the longer term, the project will integrate machine-learning interatomic potentials (MLIPs)[3] to overcome the high computational cost of DFT, which limits simulations of large systems and long timescales. By reproducing DFT-level potential-energy surfaces with near-quantum accuracy while being orders of magnitude faster than traditional ab initio molecular dynamics, MLIPs will enable extensive reactive simulations. These AI-driven approaches will facilitate the identification of preferential CO_2 binding sites and provide a detailed characterization of interaction mechanisms, distinguishing physisorption from chemisorption, while also enabling the exploration of reaction pathways and associated energy barriers.



Acknowledgements

The AUDACE! Program, the Labex ARCANE, the GRICAD infrastructure and the GENCI infrastructures.

References

(1) Alnajjar, A.; Onaizi, S. A. CO2 Capture and Conversion Using Deep Eutectic Solvents: Recent Progress and Outlooks. *J. Mol. Liq.* **2025**, *421*, 126832. https://doi.org/10.1016/j.molliq.2024.126832.

(2) Yang, X.; Rees, R. J.; Conway, W.; Puxty, G.; Yang, Q.; Winkler, D. A. Computational Modeling and Simulation of CO_2 Capture by Aqueous Amines. *Chem. Rev.* **2017**, *117* (14), 9524–9593. https://doi.org/10.1021/acs.chemrev.6b00662.

(3) David, R.; Puente, M. de la; Gomez, A.; Anton, O.; Stirnemann, G.; Laage, D. ArcaNN: Automated Enhanced Sampling Generation of Training Sets for Chemically Reactive Machine Learning Interatomic Potentials. *Digit. Discov.* **2025**, *4* (1), 54–72. https://doi.org/10.1039/D4DD00209A.

Using cold atmospheric plasma to protect surface from bacterial contamination

Florian Bitterolf[1], Guillaume Nonglaton[1], Christelle Dublanche-Tixier[2], Cédric Ducros[3]
[1] Université Grenoble Alpes, CEA, LETI, DTIS, PRISM, F-38000 Grenoble
[2] Université de Limoges, UMR 7315, IRCER, F-87000 Limoges
[3] Université Grenoble Alpes, CEA, LITEN, DTNM, SCEF, LEFC, F-38000 Grenoble

Nowadays, biological contamination especially bacterial are a major concern regarding healthcare but many other including food industry and defense. While it takes up to 10 years to put a new antibiotic on the market, bacteria could acquire resistance to an antibiotic in just a week (1). In France in 2015, more than 120 000 cases of multidrug-resistant bacteria leading to more than 5 500 deaths (2). According to forecast, by 2050 death caused by superbugs could reach 238 000 persons (3). Urging the need to finds new ways to fight against bacterial contamination. Although bacteria on their planktonic form tends to be sensitive to environmental stresses and therapeutics agents, they have a tendency to form biofilm. Surface attached communities protected by a polymeric matrix exacerbating the development of resistance(4).

Therefore, effective ways to fight against bacterial contamination would be to prevent adhesion and biofilm formation in the first place. To do so, research focus on two main strategies, preventing bacteria's adhesion through super hydrophilic, super hydrophobic or micro/nanopatterned surface (5). The second strategies consist on a biocidal approach, either by surface releasing antibacterial compound or by grafting those antibacterial compounds on the surface for a contact killing approach (6).

Among all deposition techniques in surface chemistry, cold atmospheric plasma turns out to be great versatile techniques to achieve this goal. Allowing a greener chemistry by making solvent free plasma polymer coating and having a lesser energy consumption than low pressure deposition. Moreover, those plasma are non-thermal making them suitable for a wide range of substrate materials (plastic, metals, glass, textile) (7,8).

During my PhD, my goal will be to use a DBD-CAP (Dielectric barrier discharge Cold Atmospheric Plasma) deposition to obtain a plasma polymeric thin layer that will act as an anchoring point that I'll use to integrate NPs (TiO2, ZnO) to generate ROS but also Ag NPs for a contact killing strategies. Other ways to use the plasma polymeric layer will be to use it to graft antimicrobial peptide. The possibility and effectiveness of combining NPs and AMPs for a synergistic effect will be investigated. Coating will be characterized with common physical and chemical techniques (Water contact angle, Profilometry, Ellipsometry, FTIR, XPS, QCM-d) and effectiveness toward bacterial contamination will be assessed through microbiological test of viability and adherence using model bacteria (*E. coli*, *S. Epidermidis*).

References

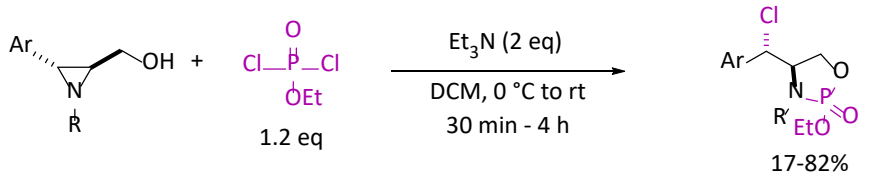
1.Harms A, Maisonneuve E, Gerdes K. Mechanisms of bacterial persistence during stress and antibiotic exposure. Science. 2016;354(6318).
2.Cassini A, Högberg LD, Plachouras D, Quattrocchi A, Hoxha A, Simonsen GS, et al. Attributable deaths and disability-adjusted life-years caused by infections with antibiotic-resistant bacteria in the EU and the European Economic Area in 2015: a population-level modelling analysis. Lancet Infect Dis. 1 janv 2019;19(1):56-66.
3.OECD (2023), Embracing a One Health Framework to Fight Antimicrobial Resistance, OECD Health Policy Studies, OECD Publishing, Paris, https://doi.org/10.1787/ce44c755-en.
4.Davies D. Understanding biofilm resistance to antibacterial agents. Nat Rev Drug Discov. 2003;2(2):114-22.
5.Durand H, Whiteley A, Mailley P, Nonglaton G. Combining Topography and Chemistry to Produce Antibiofouling Surfaces: A Review. ACS Appl Bio Mater. 2022;5(10):4718-40.
6.Ahmadabadi HY, Yu K, Kizhakkedathu JN. Surface modification approaches for prevention of implant associated infections. Colloids Surf B Biointerfaces. 2020;193.
7.Bárdos L, Baránková H. Cold atmospheric plasma: Sources, processes, and applications. Thin Solid Films. 2010;518(23):6705-13.
8.Merche D, Vandencasteele N, Reniers F. Atmospheric plasmas for thin film deposition: A critical review. Thin Solid Films. 2012;520(13):4219-36.

Synthesis of novel 1,3,2-oxazaphospholidine-2-oxides *via* ring expansion of 2-hydroxymethylaziridines

Amal Dridi,[1,2] Sandrine Py,[1] Rafâa Besbes[2]

[1] *Département de Chimie Moléculaire, UMR 5250 CNRS –Université Grenoble Alpes, 38058 Grenoble, France.*
[2] *Laboratory of Analytical Chemistry and Electrochemistry, Organic Synthesis Team, LR99ES15-University of Tunis El Manar, Faculty of Sciences of Tunis, 2092 Tunis, Tunisia.*
Email: amal.dridi@univ-grenoble-alpes.fr

2-Hydroxymethylaziridines represent valuable synthetic intermediates for the construction of diverse interesting heterocyclic systems.[1] In this communication, we report a simple and efficient approach for the synthesis of 1,3,2-oxazaphospholidine-2-oxides through the ring expansion of non-activated 2-hydroxymethylaziridines in the presence of ethyl dichlorophosphate, under mild conditions. Regio- and stereoselective aziridine ring opening yields α-chlorinated 5-membered ring heterocyclic compounds as the sole products of the reaction.



Some 1,3,2-oxazaphospholidine-2-oxides have been reported to exhibit anti-inflammatory,[2] antibacterial[3] or insecticidal[4] effects, however molecules containing such scaffold remain underinvestigated to date. Herein, we describe the preparation of 16 examples of 1,3,2-oxazaphospholidine-2-oxides, with the perspective of evaluating their applications at a later stage.

Key words: 2-hydroxymethylaziridine, 1,3,2-oxazaphospholidine-2-oxide, ring expansion.

[1] Stanković, S.; D'hooghe, M.; Catak, S.; Eum, H.; Waroquier, M.; Van Speybroeck, V.; De Kimpe, N.; Ha, H.-J. Regioselectivity in the Ring Opening of Non-Activated Aziridines. *Chem. Soc. Rev.* **2012**, *41*, 643–665.

[2] Abdou, W. M.; Sabry, E.; Shaddy, A. A. Synthesis Approach and Biological Activity Evaluation of a Series of 1,3,2-Oxazaphosphole-2-Oxides against Inflammation and Nociception. *Monatsh. Chem.* **2019**, *150*, 283–294.

[3] Krishna, B. S.; Rao, A. J.; Naidu, K. R. M.; Rao, V. K.; Raju, C. N. Synthesis and Antibacterial Activity Studies of Novel 2-Substituted- 1,3,2-Oxazaphosphole-2-Oxide Derivatives of (*S*)-(+)-Prolinol. *Org. Commun.* **2010**, *3*, 98–105.

[4] Eto, M. Functions of Phosphorus Moiety in Agrochemical Molecules. *Biosci. Biotech. Biochem.* **1997**, *61*, 1–11.

Aptamer-functionalized microneedles for cortisol optical detection

Matteo Ecolasse[1,2], Benoît Chovelon[1] and Isabelle Texier[2]

[1] Univ. Grenoble Alpes, CNRS, DPM, F-38000 Grenoble, France; [2] Univ.Grenoble Alpes, CEA, LETI, F-38000 Grenoble, France.
matteo.ecolasse@univ-grenoble-alpes.fr

Cortisol is a key biomarker of physiological stress and several pathologies, and its monitoring represents a major challenge in point of care medicine and health surveillance[1]. In this context, microneedles offer a promising and non-invasive method for sampling and analyzing interstitial skin fluid (ISF), relevant for cortisol monitoring [2].

This study aims to develop optical biosensors combining cortisol-binding aptamers and microneedles as an innovative method for measuring cortisol concentration in ISF. Aptamers are synthetic biosensing macromolecules presenting high target affinity and specificity. They are entrapped into or grafted onto a crosslinked hydrogel matrix through optimized chemical strategies[2]. The molecular reconnaissance of cortisol induces an aptamer conformational change, is transducted into an optical signal via a quencher-fluorophore displacement strategy, enabling real-time measurement and monitoring[3].

Different aptamer designs are being tested for optimizing cortisol optical detection. In parallel, microneedle arrays based on methacrylated dextran (Dex-MA) and methacrylated hyaluronan (HA-MA) have been developed and characterized (Figure 1). After entrapment of the cortisol-sensitive aptamer into the hydrogel matrix, analytic performances of the devices will be evaluated to determine their limit of detection and selectivity, in physiologically relevant conditions. This technology would pave the way for the monitoring of stress and physiological state through wearable sensors, with potential applications in diagnostics, personalized medicine, mental health, and sports monitoring.

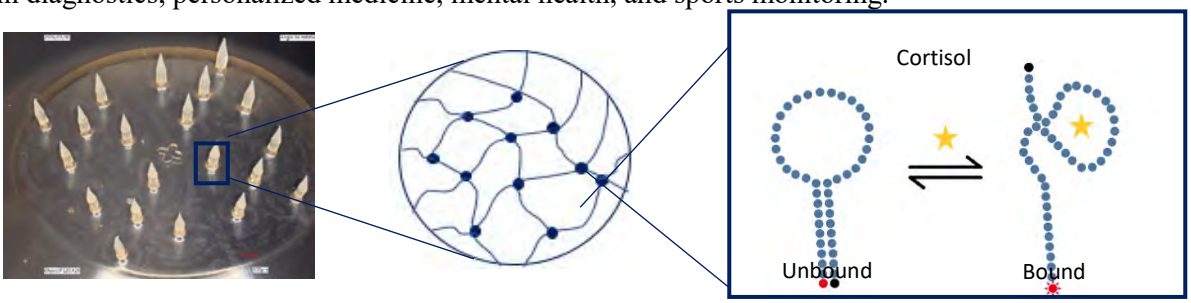


Figure 1 : Aptamer-functionalized hydrogel microneedles strategy for ISF cortisol detection

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References:

[1] Kusov & al. Cortisol Monitoring Devices toward Implementation for Clinically Relevant Biosensing in Vivo. *Molecules (Basel, Switzerland)* **2023**, *28* (5), 2353.

[2] Zhou & al. An Aptamer-Responsive Microneedle Patch Sensor Platform Combining with Hybridization Chain Reaction Amplification for Detection of Steroid Hormone Cortisol in Skin Interstitial Fluid. *Biosensors and Bioelectronics* **2024**, *269*, 116935.

[3] Saunders & al. Generalizable Molecular Switch Designs for *in Vivo* Continuous Biosensing. *Accounts of Chemical Research* **2025**, *58* (5), 703–71.

N-metala-*N*-heterocyclic carbene Re-carbonyl complexes: Study of reactivity

Daniel Elizondo-Pizarro, Sylvie Chardon-Noblat, Eder Tomás-Mendivil

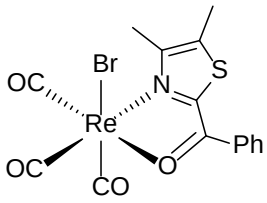
Département de Chimie Moléculaire, 301 Rue de la Chimie, 38610, Gières
daniel.elizondo-pizarro@etu.univ-grenoble-alpes.fr

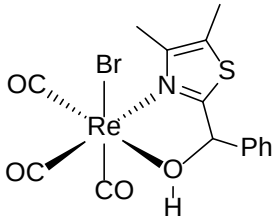
N-Heterocyclic carbenes[1] (NHC) feature a neutral carbon atom having one non-bonding orbital filled with 2 electrons and one empty orbital. The carbon only has 6 valence electrons, it is in a cyclic structure and the NHC must contain at least one nitrogen atom.

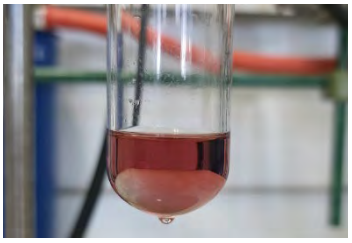
NHCs are known in organometallic chemistry for their capacity to coordinate to a metal center as a ligand, through a strong C-[M] bond. They are also known organocatalysts[2] reacting with aldehydes or acyl chlorides, forming stable organic intermediates with different redox states, such as the Breslow intermediates[3] , acylthiazolium cations, etc.

A less studied use of these carbenes is their capacity to be coordinated to a metal through the N-[M] bond; however there are still some studies that show their reactivity, revealing the tendency to tautomerize to the more stable C-[M] bond[4].

We theorized that the aforementioned properties of NHCs could be combined into one study, by the use of an acylated carbene derivative, coordinated to a rhenium metal centre through the nitrogen and oxygen atoms. These types of complexes could then show interesting reactivities and redox properties, like the formation of stabilized enolates or radicals. The stabilized enolates could be considered as an extension of the known Breslow intermediate reactivity which could be further studied by reacting them with electrophiles. Based on this we chose some acylated imidazole and thiazole ligands. The results for the synthesis, characterisation and reactivity studies of the complexes will be presented in this work.







Acknowledgements
We would like to thank Ticket 2024-2026 Labex Arcane (ANR-17-EURE-0003) for the funding of this research.

References

[1] M. Hopkinson , C. Richter , M. Schedler, F. Glorius, *Nature*, **2014**, *510*, 485-496.
[2] L.Delfau, E. Tomás, D. Martin et al, *Ang. Chem. Int. Ed*, **2021**, *60, 26783*-26789.
[3] R. Breslow, *J. Am. Chem. Soc*, **1958**, *80*, 3719-3726
[4] J. Ruiz and B. Perandones, , *J. am. Chem. Soc*. **2007**, *129*, 9298-9299.

Role of ligand clustering in multivalent recognition at biointerfaces: model study using host/guest interactions

Emily Ezewudo [a], Baptiste Chabaud [a], Bruno Espuche [a], Rémy Lartia [a], Claire Le Goff [a], Didier Boturyn [a] and Galina Dubacheva [a]*.

[a] Département de Chimie Moléculaire, CNRS UMR 5250, Université Grenoble Alpes, Grenoble, France.
* Contact: galina.dubacheva@univ-grenoble-alpes.fr

At biological interfaces, ligands are often organized into clusters rather than randomly distributed, which directly influences multivalent binding behavior. Understanding how this spatial organization affects molecular recognition is essential to better describe biological processes such as cell communication, environmental response, and immune recognition, as well as to guide the design of targeted therapeutic strategies. However, isolating the specific role of clustering in complex biological environments remains challenging. To address this, simplified and well-controlled model systems are required, enabling precise tuning of ligand density and spatial arrangement to probe structure–function relationships in multivalent interactions[1].

In this work, synthetic oligopeptide scaffolds bearing guest moieties are designed to control receptor valency and spatial distribution at surfaces. The scaffolds are immobilized on gold substrates using self-assembled monolayers combined with bioorthogonal click chemistry[2]. Hyaluronic acid functionalized with multiple cyclodextrin units is employed as a model multivalent probe to study the role of clustering on the binding kinetics and superselectivity, i.e., its ability to distinguish sharply between different densities of surface receptors. Guest surface density and polymer binding are characterized using electrochemistry and quartz crystal microbalance with dissipation monitoring. We will present our synthetic strategy used to obtain well-defined and tunable oligopeptide scaffolds together with our first results on their immobilization on surfaces at controlled density and on the impact of their valency on multivalent recognition.

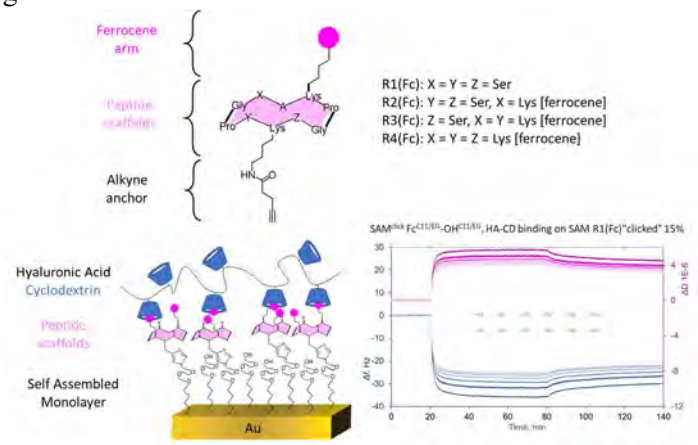


Figure 1: Model system for studying clustering effects in multivalent host–guest interactions between functionalized surfaces and polymers

References

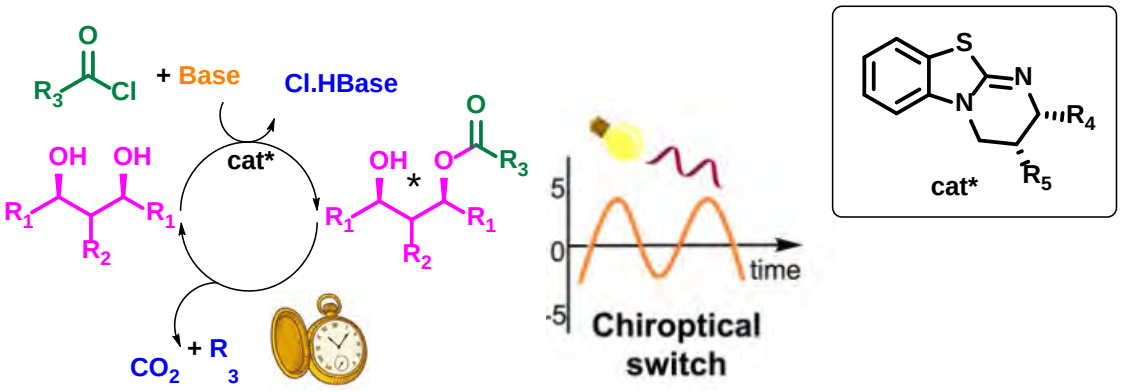
(1) Dubacheva, G. V.; Curk, T.; Richter, R. P. *Acc. Chem. Res.* **2023**, *56* (7), 729–739. DOI: 10.1021/acs.accounts.2c00672.
(2) Chabaud, B.; Bonnet, H.; Lartia, R.; Van Der Heyden, A.; Auzély-Velty, R.; Boturyn, D.; Coche-Guérente, L.; Dubacheva, G. V. *Langmuir* **2024**, *40* (9), 4646–4660. DOI: 10.1021/acs.langmuir.3c03279.

Catalysis as enabling tool for innovative chiroptical switches

Adrien Lefebvre[1] and Adrien Quintard*[1]

[1] *Université Grenoble Alpes, CNRS, DCM, 38000 Grenoble, France*
adrien.lefebvre@univ-grenoble-alpes.fr

Chiroptical switches, where reversible changes between different states triggers a change in the chiroptical properties, hold tremendous potential for the development of a diverse range of tools, including chiral logic gates, chiral separation, asymmetric catalysis, and data storage. However, up to this point, chiroptical switching materials have primarily relied on altering the structure of pre-existing chiral molecules. In this work, the application of modern organic synthetic methodologies enables the development of an efficient chiroptical switch. By taking advantage of an organocatalyzed desymetrization of an achiral diol, we were able to access a temporary enantioenriched compound, evolving back to the achiral diol upon time. The evolution of this innovative chiroptical switch can be followed by the fluctuation of the chiroptical properties of the system.



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The Centre National de la Recherche Scientifique (CNRS), Université Grenoble-Alpes, IRGA funding from the IDEX-UGA (15-IDEX-0002) are warmly acknowledged for financial support of our research on molecular machine.

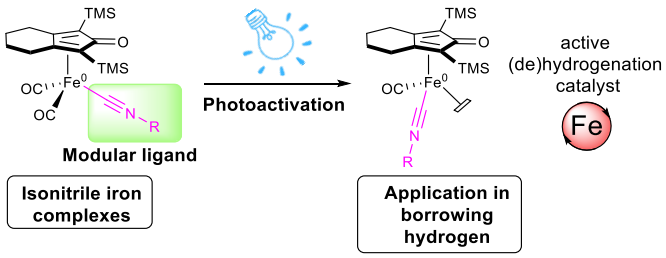
Novel iron-based catalysts for enantioselective photoinduced reversible hydrogen transfer reactions

Marine Olivier,[a,b] Gaëtan Quintil,[a,b] Adrien Quintard[a]*, Amélie Kochem[b]*

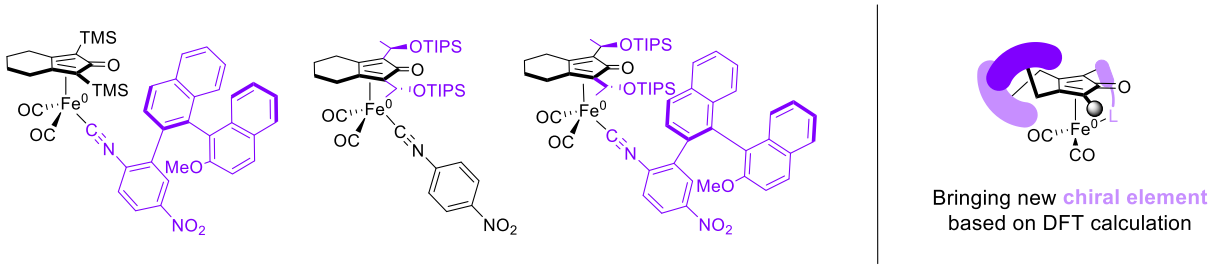
[a] *Univ. Grenoble Alpes, CNRS, DCM, 38000 Grenoble, France.*
[b] *Université Grenoble Alpes, CNRS, CEA, LCBM (UMR 5249), 38000 Grenoble, France.*

marine.olivier@univ-grenoble-alpes.fr

The quest for sustainable and cost-efficient synthetic processes has led to the development of iron cyclopentadienone catalysts, replacing costly noble metal complexes notably for hydrogen transfer reactions. These catalysts, featuring cooperativity between iron and the cyclopentadienone ligand, provided unique reactivities, particularly in borrowing hydrogen reactions.[1-2] Modification of these catalysts has mainly focused on changing the cyclopentadienone core, but little has been done with the iron tricarbonyl structure. In order to potentially enhance the activity of these complexes and obtain different reactivities, the CO ligands has been replaced by different isonitrile ligands, creating a library of modular complexes efficient in catalysis.[3]



On the other hand, the ongoing challenge also involves developing potent chiral iron cyclopentadienone complexes to enantioselectively reduce ketones. Indeed, despite numerous efforts to design new chiral cyclopentadienone complexes, it usually only provided moderate enantiocontrol while requiring above 30 bar of H_2 to obtain a good reactivity. To overcome such limitations, various strategies have been tested such as introducing chiral isonitrile ligands, chiral cyclopentadienone ligands or a combination of both to reduce ketone under milder conditions with isopropanol as an hydrogen donor. Excellent reactivity has been observed in the reduction of a broad range of substrates, providing up to 78:22 er. To increase the enantioselectivity of this process, we aim to design new chiral iron cyclopentadienone catalyst based on DFT calculations.



References:

(1) Roudier, M.; Constantieux, T.; Quintard, A.; Rodriguez, *J. Org. Lett.* **2014**, 16.
(2) Quintard, A.; Constantieux, T.; Rodriguez, J. Angew. Chem. Int. *Ed.* **2013**, *52*.
(3) Gounon, C.; Quintil, G.; Pécaut, J.; Clémancey, M.; Bjornsson, R.; Quintard, A.; Kochem,A. *Dalton Trans.* **2025**, *54*.
(4) Quintil, G.; Pécaut, J.; Bjornsson, R.; Kochem, A.; Quintard, A. *Eur. J. Org. Chem.***2026**, *29*.

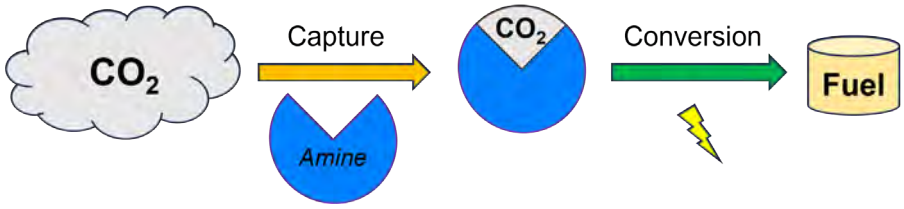
DECIPHERING THE EFFECT OF AMINE-BASED CAPTURE AGENTS IN DIRECT CO2 CAPTURE AND CONVERSION

Laurent Severy, Gabrielle Mpacko Priso, Alicia Gomis-Berenguer, Isabelle Rougeaux, Yassine Naciri, Bertrand Reuillard, Koushik Ranu, Vincent Artero

Laboratoire de Chimie et Biologie des Métaux, Université Grenoble Alpes, CEA, CNRS, 17 rue des Martyrs, 38000 Grenoble, France

Laurent.severy@cea.fr

Direct capture and conversion of CO_2 from dilute sources is essential for closing the carbon cycle and reducing net greenhouse emissions, particularly for sectors that are difficult to decarbonize. However, there are currently only few studies on integrating existing CO_2 capture systems with the electrochemical reduction [1,2]. To address this gap, we are investigating heterogenized molecular catalysts in combination with aqueous amine-based capturing agents [3] to achieve direct conversion of dilute CO_2 into C1 products such as CO and formic acid.
The efficiency of the conversion process is shown to depend on a variety of parameters, including the type of amine and its pKa, the concentration of capturing agent, the concentration of additives and most importantly the concentration of CO_2.
We report on the effect of different amine-based capturing agents on the conversion of CO_2 using a manganese-based catalyst immobilized on carbon nanotubes [4]. Speciation and amine type are shown to have a major effect on the selectivity of electrocatalytic reduction.



Acknowledgements
This work is funded by CEA's Audace ! program (ANR-24-RRII-0004).

References

[1] G. Leverick *et al.*, *ACS Catal.* 2023, *13*, 18, 12322.
[2] J. Chang *et al.*, *Renew. Sust. Energ. Rev.* 2026, *231*, 116754.
[3] A. Qayoom Mir *et al.*, *J. Am. Chem. Soc*. 2025, *147*, 43, 39123.
[4] B. Reuillard *et al., J. Am. Chem. Soc.* 2017, *139*, 41, 14425.

Design of artificial metalloenzymes for enantioselective sulfoxidation

Stann Van Baaren,[a] Yohann Moreau,[b] Christine Cavazza[c], Caroline Marchi Delapierre[a], and Stéphane Ménage[a]

[a] UGA-CNRS-CEA UMR 5249, LCBM-BioCE, [b] UGA-CNRS-CEA UMR 5249, LCBM-CoMX, [c] UGA-CNRS-CEA UMR 5249, LCBM-BEE

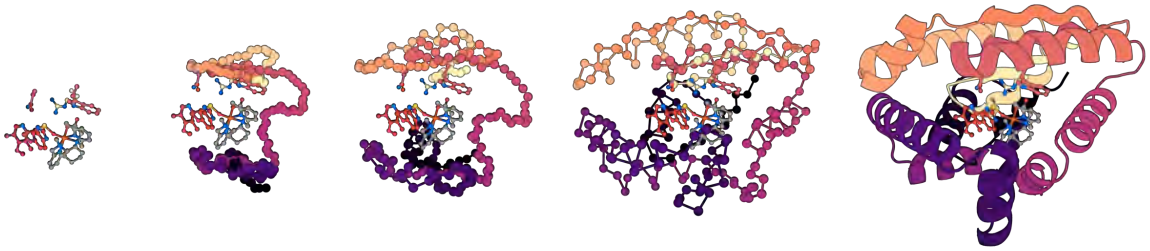
stann.van-baaren@univ-grenoble-alpes.fr

Natural enzymes are exceptional catalysts with high selectivity and efficiency under mild conditions. However, their industrial application is limited to natural transformations. On the other hand, artificial metalloenzymes allow for a larger range of reactivities but often lack enantioselectivity.[1] This work presents an innovative approach to improving artificial metalloenzymes stereoselectivity by using artificial intelligence for their design.

Our research focuses on developing artificial metalloenzymes capable of enantioselective oxidation of thioethers to sulfoxides, a transformation critical in pharmaceutical synthesis, particularly for proton pump inhibitors like Esomeprazole.

The strategy we use consist of designing from scratch artificial proteins around an ideal active site containing an inorganic complex. This presentation will explain the construction of the design pipeline and its different inputs. Starting from the theoretical active site construction and optimization with QM tools, it will address the AI assisted design of the backbone containing this theoretical active site using a RFdiffusion, the generation of corresponding sequences, their computational testing and filtering that lead to the selection of 24 candidates.[2,3]

Finally, we will present data on the high-throughput expression of these proteins from synthetic genes and discuss preliminary findings regarding their catalytic performance.



References

(1) Marchi-Delapierre, C.; Cavazza, C.; Ménage, S. EcNikA, a Versatile Tool in the Field of Artificial Metalloenzymes. *J. Inorg. Biochem.* **2025**, *262*, 112740. https://doi.org/10.1016/j.jinorgbio.2024.112740.

(2) Watson, J. L.; Juergens, D.; Bennett, N. R.; Trippe, B. L.; Yim, J.; Eisenach, H. E.; Ahern, W.; Borst, A. J.; Ragotte, R. J.; Milles, L. F.; Wicky, B. I. M.; Hanikel, N.; Pellock, S. J.; Courbet, A.; Sheffler, W.; Wang, J.; Venkatesh, P.; Sappington, I.; Torres, S. V.; Lauko, A.; De Bortoli, V.; Mathieu, E.; Ovchinnikov, S.; Barzilay, R.; Jaakkola, T. S.; DiMaio, F.; Baek, M.; Baker, D. De Novo Design of Protein Structure and Function with RFdiffusion. *Nature* **2023**, *620* (7976), 1089–1100. https://doi.org/10.1038/s41586-023-06415-8.

(3) Dauparas, J.; Anishchenko, I.; Bennett, N.; Bai, H.; Ragotte, R. J.; Milles, L. F.; Wicky, B. I. M.; Courbet, A.; de Haas, R. J.; Bethel, N.; Leung, P. J. Y.; Huddy, T. F.; Pellock, S.; Tischer, D.; Chan, F.; Koepnick, B.; Nguyen, H.; Kang, A.; Sankaran, B.; Bera, A. K.; King, N. P.; Baker, D. Robust Deep Learning–Based Protein Sequence Design Using ProteinMPNN. *Science* **2022**, *378* (6615), 49–56. https://doi.org/10.1126/science.add2187.

Clicked Bioinspired Copper Complexes at Carbon Nanotubes for Oxygen Reduction Reaction

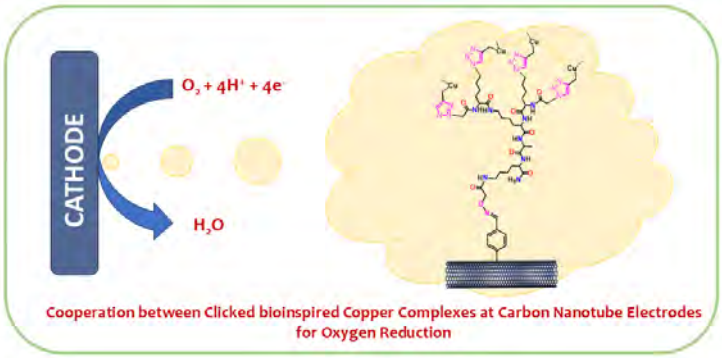
Sunita Birara[1]*, Aurore Thibon-Pouret[1], Catherine Belle[1], Alan Le Goff[1]

[1] Université Grenoble Alpes, CNRS UMR 5250, DCM, Grenoble, France

catherine.belle@univ-grenoble-alpes.fr, alan.le-goff@univ-grenoble-alpes.fr

Proton-exchange membrane fuel cells (PEMFCs) that operate at low temperatures are key technologies for clean energy systems aimed at reducing reliance on fossil fuels. However, the catalysts used at both the anode and cathode are largely based on platinum group metals (PGMs). The scarcity and limited availability of platinum worldwide therefore represent a major challenge to the large-scale deployment of these devices. Copper-based enzymes, such as laccase, are capable of performing the Oxygen Reduction Reaction at the cathode side with efficiencies comparable to platinum-based catalysts.[1] However, their poor stability prevents their direct and practical incorporation into conventional PEMFCs. Despite notable progress in the design of complexes inspired by hydrogenases at the anode, where hydrogen oxidation occurs, there is still no effective substitute available for the cathode.

The objective of the project is the development of novel bioinspired copper catalysts utilizing BMPA (bis(2-picolyl)amine) derivatives bearing click-chemistry synthons and their immobilization on carbon nanotubes by taking advantage of clickable multivalent peptidic/dendrimeric scaffolds.[2] These scaffolds will provide multiple anchor points for mono- and dinuclear copper complexes while providing spatial control. This control is aimed at triggering cooperation between mono- and dinuclear copper complexes towards oxygen activation and reduction. Finally, these novel nanohybrid catalysts will be implemented in a fully bioinspired Pt-free H_2/air fuel cell.



Cooperation between Clicked bioinspired Copper Complexes at Carbon Nanotube Electrodes for Oxygen Reduction

Acknowledgements

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References

[1] Le Goff, A.; Holzinger, M.; Cosnier, S. Recent Progress in Oxygen-Reducing Laccase Biocathodes for Enzymatic Biofuel Cells. Cell. Mol. Life Sci. 2015, 72 (5), 941–952.

[2] Gentil, S.; Pifferi, C.; Rousselot-Pailley, P.; Tron, T.; Renaudet, O.; Le Goff, A. Clicked Bifunctional Dendrimeric and Cyclopeptidic Addressable Redox Scaffolds for the Functionalization of Carbon Nanotubes with Redox Molecules and Enzymes. Langmuir 2021, 37 (3), 1001–1011.

Polyfunctionalization of allylic alcohols via borrowing hydrogen catalysis

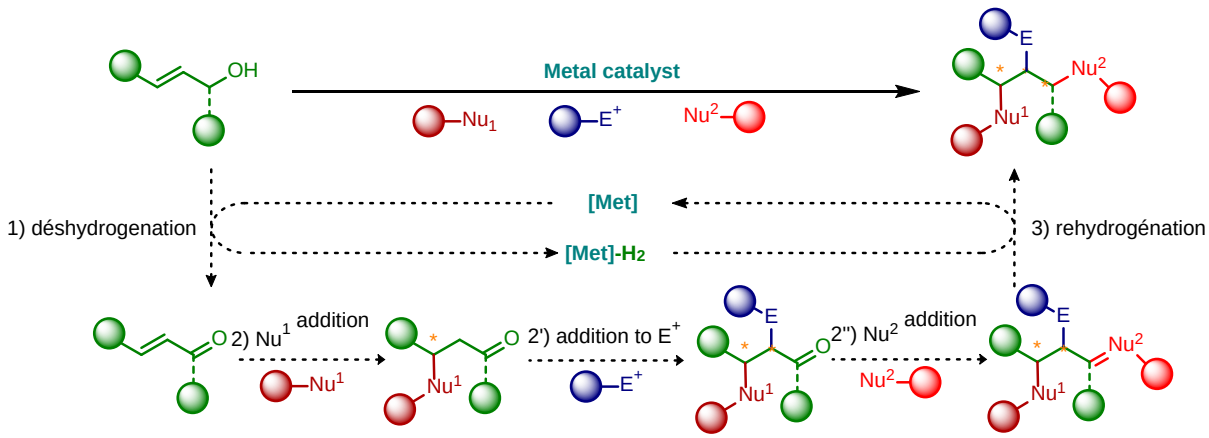
Michaël Vaglio-Pret[1], Adrien Quintard[1] and Amélie Kochem[1].

michael.vaglio-pret@univ-grenoble-alpes.fr[1]

adrien.quintard@univ-grenoble-alpes.fr[1]

amélie.kochem@cea.fr[1]

Borrowing hydrogen reactions are among the greenest approaches for creating complex molecules from simple materials. The use of allylic alcohols within this catalysis is interesting because it gives access to transient α,β-unsaturated carbonyls, thus expanding the possibilities of functionalization at different positions of the alcohol substrate. Our team has exploited this reactivity by making an innovative borrowing hydrogen cascade reaction, combining an amination and an intramolecular oxa-Michael reaction. This stereoselective synthesis permits access to various THP moieties, notably potentially bioactive molecules.



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[1] Michaël Vaglio-Pret, Mattéo Favre, Milly Ogden, Amelie Kochem and Adrien Quintard, *Org Chem Front*, **2026,** Advance Article, DOI : https://doi-org.sid2nomade-1.grenet.fr/10.1039/D6QO00148C