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Ecole Nationale Supérieure de Chimie de Rennes

COLLEGE DOCTORAL BRETAGNE — SCIENCES DE LA MATIERE DES MOLECULES ET MATERIAUX

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Abstract booklet

Plenary conferences :

Dr. Guillaume Lefèvre
CNRS, Chimie ParisTech
Unlocking the access to unsaturated iron synthons in homogeneous catalysis: key role of s and p-block salts.

Dr. Maxime Vassaux
CNRS, Institut de Physique de Rennes
Simulation of the mechanical properties of materials across scales, starting from the atoms.

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Amphitheatre C

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Gold bis(dithiolene) complexes: a dual interest in single-component molecular conductor and biological activity

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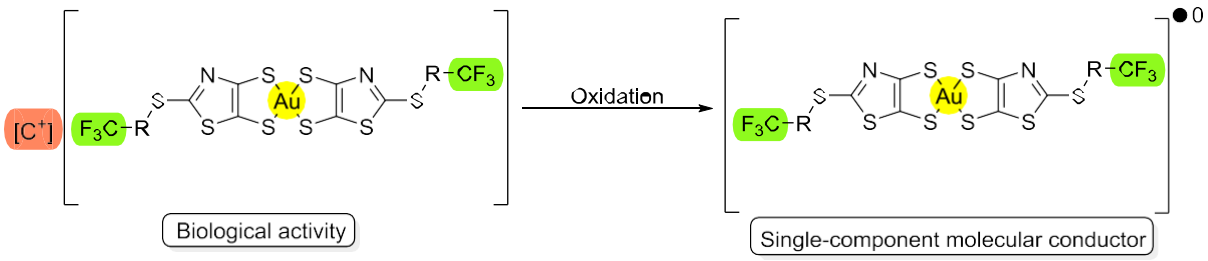
Gold bis(dithiolene) complexes exhibit a dual interest: in the neutral radical state, they constitute precursors for single-component molecular conductors [1], while in the monoanionic state, they display biological activities [2]. Fluorination of the dithiolene ligands makes it possible to investigate both its influence on the antibacterial properties of monoanionic complexes and the role of fluorinated group segregation in the organization and intermolecular interactions of neutral complexes. To date, only one neutral fluorinated gold complex has been reported, revealing a highly ordered organization characterized by the formation of distinct bilayers of fluorinated chains [3]. In this work, we present a synthetic strategy leading to fluorinated gold bis(dithiolene) complexes, enabling the study of fluorine atom segregation and molecular interactions both in the radical state, with a view toward the development of organic conductive materials, and in the monoanionic state in the context of biological applications.



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Adding value to terpenoids: from pseudoionone to 1-methyl-1,3-cyclohexadiene

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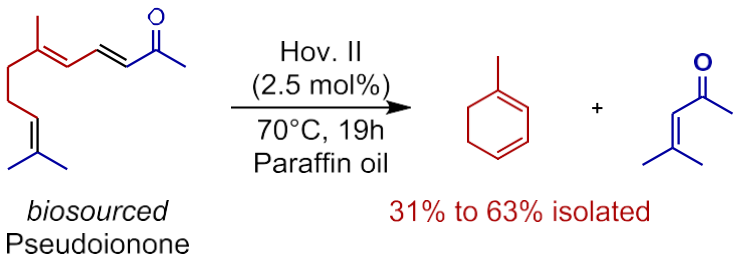
The rising importance of bio-sourced alternatives to fossil-based feedstocks and base chemicals marks one of the most important and demanding tasks for the modern chemical society.[1,2] It is therefore essential to continue to expand research and the development of new techniques and applications to ensure the aforementioned transition.[3] Herein, we report a new approach towards the synthesis of 1-methyl-1,3-cyclohexadiene 1 as well as mesityl oxide 2 from bio-sourced pseudoionone. With the everlasting demand of small olefinic molecules in polymer chemistry as well as pharmacy, these results may contribute to said transition.

The approach involves the synthesis of isomerically pure 3E, 5Z-pseudoionone, starting from bio-sourced and commercially available nerol. The spatial orientation of the resulting triene enables selective ring-closing metathesis using the commercially available Hoveyda 2nd generation catalyst. When utilizing commercially available pseudoionone, available as isomeric mixture of 3E, 5E and 3E,5Z-pseudoionone (~70%/30, respectively), the reaction proceeds, giving mostly cross-metathesis products. However, the roughly 30% of 3E,5Z-Isomer proceed to the desired products selectively. Due to the high volatility of the products and their close proximity in boiling points, proper isolation and separation of the products became an integral part of this project.



Citation: *Green Chem.*, **2025**,27, 11809-11815.

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Insights into self-assembly mechanisms and electrical properties of tetrazine-based supramolecular polymers

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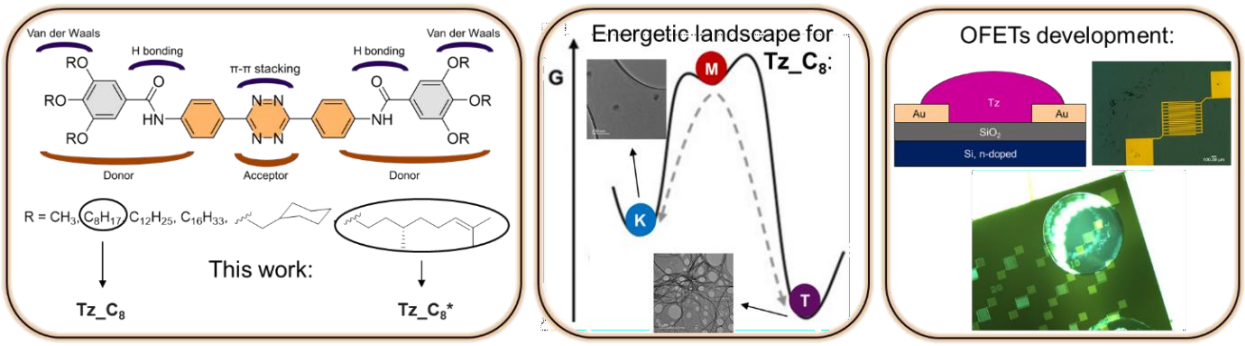
Supramolecular polymers are composed of monomeric units held together by highly directional and reversible secondary non-covalent interactions, resulting in dynamic species that can exhibit properties such as self-healing functions and responsiveness towards external stimuli.[1] Originally, supramolecular polymerization was regarded as a process entirely driven by thermodynamics. However, as the understanding of this process broadened, kinetic contributions started to emerge as impactful factors towards the outcome of the self-assembly, and multiple pathways in competition for the same monomer can occur. In particular, experimental conditions (*e.g.*, temperature or solvent modulation) and specific interactions (*e.g.*, donor-acceptor interactions) can have significant impact on the polymerization.[2,3] We recently developed a new family of supramolecular polymers, featuring a central tetrazine core and different aliphatic side chains, resulting in donor-acceptor-donor structures with interesting self-assembly mechanisms. In determined conditions, supramolecular gels can be obtained, and given the electron properties (*e.g.*, available reduction potentials, electron deficiency) exhibited by tetrazine, these materials can be studied towards the development of novel n-type organic semiconductors.[4] In this work, the self-assembly of two of these platforms (**Tz_C$_8$** and **Tz_C$_8$***) is explored, describing how subtle structural differences can not only impact the morphologies of these systems, but also their evolution towards thermodynamic equilibrium. Additionally, preliminary studies on their conductive capabilities are reported, with the development of organic field effect transistors (OFETs) featuring the tetrazine-based supramolecular gels.



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Magneto-Chiral Dichroism Modulation in Single-Molecule Magnets of Lanthanide Ions

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Single-Molecule Magnets (SMMs) are promising candidates for next-generation data storage applications because they exhibit magnetic bistability at the single-molecule scale. In parallel, magneto-chiral dichroism (MChD) has been proposed as an optical alternative for the readout of magnetic information[1]. Thus, SMMs exhibiting MChD could serve as ideal candidates for optically readable data storage media. Furthermore, incorporating molecular switches into such systems would enable access to different magnetic states of the SMMs[2]. The main objective of this project is to design, synthesize, and investigate chiral lanthanide-based SMMs with switching capabilities. In these systems, the lanthanide ion is the source of the SMM behavior, while the MChD response arises from the coordination of the metal center with chiral ligands. Here, the systems under investigation are chiral lanthanide complexes based on dithienylethene (DTE) derivatives, which are well known for their ability to undergo reversible photoinduced isomerization between two forms[3]. Upon switching, the lanthanide crystal field—and consequently the magnetic anisotropy—is expected to be modulated, resulting in variations in both the SMM properties and the MChD response.

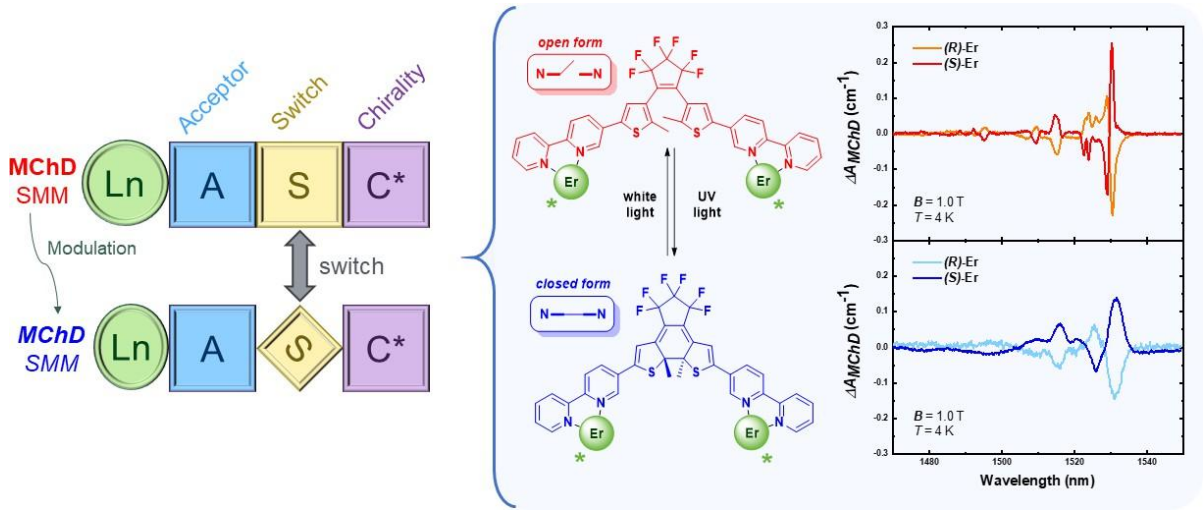

Figure. (Left) Schematic representation of the studied systems. (Right) Open and closed forms of the chiral photoactive Er(III) bis(bipyridyl)-DTE complex and the corresponding MChD signals.

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Design of Molecular Catalysts for Renewable Electrochemical CO_2 Valorization

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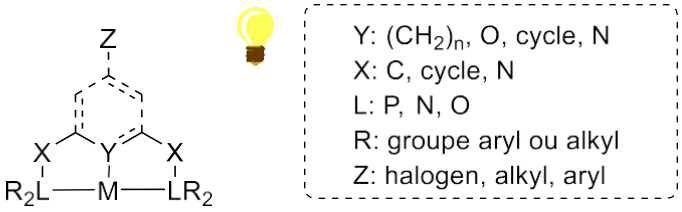
The electrochemical reduction of carbon dioxide (CO_2) represents a promising strategy for converting a greenhouse gas into value-added chemicals and fuels.[1] Transition metal complexes with tailored ligands have demonstrated high efficiency and selectivity in catalyzing CO_2 reduction reactions. In this study, we focus on the design and synthesis of pincer ligands coordinated to first-row transition metals, aiming to develop robust catalysts for electrochemical CO_2 reduction. Pincer ligands are known for their rigid tridentate framework, which provides stability to the metal center and allows fine-tuning of electronic and steric properties. [2,3]



We report the synthesis of several novel pincer-metal complexes and characterize them using spectroscopic techniques, including NMR and UV-Vis, as well as electrochemical methods such as cyclic voltammetry. Preliminary electrochemical studies indicate that these complexes facilitate CO_2 reduction at relatively low overpotentials. The results suggest that the choice of metal center and ligand architecture strongly influences catalytic activity and product distribution. This work provides insights into the ''structure-activity'' relationships of pincer-based catalysts and highlights their potential in sustainable CO_2 conversion technologies. Future studies will focus on mechanistic investigations and optimization of catalytic performance under practical electrochemical conditions.

Acknowledgments:

The authors acknowledge financial support from UBO and CNRS. CC thanks region Bretagne (ARED) and UBO for PhD funding.

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Reactivity and electronic structure of low-valent phopshino-α-iminopyridine based iron imido and amido complexes

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Compounds containing iron-nitrogen multiple bonds have long been considered intermediates in nitrogen reduction[1] and have proven valuable for the synthesis of nitrogen-containing compounds through powerful transformations such as C–H bond amination[2,3] and olefin aziridination.[4] Accordingly, there is a natural interest in understanding the structural and electronic properties of metal imido units for controlling and predicting their reactivity.[5]

To this end, di-*tert*-butylphosphine-α-iminopyridine ($^{t\text{Bu}}$PNN$^{\text{Dipp}}$) iron imido complexes were synthesized by reacting a PNN iron-nitrogen precursor (**1**) with a series of organoazides (**2–6**). The PNN framework employed combines structural motifs capable of both redox and chemical metal–ligand cooperativity.[6]

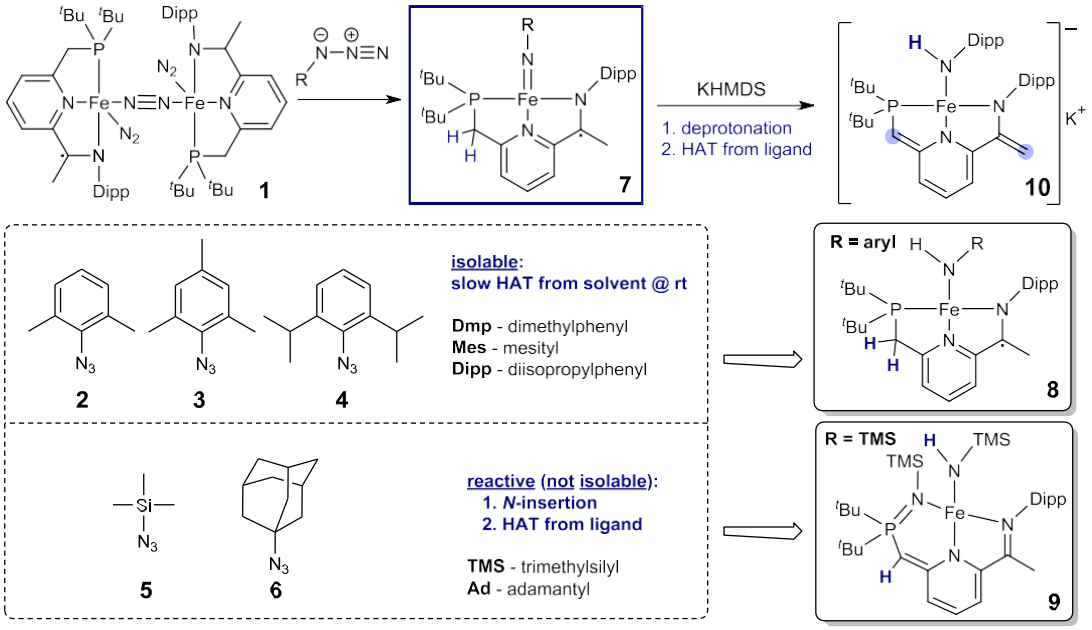

Figure 1. Synthesis of various $^{t\text{Bu}}$PNN$^{\text{Dipp}}$ iron imido complexes and their reactivity.

The PNN iron imido complexes **7** displayed distinct reactivities depending on the nature of the imido *N*-substituent. Complexes bearing R = aryl groups (**2–4**) afforded the isolable complexes, which undergo slow intermolecular hydrogen-atom transfer (HAT) forming the corresponding amido complexes **8**. In contrast, imido complexes featuring the substituents R = **5,6** proved to be non-isolable, *e.g.* decomposing *via* a *N*-insertion pathway to form complex **9**. Deprotonation of the PNN ligand backbone in an aryl iron imido complex (**7**) using a mild base was proposed as a strategy to enhance the overall reactivity of the complex and render it applicable in homogeneous catalysis.

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Combining photochemistry and oxidative couplings to access innovative heteroatom-containing Polycyclic Aromatic Hydrocarbons

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Over the last century, chemists have shown great interest in polycyclic aromatic hydrocarbons (PAHs).[1] This interest increased after the discovery of graphene, a two-dimensional material made exclusively of sp²-hybridized carbon atoms and exhibiting exceptional electronic properties.[2] Since then, increasingly extended π-conjugated systems have been developed, leading to the synthesis of molecular nanographenes (PAHs whose dimensions exceed one nanometer). These compounds show great potential for the development of organic optoelectronic devices such as OLEDs (Organic Light-Emitting Diodes), OPVs (Organic Photovoltaics), and batteries. [2]

Introducing heteroatoms into PAHs provides a powerful strategy to modulate their structure, reactivity, and electronic properties.[3] For instance, incorporating nitrogen atoms enables coordination chemistry, combining the photophysical properties of transition metals with those of the PAH framework.[4] Our research group pioneered the insertion of phosphorus into PAHs, taking advantage of the specificities of this heteroatom.[5]

This research project aims to develop new synthetic routes for the incorporation of heteroatoms particularly phosphorus and silicon into extended PAHs (Figure 1). To this end we will combine photocyclization and chemical cyclodeshydrogenation.[6] To reach our objective, we plan to synthesize literature-known alkynes containing large PAHs frameworks. These intermediates will serve as key building blocks for the preparation of the target heterocycles, using original methodologies: the silver-mediated phosphole cyclization[7, 8] and the silirene to silole methodology.[9]

We aim to investigate how extended conjugation and the incorporation of heteroatoms will influence the optical, redox, and possibly chiroptical properties of the target molecules.

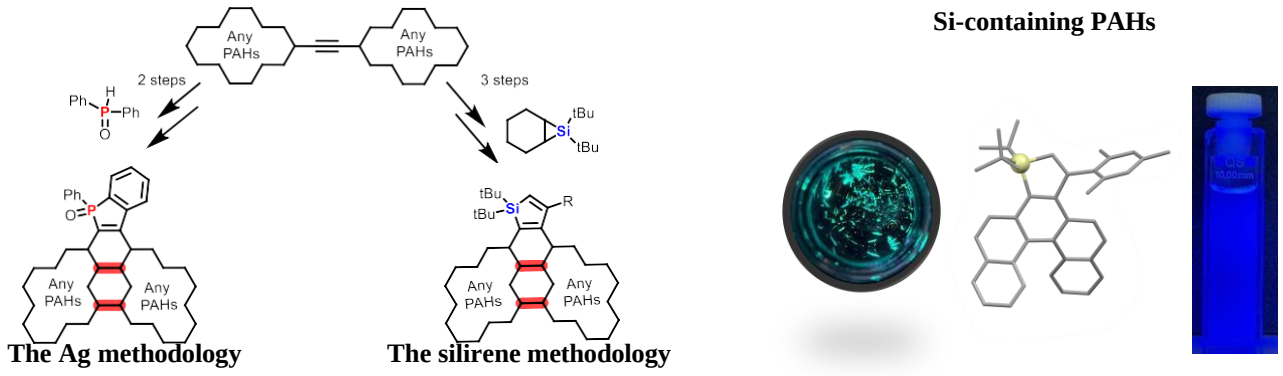

Figure 1 : Synthetic strategy toward Phosphole and Silole derivatives and exemple of structural characterization of the Silole with photoluminescence in Solution and the Solid State.

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Synergic Partnership of Iron Catalysis and Blue Light Activation for Hydrogen Borrowing Transformation at Room Temperature

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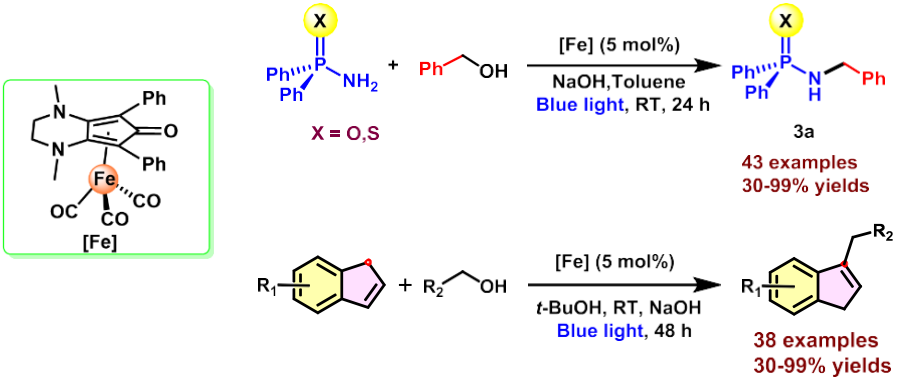
Sustainability and efficiency have become crucial priorities in modern molecular synthesis. With the increasing environmental awareness and the global drive to reduce chemical waste, energy consumption, and dependence on precious metals, the development of **greener, atom-economical catalytic methodologies** is of growing importance. The **borrowing hydrogen (BH)** or **hydrogen auto-transfer** strategy has emerged as a powerful and sustainable tool to build new C–C and C–N bonds by using readily available (bio)alcohols as electrophilic alkylating agents.[1] This transformation offers a **benign alternative** to conventional alkylation methods,[2] generating **water as the only by-product** while avoiding stoichiometric reagents or halogenated intermediates. In this context, our research focuses on two representative and complementary case studies involving iron-catalyzed hydrogen borrowing methodology: the ***C*-alkylation of indenes**[3] and the ***N*-alkylation of phosphinic (thio)amide derivatives**.[4] We aim to demonstrate that accurate catalyst design associated to blue-light activation permitted to perform energy-efficient activation technologies, notably at room temperature. To the best of our knowledge, **no previous examples** of either **indene alkylation** or **phosphinic (thio)amide *N*-alkylation at room temperature** have been achieved **using iron catalysis.**



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Magneto-Chiral Dichroism of Helicene-based Er(III) Complexes

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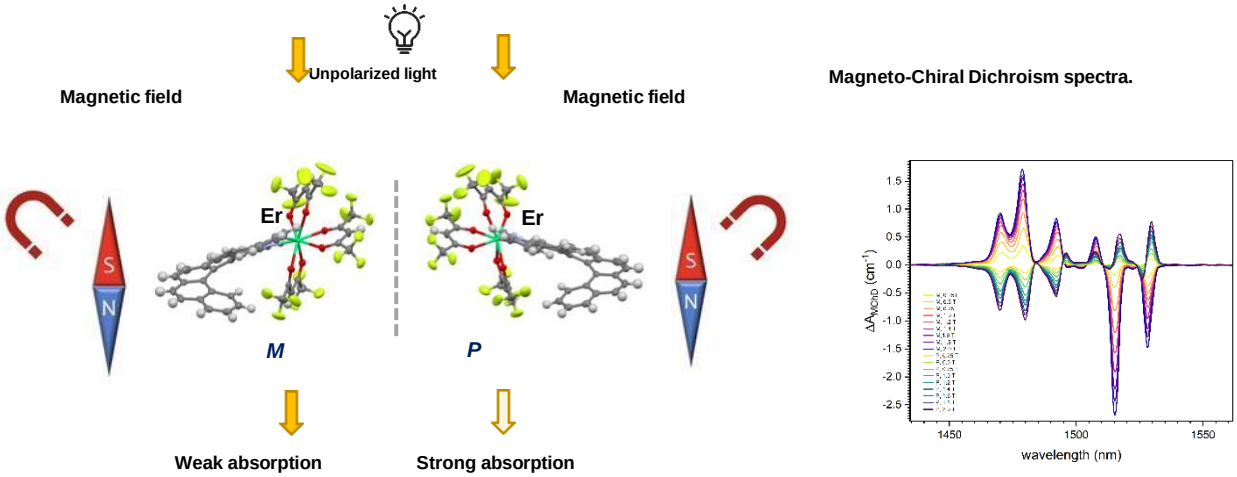
Magneto-Chiral dichroism (MChD)[1] is a cross effect between chirality and magnetism. It corresponds to the differential optical response between a magnetic field being either parallel or antiparallel to the incident light. It gives rise to a dichroic response which depends on the handedness of the chiral molecule. Given that the majority of lanthanide complexes are paramagnetic systems[2] with intrinsic spin-orbit couplings, they are valuable motifs for designing chiral chemical structures, which can be used to study the Magneto-Chiral effect. Helicenes are representative chiral motifs formed of *ortho*-fused aromatic or heteroaromatic rings[3]. They have a helical shape and display remarkable chiroptical properties[4,5]. From previous work, our group has reported Ln-helicene complex showing great SMM behavior and strong MChD response.[6,7] In this context, the Magneto-Chiral Dichroism of Er(III)[6]helicene-bipyridine was investigated for the first time in the NIR region and in high magnetic fields, up to 9T.



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Copper-64 PET imaging radiopharmaceuticals based on bicyclic peptide-triazamacrocycle conjugates

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Nuclear medicine plays a central role in cancer diagnosis and therapy through the use of radiopharmaceuticals. These agents combine a biological targeting vector labeled with a radionuclide, which can be a metal ion such as [^{68}Ga] or [^{64}Cu] for diagnosis, or [^{177}Lu] for therapy. Efficient chelation is essential to ensure *in vivo* stability of the radiometal complex. A well-established clinical example is the theranostic pair [^{68}Ga]Ga-DOTA-TATE/[^{177}Lu]Lu-DOTA-TATE targeting somatostatin receptor (SSTR2) overexpressed in neuroendocrine tumors,[1] where the use of the same peptide vector (TATE or TOC) and chelator (DOTA) ensures comparable biodistribution in imaging and therapy. Cyclic polyamines such as DOTA are widely recognized for their excellent chelation properties.

Peptides are well-known targeting vectors in nuclear medicine, particularly cyclic peptides that offer enhanced metabolic stability and high affinity for tumor-associated receptors.[2] Recently, bicyclic peptides have attracted increasing interest due to their rigid two-loop architecture enabling stronger affinity and improved selectivity toward complex tumor targets such as integrin $\alpha_v\beta_3$.[3]

In this work, we aim to develop innovative radiometal-based radiopharmaceuticals using a trifunctionalized triazacyclononane (tacn) chelator as a central scaffold for the development of ^{64}Cu-labeled bicyclic peptides. We will present the design and synthesis of tacn-based chelators, their bioconjugation to peptides provided by our collaborators, and the first proof-of-concept [^{64}Cu] radiolabeling experiments.

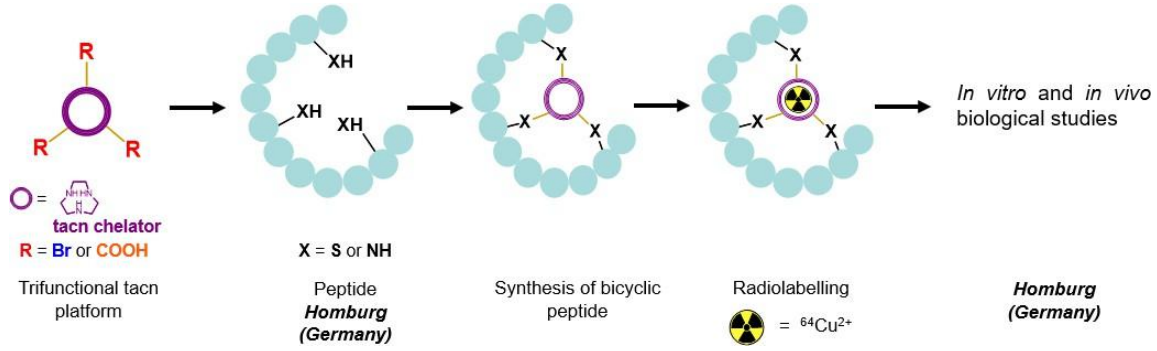

Figure 1. Schematic illustration of the concept for the development of bicyclic peptide conjugates based on trifunctionalized metal chelators as central structural scaffolds, enabling radiolabeling of the bicyclic conjugates with copper-64.

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Coordination polymers based on lanthanides and poly-halogenated benzene-carboxylate ligands: structural and optical insights for comparative analysis

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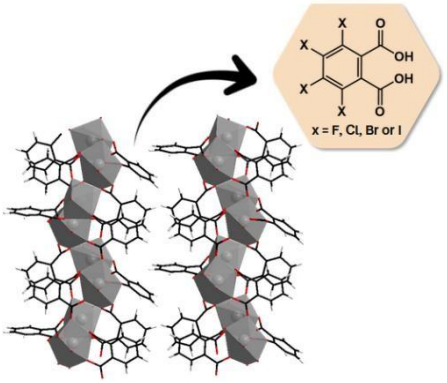
In recent decades, coordination polymers have attracted considerable attention due to their remarkable optical properties, particularly for applications in lighting and anti-counterfeiting technologies.[1] These materials consist of metal centers coordinated to various organic ligands, forming extended one-, two-, or three-dimensional frameworks. The organization of these crystalline structures is governed by a variety of supramolecular interactions, including hydrogen bonding, halogen bonding, and π-stacking interactions.[2]

The incorporation of halogenated benzene-poly-carboxylate ligands enables coordination to metal centers through their carboxylate groups, while also offering the possibility of halogen bonding or short halogen···halogen interactions. Previous studies have suggested that coordination polymers based on such ligands are promising candidates for the development of new luminescent materials.[3,4] Nevertheless, much remains to be explored, as complete structural investigations covering all halogenated benzene-carboxylate derivatives with rare earth elements have not yet been fully reported.

Crystallogenesis experiments were conducted to obtain new crystalline structures of coordination polymers by varying the number, the nature, and the position of the halogen substituents on the ligand. The impact of these modifications on the resulting crystal structures was examined, and the results of this study will be presented.



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Incorporation of photoswitches into nitronylnitroxide ligands

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The development of light-responsive supramolecular systems capable of controlling metallogels properties remains a significant challenge. The deposition of Single-Chain Magnets (SCMs) onto surfaces can be facilitated by metallogels. Opening the way to efficient organisation of molecule-based magnet memories.[1] The incorporation of photoactive units into nitronyl–nitroxide radical ligands intended for the assembly of lanthanide-based SCMs capable of undergoing sol–gel transitions is investigated as a strategy to introduce light-driven structural control.[2] In this context, ligands bearing a fluoroazobenzene photochromic unit were designed. These fluoroazobenzene-functionalized radicals contain a reversible trans–cis photoswitch positioned at varying distances from the coordinating site, enabling light-induced geometrical perturbations of the supramolecular assembly.

Various nitronyl–nitroxide ligands incorporating azobenzene moieties were synthesized. The influence of the radical on the photochromic behaviour was evaluated, and several ligands retain good photochromic performance. Initial explorations toward the formation of photochromic gels based on these ligands are also presented.

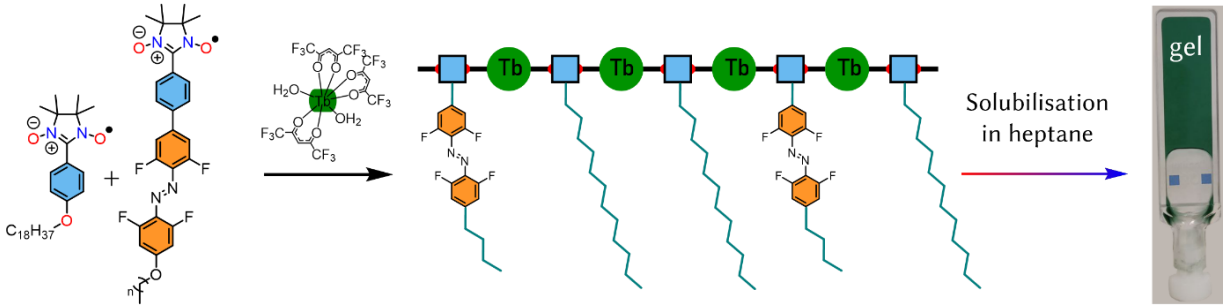

Figure 1 : From ligands to doped metallogels

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Sergeants & Soldiers approach for chirality control in gels of supramolecular nanotubes of Ln^{3+} based 1D coordination polymers

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Coordination polymers are highly tunable and versatile objects opening real perspectives in the technological use of these unique systems. In particular, peculiar magnetic and chiroptical properties can be observed on lanthanide–radical chains with original topologies such as helical chains. Unfortunately, their surface deposition is tricky and restrain their uses. A strategy is to form metallogels of supramolecular nanotubes out of these objects using radicals with long alkyl chains such as 2-(4'-(octadecyloxy)phenyl)-4,4,5,5-tetra-methylimidazolin-1-oxyl-3-oxide) (NIT-C18).
Herein, we demonstrate that the chirality of the supramolecular nanotubes can be controlled using (R/S)-2-(4'-(octadecan-2-yloxy)-4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide (NIT-C18(R/S)) radicals. We also show that the combination of chiral and achiral radicals in a Sergent & Soldiers approach allows the formation of enantiomerically pure nanotubes which can be deposited on surface via wet chemistry techniques. Thus, it gives a hint to better control their supramolecular organization on surface.

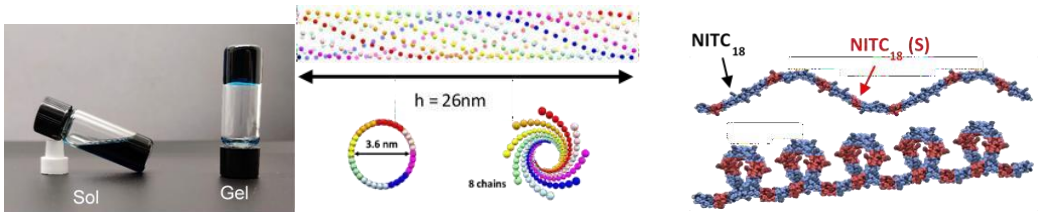

Figure 1 Left: Gelation test. Middle: Supramolecular nanotube representation extracted from SAXS measurements. Right: Sergent & Soldiers 1D coordination polymer.

Acknowledgments We thank the ANR-23-C009-0020 NANOCHAINS, CNRS, INSA Rennes, Rennes metropole, Collège doctoral de Bretagne, région Bretagne, IRIS-E and EUR CAPS for the funding.

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Luminescence of the Protactinium in solution

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Actinides are the heaviest naturally occurring elements in both the universe and the Earth's crust[1]. Although substantial experimental and theoretical work has been devoted to these species, their chemistry remains only partially elucidated, especially regarding oxidation states and speciation[2–4]. This gap arises from the intrinsic radioactivity of actinides and the difficulty of accurately treating electronic correlation in quantum-chemical calculations.

Protactinium is a suitable candidate for study: it exhibits an f^1 electronic configuration in the +IV oxidation state and has experimentally accessible absorption and emission spectra in aqueous solution[5–8]. Theoretical investigation of protactinium's absorption was previously conducted by Hanna Oher and Florent Réal at the University of Lille; the present work focuses on the emission mechanism.

Quantum-chemical calculations of protactinium fluorescence in aqueous solution indicate a strong influence of solvation on the excited-state geometry and a change in coordination relative to the ground state. The calculated spectra match the measured data and also predict a second, previously unobserved transition, which is interpreted through a second-order crystal-field analysis performed with the NewMag program[9].

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Synthesis of new conducting materials by mechanochemistry to elaborate solids electrolytes in $[Na_2S]_{1-x}[(In_2S_3)_{1-y}(Sb_2S_3)_y]_x$ system

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For many years, several solid electrolytes have been developed. By replacing the liquid electrolyte with a solid electrolyte, the device is protected from the risk of leaks and therefore enhances the safety of the system. Moreover, the use of sodium, more abundant than lithium, allows to bypass the geopolitical constraints related to the latter.

Among the systems present in the literature, Na_3PS_4 and Na_3SbS_4 have been extensively studied due to their ionic conductivity with room temperature values of $2x10^{-4}$ S/cm [1] and $3x10^{-3}$ S/cm [2], respectively. In order to improve the conductivity properties of these materials, a large number of researches based on computational methods have also focused on the substitution of antimony by other elements. More particularly to the material Na_3SbS_4, by substituting antimony with other elements such as tungsten ($Na_{3-x}Sb_{1-x}W_xS_4$ [3]) or silicon ($Na_{3-x}Sb_{1-x}Si_xS_4$ [4]), it has been demonstrated that the rate of sodium vacancies increased. The formation of conduction network results directly from this increase and thus improves the diffusion properties of the Na^+ ions of the material.

Thus, in order to develop new sodium ion conducting materials, the choice was oriented towards the study of the substitution of antimony by indium which is a known element for the formation of amorphous compounds in the Na_2S-In_2S_3 [5] system. In addition, glassy materials due to their disordered structure attract great interest from the ionic conductivity. The classic synthesis method for obtaining vitreous compounds is melt-quenching in a silica ampoule. However, the sodium contained in our materials diffuses into the silica used in these processes, making it very fragile until the breaking of the ampoule. That is why the chosen method for making such materials is mechanochemistry.
In this presentation, we focus on the synthesis by mechanical milling and the study of compounds of the system $[Na_2S]_{1-y}[(In_2S_3)_{1-x}(Sb_2S_3)_x]_y$. The addition of Na_2S in the $(In_2S_3)_{1-x}(Sb_2S_3)_x$ matrices studied allows obtaining different amorphous compounds but also amorphous-crystal composites. Moreover, the Le Bail refinements carried out on XRD patterns highlight a decrease in the mesh parameter when indium is substituted by antimony.

Key words: solid electrolyte; mechanochemistry; amorphous; amorphous-crystalline composites

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Nanostructuration of sillicate glasses using water: a multiscale simulation investigation

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Abstract

Understanding how water interacts with glass remains a central question in glass science, as the glass industry moves toward decarbonized processes using innovative process such as hydrogen-fired furnaces, here water becomes an inherent by-product. Water is expected to lower key characteristic temperatures of glass, such as the glass transition, softening, or crystallization temperatures, but its broader impact remains uncertain: How will hydration affect structural, mechanical and optical properties.

Nanoconfined water is known to exhibit slow dynamics, high viscosity, and can even adopt a glassy state(1). Exploiting these distinctive features, we examine how confined water modi- fies the mechanical behaviour of silica glass across nano to macroscopic scales. Specifically, we vary the hydration level and perform a thorough comparison of different interatomic potentials, including ReaxFF(2) and DCRP(3), to capture the diversity and evolution of water–silica interactions.

We further investigate the influence of water content, pore sizes, and spatial distributions on the structural and mechanical responses of the glass network.

This work offers new insight into the interplay between hydration, nanoconfinement, dy- namics of water and mechanical properties in silicate glasses, and opens perspectives for understanding water-rich environments relevant to materials engineering, geosciences, and industrial process.

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Keywords: LAMMPS, Molecular Dynamics, Water–glass interactions, Nanoconfined water, Silicate glasses, Hydrous Glasses, Mechanical properties, Interatomic potentials, Pores, Nanoconfinement, Nanoporosity

*Speaker

Ice-Induced Structural Reconfigurations in Nanoconfined Water-Glycerol Mixtures

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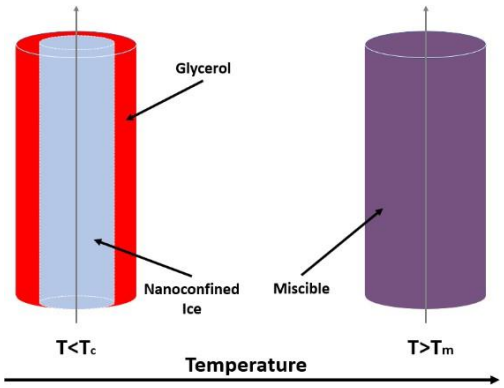
We elucidated the mesoscopic organization emerging in water-glycerol mixtures confined within the nanoporous cylindrical pores of SBA-15 and MCM-41 silicas, with pore diameters of 8.1 nm and 3.5 nm, respectively. Neutron diffraction was used to track variation in the intensity of Bragg reflections originating from the crystalline pore arrangements after filling and as a function of composition and temperature. Additionally, isotopic substitution was employed to systematically adjust the scattering length density contrast between the different components of the mixtures. The radial concentration profile within the pore was determined by fitting various form factor models to the experimental intensity data. At room temperature, our findings support a uniform compositional distribution within the pore. Upon cooling, we observe partial ice crystallization at $T_f \approx 200$-230 K in solutions where the water content exceeds the maximally freeze-concentrated solution threshold (30% w/w), while vitrification of the entire solution is observed otherwise. The partial freezing triggers phase separation into distinct ice and liquid domains. Remarkably, the morphology adopted by these domains is shaped by the geometry of the confining cylindrical nanopore, resulting in a core-shell structure: a pure ice core surrounded by a glycerol-rich layer adjacent to the pore surface. In contrast to the unfreezable layer commonly found in pure confined water, typically around 0.6 nm thick, our findings demonstrate that the size of the interfacial glassy solution is governed by both the pore size and the overall mixture composition. In the systems studied, this interfacial thickness varies between 0.3-1.4 nm, with its composition aligning with



that of the MFCS.

Acknowledgments: The experiments were conducted as part of the Ph.D. project of M. N. Kamar, who gratefully acknowledges funding from the University of Rennes. We express our gratitude to the Institut Laue-Langevin (ILL) for providing neutron beam time, which was central in the success of this study. We acknowledge the funding by ANR-22-CE50-0002 and ANR-23-CE29-0028.

Reference: This manuscript was accepted for publication in ***The Journal of Chemical Physics*** on March 23, 2026 (Manuscript No. JCP26-AR-00724R).

Title: Impact of farming and livestock production methods on the metabolic profiles of foods: a transdisciplinary approach for a better understanding of food choices.

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Agroecology, a holistic approach to agricultural production, is attracting increasing interest for its capacity to restore soil and ecosystem health and to improve the nutritional quality of food. However, although its environmental benefits are well documented, its effects on nutritional composition remain little studied [1]. Moreover, consumers' willingness to pay (WTP) for sustainability remains low, except when individual benefits such as taste or health are perceived [2, 3]. This thesis adopts a transdisciplinary approach to analyze the links between agroecology, nutritional quality, and consumer valuation. It aims to compare the micronutritional composition of agroecological and conventional products (notably antioxidants), identify the mechanisms explaining these variations, develop analytical methods and biomarkers based on a global metabolomic approach, and assess consumers' WTP.

We studied four tomato varieties (Belmandia, Diamandia, cherry, Côtelées), grown in greenhouses under two production systems: soilless (conventional) and living soil (agroecological). The Belmandia variety was analyzed seven times from May to September 2025, while the others were analyzed occasionally. Their nutritional composition was evaluated through antioxidant capacity (FRAP/DPPH) and metabolic profile (HPTLC). A pilot study in experimental economics, focused on cherry tomatoes, measured consumers' willingness to pay (WTP) (students) according to three types of information: definitions of the production systems, environmental impacts, and health impacts.

The first analyses reveal that Belmandia and cherry tomatoes grown in living soil (agroecological) show higher antioxidant capacity (FRAP/DPPH) and a stronger metabolic profile (HPTLC) during peak season (May–August), but not in September. The other varieties, which were degraded, were excluded. The pilot study shows that consumers are willing to pay more for tomatoes grown in living soil, and even more when information is provided.

The initial results of this thesis reveal significant differences between agroecological and conventional production systems, confirming the potential of agroecology. To further investigate these observations, additional measurements will be conducted on other foods (apples, soybeans), and a rigorous experiment will need to be carried out in order to validate and generalize these conclusions.

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Infrared interferometry for precision spectroscopy of complex molecular processes

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Observational data obtained from ground-based and space telescopes cannot be fully interpreted in isolation; they must be complemented by theoretical modeling and laboratory astrophysics. Together, these three approaches enable the validation and refinement of chemical network models relevant to the interstellar medium and planetary atmospheres.
Here we develop a Fourier Transform Spectrometer designed [1] for the acquisition of molecular absorption spectra in the mid-infrared range (3–10 μm). The instrument provides high-resolution spectral measurements, essential for fundamental spectroscopic investigations. Preliminary results from CO_2
spectroscopy in a plasma environment are reported, demonstrating the instrument's capabilities. Coming work on coupling the current setup to a supersonic expansion chamber will be discussed. The experimental setup and associated technical challenges encountered during the development process are also reviewed.

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Development of radial and spherical GRadient INdex (GRIN) optics by ionic exchange to improve the performance of infrared optronic systems

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Currently, high-performance imaging systems covering the SWIR–LWIR bands[1,2] are subject to strict constraints in terms of size, weight, optical power, and cost, requiring simplified optical architectures[3–5]. In this context, gradient-index (GRIN) optics offer an attractive alternative to conventional complex systems composed of multiple lenses. GRIN optics enable control of light propagation through a continuous spatial variation of the refractive index, allowing the design of more compact systems with reduced aberrations and fewer optical elements[6]. Although they are widely used in the visible range, their development in the infrared remains limited, mainly due to the difficulty of achieving stable and well-controlled refractive index gradients in materials that are transparent in the MWIR–LWIR ranges. Chalcogenide glasses are promising candidates for these applications due to their broad transmission window, high refractive index ($n \approx 2–3$), and ease of shaping. However, achieving reproducible radial profiles with sufficient index contrast remains a major challenge. Recent studies by C. Fourmentin and J. Guichard[7] have demonstrated the fabrication of infrared GRIN lenses via Na^+ /Ag^+ ionic exchange in chalcogenide glasses, achieving significant refractive index variations. However, these methods suffer from limitations such as crack formation and interface degradation. In order to further reduce corrosion caused by silver ions, better control of the ionic exchange rate is required. Thus, a new method of solid– solid Na^+ /Ag^+ ionic exchange has been developed. This process uses pure silver nitrates "diluted" in silica powder in order to limit contact between the silver nitrates and the glass sample. In addition, the process is carried out at a higher temperature, enabling the accumulation and diffusion steps to be combined. This approach significantly reduces internal mechanical stresses responsible for the formation of microcracks observed in previous studies[8]. The resulting lenses exhibit improved structural integrity and good reproducibility, with very few sample losses. Optical characterization reveals a pronounced refractive index gradient, with a higher index at the periphery and a parabolic profile, indicating ion diffusion toward the core.

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Towards Accurate Molecular Dynamics: Developing Diabatic Dipole Moment Surface with Artificial Neural Network

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To accurately simulate spectra in situations where the Born–Oppenheimer approximation breaks down, we need more than just a high-quality potential energy surface (PES). We also require good representations of other molecular property operators, such as the dipole moment and the angular momentum. These operators are often not totally symmetric, which makes their description more challenging.

In this work, we develop a method that uses a diabatic basis together with symmetry considerations for representing all these operators. The artificial neural network was employed to fit both the potential energy surface and dipole moment surface. We apply this approach to radical systems, constructing both dipole-moment surfaces and dipole-transition-moment surfaces.

Room-Temperature Ferromagnetic Oxide Nanosheets for Spintronic Applications

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Spintronics intends to further develop electronic systems with the aim of reducing energy consumption while maintaining growing performances. In this framework, 2D oxide materials are a promising platform offering model properties ranging from high-k 2D dielectrics [1] to 2D ferroelectrics [2] or 2D ferromagnets [3] while being intrinsically air stable, an overall key asset for 2D spintronics.

This presentation focuses on the development of 2D-TFCO ($[Ti_{0.8-x/4}Fe_{x/2}Co_{0.2-x/4}O_2]^{0.4-}$) doped-titanate oxide nanosheets, an original 2D oxide stable in ambient atmosphere with ferromagnetic properties at room temperature [3]. TFCO oxide nanosheets are produced via the exfoliation of the bulk layered parent oxide KTFCO ($K_{0.8}Ti_{1.6-x/2}Fe_xCo_{0.4-x/2}O_4$), synthesized by solid-state chemistry methods. The optimization of synthesis parameters has led to the growth of millimetric KTFCO single crystals (see Fig.1a) suitable for bulk properties analysis prior to the exfoliation of large area TFCO nanosheets.

Latest results on KTFCO crystals characterizations will be presented, especially their magnetic properties with Curie point above room temperature. Structural properties of the layered phase will also be presented. Exfoliation of KTFCO crystals into TFCO-nanosheets (Fig.1b) will be demonstrated as a first step towards the integration of this 2D ferromagnetic insulator as a functional material in spintronics heterostructures (Fig.1c). Finally, a specific focus will be dedicated to the investigation of the electronic, magnetic, transport and magneto-transport properties of 2D-TFCO single and multilayers.

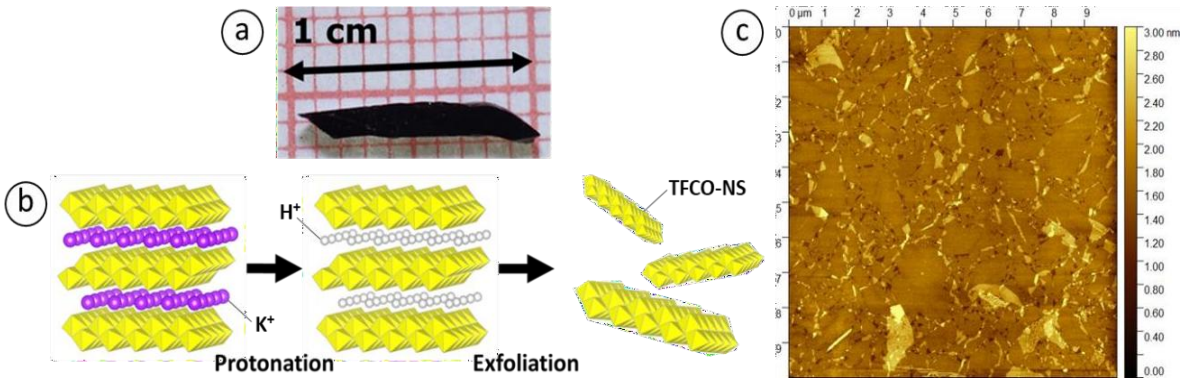

Fig.1. a) Picture of millimetric KTFCO layered crystal grown using molten salts method; b) Detailed diagram of KTFCO chemical exfoliation process; c) AFM image of single-layer film of TFCO nanosheets

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Tracking and Controlling Reaction Intermediates in Transition Metal Oxides with Ultrafast Spectroscopy

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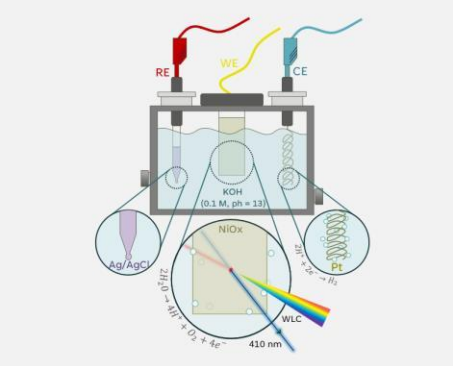
Earth-abundant transition metal oxides (TMOs) based on Ni, Fe, and Co are being widely explored as potential electrocatalysts. [1,2] Their low production costs and high availability make them promising candidates for applications in energy and chemical product generation. [3] However, achieving the high catalytic efficiencies and stabilities required for industrial implementation remains challenging. [4] Electrochemical reactions, driven by an external electric field, occur as a series of proton-coupled electron transfer steps in which reaction intermediates are generated. [5] However, the exact mechanism behind the generation and stabilisation of those intermediates in TMOs is not well understood. [6] In this presentation, I will discuss how ultrafast spectroscopy can be used as a tool to monitor and control the formation of reaction intermediates at the electrochemical interface. Specifically, I will report data on Ni-based oxides used for the oxygen evolution reaction (OER), tracking the spectroscopic fingerprints of different intermediates, and demonstrating how they can be manipulated using light. Finally, I will examine the opportunities and constraints associated with light-driven control of pre-catalytic species and the reaction mechanism.



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Computational Design of Excited-State Absorption for Optical Limiting

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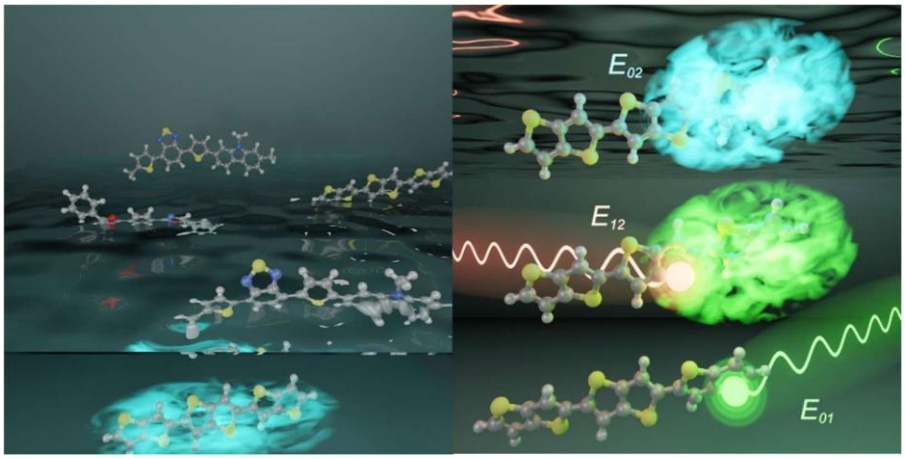
During excited-state absorption (ESA), an electron residing in an electronically excited state, typically populated via prior ground-state absorption, absorbs a photon and is further promoted to a higher energy level. ESA plays a key role in applications such as transient absorption spectroscopy and optical limiting devices. In optical limiting, ESA, combined with other nonlinear optical phenomena, causes materials to absorb strongly at high incident light intensities while remaining nearly transparent at low intensities.

In this contribution, I introduce the key aspects that ought be considered when performing static quantum- chemical ESA calculations on organic molecules. The general introduction is followed by an overview of the four consecutive parts of my PhD project. The project itself focuses on the development of an efficient computational model for calculating ESA intensities, i.e. oscillator strengths (*f*), as well as the formulation of design rules for enhancing ESA in potential organic optical limiters.

The individual subprojects comprise: *i)* benchmarking quadratic-response methods for ESA oscillator strength calculations against high-level theoretical references [1]; *ii)* evaluating and correcting an alternative approximate unrelaxed linear-response TD-DFT approach [2]; *iii)* developing a solvation protocol within the unrelaxed linear-response framework [3]; and *iv)* investigating the effect of various substitutions on ESA intensity in an azulene molecule.



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