

Congrès SCF Nord Est 2026



*14 - 16 janvier 2026
Novotel Metz Centre
(France)*



Société Chimique de France
Événements SCF Nord-Est

Association des sections régionales
Alsace, Bourgogne Franche-Comté,
Champagne-Ardenne et Lorraine

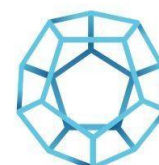
Recueil des résumés

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Chimie & Société



Bienvenue au Congrès SCF Nord-Est 2026

Chers collègues, chères et chers congressistes,

C'est un plaisir tout particulier de vous accueillir à Metz, au sein de l'Hôtel Novotel Centre, pour le **congrès SCF Nord-Est 2026**. Ce recueil de résumés reflète l'excellence et la diversité des travaux qui seront présentés durant ces trois journées de rencontre, du **14 au 16 janvier 2026**.

Véritable trait d'union entre les anciennes régions **Alsace, Bourgogne-Franche-Comté, Champagne-Ardenne et Lorraine**, ce congrès est avant tout un lieu d'échanges privilégié. Il a pour ambition de fédérer notre communauté — académiques comme industriels — autour des avancées les plus récentes de la chimie, qu'elles soient fondamentales ou finalisées.

La chimie au cœur des enjeux sociétaux

Ce recueil illustre la richesse de nos thématiques. À travers les conférences plénières, les présentations invitées et vos communications, nous explorerons ensemble des domaines aussi variés que :

- La protection de l'environnement et la transition énergétique ;
- La santé et les nouveaux matériaux ;
- L'interaction lumière-matière, la chimie des métaux et l'instrumentation.

Un espace de dialogue et de proximité

L'une des forces de ce rendez-vous est sa convivialité. En réunissant pratiquement soixante-dix participants dans un même lieu, nous souhaitons favoriser des interactions scientifiques fructueuses et resserrer les liens entre les laboratoires du Nord-Est de la France.

Nous remercions l'ensemble des contributeurs pour la qualité de leurs résumés, ainsi que nos partenaires et sponsors qui soutiennent la vitalité de la chimie régionale.

Nous vous souhaitons un excellent congrès, riche en découvertes et en nouvelles collaborations.

Le Comité d'Organisation du Congrès SCF Nord-Est 2026

Comité d'organisation

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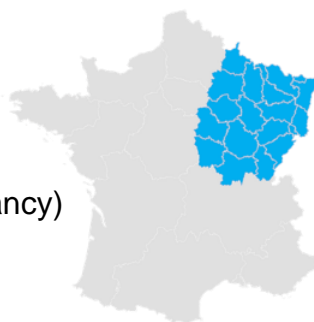
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Programme

Mercredi 14 janvier	
13H45 - 14H45	Accueil et enregistrement (Hall)
14H45 - 15H00	Ouverture SCF Nord Est 2026 (Amphithéâtre)
15H00 - 15h50	PL1 - Hydrometallurgical recovery of tin and copper from mobile phone printed circuit boards (THYMO project) <i>Éric Meux</i>
15H50-16H30	Pause-café (Hall)
16H30 - 17h00	Prix thèse SCF Alsace - <i>Valentyn Pozhydaiev</i>
	A Povarov-type reaction to access tetrahydroquinolines from N-benzylhydroxyl amines and alkenes in HFIP
17H00 - 17h30	Prix thèse SCF Bourgogne Franche Comté - <i>Leya Liu</i>
	Towards LSPR-based detection of lipopolysaccharides using gold nanorods
17H30 - 18h00	Prix thèse SCF Champagne Ardenne - <i>Rémi Pereira</i>
	Building Molecular Complexity: Catalytic Access to Chiral Polycycles with Quaternary Centers
18H00 - 18h30	Prix thèse SCF Lorraine - <i>Lyns Verel Che Dji</i>
	Low-field NMR relaxometry methods for studying and designing superparamagnetic iron oxide contrast agents
18H30 - 19h00	Femmes & Sciences
19H30	Cocktail (Hall)

Jeudi 15 janvier - matinée		
8H40 – 9H30	PL2 - On the chelation of radionuclides by siderophores and bioinspired analogs: environmental and health-related applications <i>Michel Meyer</i>	
9H30-10H00	Pause-café (Hall)	
	Session 1 (Salle 1)	Session 2 (Salle 2)
10H00-10H30	IL1 - Engineering surface-active nanomaterials for selective catalysis and emerging nanozyme applications <i>Almudena Marti-Morant</i>	IL2 - On-surface synthesis: the role of halogen bonding <i>Frédéric Chérioux</i>
10H30-10H45	OC01 - Colloidal synthesis of twisted gold nanoparticles <i>Thomas Girardet</i>	OC06 - New L-proline-based deep eutectic solvents in heterocyclic syntheses <i>Stéphanie Hesse</i>
10H45-11H00	OC02 - Engineering assemblies of viologens <i>Eleanna Nikolopoulos</i>	OC07 - Isothiazolones: heterocyclic compounds of therapeutic interest <i>Antoine Lesure</i>
11H00-11H15	OC03 - Alternative methodological approaches for Taylor dispersion analysis - Application to AuNP-Protein <i>Jérémy Gouyon</i>	OC08 - The Viridium-Acrinium conjugate: a multi-responsive molecule <i>Guijun Sun</i>
11H15-11H30	OC04 - Ion exchange on colloidal Mg/Al LDH nanoparticles: when kinetics leads to thermodynamics irreversibility <i>Marc Hébrant</i>	OC09 - Towards sustainable chemistry: plasmonic catalysis for biomass-derived HMF oxidation <i>Filippo Pieretti</i>
11H30-11H45	OC05 - Development of Recovery Processes for Gadolinium Present in Hospital Effluents Using Modified and/or Eco-Designed Natural Biosorbents <i>Fatima Kaabouch</i>	OC10 - Synthesis and bioevaluation of N-heterocyclic/M-M bonded complexes <i>Isabelle Jourdain</i>
	Déjeuner + Session Posters	

Jeudi 15 janvier – après-midi		
	Session 3 (Salle 1)	Session 4 (Salle 2)
13H45-14H15	IL3 - From molecules to aggregates: in silico rationalization of optoelectronic properties of conductive materials <i>Laura Le Bras</i>	IL4 - Reconfigurable and programmable materials or light-induced 3D &4D <i>Arnaud Spangenberg</i>
14h15-14h30	OC11 - Development of a hard carbon/tin composite negative electrode for sodium-ion batteries via electrodeposition <i>Stan Viaud</i>	OC15 - Azaullazine meets iron: orbital design unlocking long-lived emission in Fe(II) complexes <i>Philippe Pierrat</i>
14H30-14H45	OC12 - Solvothermal elaboration of tridimensional nitrogen and iron co-doped graphenic materials (ORR catalysis in PEMFC) <i>Mélodie Becker</i>	OC16 - Design and synthesis of new iron complexes for photophysical applications <i>Johanne Coutard</i>
14H45-15H00	OC13 - Variations around the CoNiFeMnCr equimolar composition: high temperature properties of some HEA or MEA <i>Patrice Berthod</i>	OC17 - Integrated absorption-emission spectroscopy under one- and two-photon excitation for styryl-substituted cyclic enones <i>Cédric Mittelheisser</i>
15H00-15H15	OC14 - Optical imaging electrochemical reactivity through an electrochromic counter electrode <i>Claire Hugon</i>	OC18 - Engineering NIR-active photosensitizers from supramolecular NHC platforms for photodynamic <i>Florence Dumarçay</i>
15H30-16H00	Pause-café (Hall)	
16H00-16H50	PL3 - Exploring the chemistry of protein-nucleic acids complexes by computational approaches <i>Emmanuelle Bignon</i>	
17H30-19H30	Sortie culturelle - Temps libre	
19H30	Dîner de Gala	

Vendredi 16 janvier		
8H30 – 9H20	PL4 - Porphyrins at work: from molecular recognition to light-activated therapy <i>Valérie Heitz</i>	
9H20-9H50	Pause-café (Hall)	
	Session 1 (Salle 1)	Session 2 (Salle 2)
9H50-10H20	IL5 - Some examples of carbohydrate-templated chemical tools for biological purposes <i>Jean-Bernard Behr</i>	IL6 - Complex mixtures analysis by ViscY NMR experiments: at the limit of NOE <i>Pedro Lameiras</i>
10H20-10H35	OC19 - SIRT6–Nucleosome Interactions: C-Terminal Domain Binding Modes That Modulate DNA Unwrapping <i>Yuya Qiu</i>	IL7 - Exploring archaeological organic substances: molecular, isotopic and radiocarbon-dating approaches <i>Pierre Adam</i>
10H35-10H50	OC20 - Synthesis and Functionalization of Cyanine-7 Dyes for Theranostic Applications <i>Khaoula Cherkani El Hassani</i>	
10H50-11H05	OC21 - Near infrared photodynamic therapy for pancreatic cancer: design of porphyrin-based photosensitizers <i>Emmanuel Valzer</i>	OC22 - Discrimination of racemic and enantiopure phenylalanine crystals by low frequency polarized Raman spectroscopy <i>Yechi Romiald Yavo</i>
11H10-12H00	PL5 - From the search for structural chemodiversity to applications in medicinal chemistry <i>Stéphane Gérard</i>	
	Clôture congrès SCF Nord Est 2026	

Conférences Plénières

Conférenciers en séance plénière



Emmanuelle BIGNON

CNRS Research Scientist — UMR 7019 (CNRS-UL)

Laboratory of Theoretical Physics and Chemistry, University of Lorraine (Nancy)

Exploring the chemistry of protein-nucleic acids complexes by computational approaches

Molecular modeling, DNA



Stéphane GÉRARD

Professor — UMR 7312 (CNRS-URCA)

Institute of Molecular Chemistry of Reims, University of Reims Champagne Ardenne (Reims)

From the search for structural chemodiversity to applications in medicinal chemistry

Chemobiology, MedChem



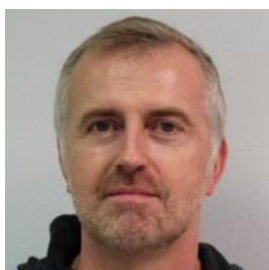
Valérie HEITZ

Professor — UMR 7177 (CNRS-UniStra)

Synthesis of Multifunctional Molecular Assemblies, University of Strasbourg (Strasbourg)

Porphyrins at work: from molecular recognition to light-activated therapy

Supramolecular Chemistry, Health



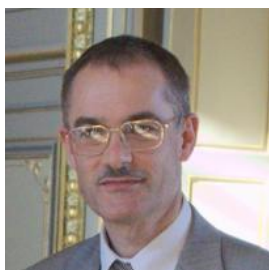
Éric MEUX

Professor — UMR 7198 (CNRS-UL)

Jean Lamour Institute, University of Lorraine (Metz)

Hydrometallurgical recovery of tin and copper from mobile phone printed circuit boards (thymo project)

Materials, Durability



Michel MEYER

CNRS Research Scientist — UMR 6302 (CNRS-UBE)

Institute of Molecular Chemistry, Université Bourgogne Europe (Dijon)

On the chelation of radionuclides by siderophores and bioinspired analogs: environmental and health-related applications

Coordination Chemistry, Speciation

PL1 - HYDROMETALLURGICAL RECOVERY OF TIN AND COPPER FROM MOBILE PHONE PRINTED CIRCUIT BOARDS (THYMO PROJECT)

Eric Meux,¹ Marianne L'hôte,¹ Nathalie Leclerc,¹ Sébastien Diliberto,¹ Stéphanie Michel,¹ Pierrat,² Hervé Muhr,³ Yosri Khalsi,⁴ Abdel Tazibt,⁴ Frédéric Diot,⁴

¹ Institut Jean Lamour, 57000 Metz (eric.meux@univ-lorraine.fr)

² Laboratoire Lorrain de Chimie Moléculaire, 57000 Metz

³ Laboratoire Réactions et Génie des Procédés, 54000 Nancy

⁴ CRITT-Techniques Jet Fluide et Usinage, 57000 Bar-le-Duc

⁵ GeoRessources, 54500 Vandœuvre-lès-Nancy.

Keywords: hydrometallurgy, mobiles phones, PCBs, copper, tin

Summary: every year, around 24 million mobile phones are sold in France. The collection rate for end-of-life phones is low, with only 0.5 million being recycled. [1] According to the eco-organization ECOLOGIC [2], at least 46 million smartphones are “hibernating” in French people's drawers. Smartphones Printed Circuit Boards (PCBs) are considered “rich” and their market value can be very high (more than €230,000/t) due to the presence of gold, palladium, and silver. Currently, PCBs are recycled using pyrometallurgical processes, which are energy-intensive and do not allow all metals to be recovered. The THYMO project aimed to develop a hydrometallurgical process with low environmental impact that allows for the recovery of as many metals as possible. The automated dismantling of mobiles phones was developed by CRITT TJFU. GeoRessources was responsible for grinding PCBs and enriching the ground material with metals using various physical techniques. After thoroughly characterizing the ground material, a hydrometallurgical process was developed to recover tin and copper (Fig. 1).

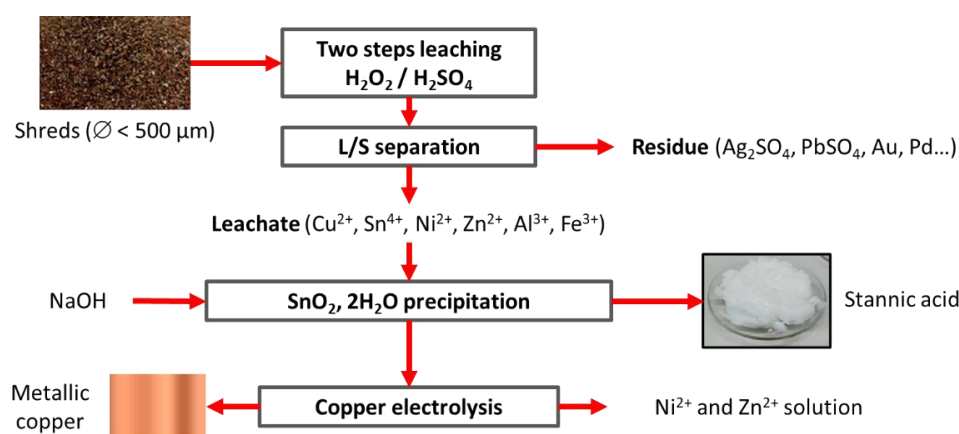


Fig. 1: flow-sheet of the hydrometallurgical process developed

The leaching stage, optimized using Design Of Experiments, enabled more than 97% of Cu and Sn to be dissolved using a green reagent. Sn^{4+} cations were then selectively precipitated in the form of $\text{SnO}_2 \cdot 2\text{H}_2\text{O}$. Copper was then in metallic form by electrolysis with a purity greater than 99.99%. The leaching residues, mainly composed of non-metallic compounds (Al_2O_3 , SiO_2), contain the unleached precious metals. A complete mineralogical characterization of these residues is currently underway at GeoRessources in order to consider the possibility of enriching them in precious metals using physical methods.

References:

[1] *Sofies and Bio Innovation Service*. 2019. Étude du marché et parc de téléphones portables français en vue d'augmenter durablement leur taux de collecte [2] *Harris Interactive et CREDOC pour Ecologic*. 2023. Evaluation du nombre de téléphones portables usagés stockés en France.

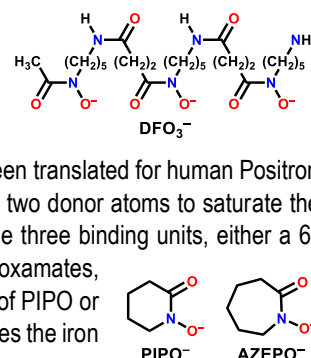
PL2 - ON THE CHELATION OF RADIONUCLIDES BY SIDEROPHORES AND BIOINSPIRED ANALOGS: ENVIRONMENTAL AND HEALTH-RELATED APPLICATIONS

Michel Meyer,¹

¹ Université Bourgogne Europe, CNRS, Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB, UMR CNRS 6302), 9 avenue Alain Savary, 21078 Dijon Cedex, France (michel.meyer@u-bourgogne.fr)

Keywords: hydroxamic acids, actinides, zirconium, speciation, DGT samplers, radiopharmaceuticals

Summary: Siderophores are secondary metabolites excreted by some bacteria, yeasts, and a few plants into their environment to scavenge iron(III) from insoluble oxohydroxides, transport this essential nutrient across the membrane and finally deliver it to the cytosol in the reduced iron(II) form. Among the more than 600 siderophores isolated so far, most of the bacterial and fungal chelators are hexadentate, incorporating mainly hydroxamate or catecholate binding units. Desferrioxamine B (DFO) is an emblematic trishydroxamic siderophore of linear topology produced by numerous terrestrial and marine actinomycetes, including the soil bacterium *Streptomyces pilosus* from which it was isolated for the first time in 1958. It became in the mid 1960's an authorized drug for treating iron or aluminum overloads in humans and is nowadays entitled as the "gold standard" for chelating the positron emitting radionuclide $^{89}\text{Zr}^{4+}$ [1]. Currently, ^{89}Zr -labeled DFO immunobioconjugates are the only Zr-based radiopharmaceuticals that have been translated for human Positron Emission Tomography (PET), although DFO^{3-} is far from being an ideal chelator as it lacks two donor atoms to saturate the coordination sphere of Zr^{4+} . More seldom, some mixed siderophores incorporate among the three binding units, either a 6- (PIPO) or a 7-membered (AZEPO) cyclic hydroxamic chelating group. While open-chain hydroxamates, as those found in DFO, prevail in aqueous solutions as the *E* conformer, the cyclic structure of PIPO or AZEPO enforces a *Z* orientation of both oxygen donor atoms [2]. This preorganization stabilizes the iron and uranyl complexes by ca. 5 kJ mol⁻¹ per bound unit [3].



The lecture will provide an overview of our contribution to the field of siderophore chemistry [2–8], with a strong emphasis on the coordination properties of natural and abiotic hydroxamic acids of linear or branched topologies with respect to 5f and 3d radionuclides, including U(VI), Th(IV), Pu(IV), and $^{89}\text{Zr(IV)}$. Owing to their high binding affinity towards strongly acidic cations, water solubility, and low toxicity, these ligands could find valuable applications in analytical and environmental sciences, but also in nuclear medicine. An in-depth speciation study of the $\text{UO}_2^{2+}/\text{DFO}^{3-}$ system [4] prompted us to covalently graft DFO onto organic resins [5,6], producing thereby solid/liquid extracting materials that were incorporated in Diffusive Gradients in Thin-films (DGT) devices. The resulting passive samplers allowed us to monitor over several days the U content in natural fresh- and seawaters, overcoming the limitations of commercial DGT's. Extension of DFO by a fourth but cyclic hydroxamate moiety afforded octadentate high-affinity chelators for $^{238}\text{Pu}^{4+}$ (DGT binding gels) [6], $^{227}\text{Th}^{4+}$ (targeted radionuclide α therapy) [7], but also $^{89}\text{Zr}^{4+}$ (PET imaging) [8]. According to both in vitro and preclinical in vivo studies, the most promising $^{89}\text{ZrDFOcylo}^*$ radioimmunoconjugate of Trastuzumab was found to clearly surpass the analogous $^{89}\text{ZrDFO}$ construct.

References:

- [1] *ACS Chem. Biol.* **2018**, 13, 11-25.
- [2] *J. Inorg. Biochem.* **2015**, 151, 164-175.
- [3] *New J. Chem.* **2018**, 42, 7765-7779.
- [4] *J. Environ. Radioact.* **2021**, 235-236, 106645.
- [5] *New J. Chem.* **2023**, 47, 13436-13449.
- [6] *New J. Chem.* **2025**, 49, 20151-20160.
- [7] *J. Nucl. Med.* **2023**, 64, 1062-1068.
- [8] (a) *Eur. J. Nucl. Med. Mol. Imaging* **2019**, 46, 1966-1977. (b) *ChemPlusChem* **2024**, 89, e202400062.

PL3 - EXPLORING THE CHEMISTRY OF PROTEIN-NUCLEIC ACIDS COMPLEXES BY COMPUTATIONAL APPROACHES

Emmanuelle Bignon,¹ Antonio Monari,² Yuya Qiu,¹ Ekaterina Smirnova³, Patrick Schultz³, Gabor Papai,³ Adam Ben Shem³

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²Université Paris Cité and CNRS, ITODYS, Paris, France

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Keywords: Computational biochemistry, protein-nucleic acids complexes

Summary: Protein–nucleic acid complexes lie at the heart of nearly every fundamental process in biology, from genome maintenance and gene regulation to viral RNA recognition and cellular signaling. Their dynamic behavior, chemical diversity, and structural complexity present major challenges for experimental investigations alone, and many key aspects remain to be elucidated. In this presentation, two case studies will highlight how state-of-the-art computational chemistry is transforming our ability to decipher the mechanisms that govern these essential assemblies [1]. By integrating quantum mechanical methods, advanced molecular dynamics, enhanced-sampling strategies, and multiscale modeling, we can now probe the energetics of complex enzymatic reactions, the dynamics of protein-nucleic acids interactions, and the role of conformational flexibility with unprecedented resolution.

The two case studies, focusing on the enzymatic replication of viral RNA [2] and on regulatory mechanisms of epigenetic marks [3], will illustrate how computational approaches complement structural and biochemical data, enabling us to visualize transient states, interrogate the dynamics of macromolecular assemblies, and predict reaction mechanisms. Together, these advances pave the way for a deeper understanding of protein–DNA and protein–RNA interactions and their underlying chemistry, ultimately guiding the design of novel modulators and therapeutic strategies.

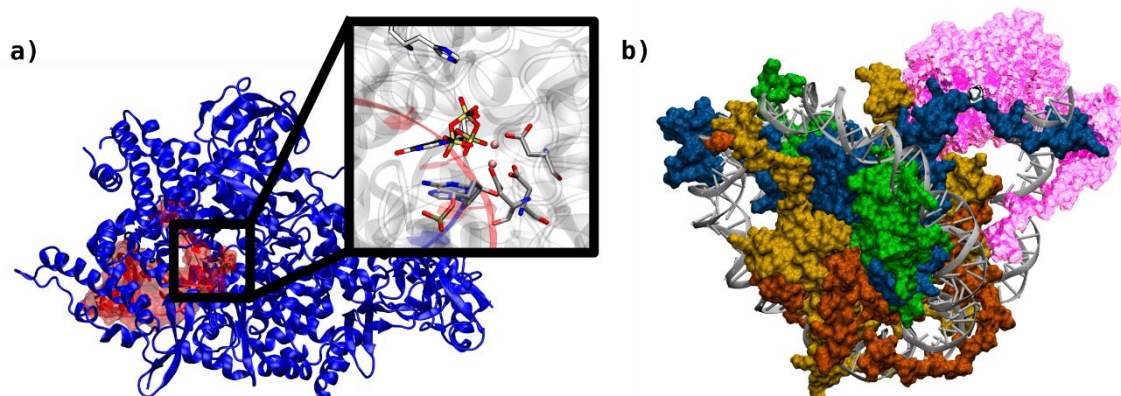


Fig. 1 : Two case of studies detailed in this presentation: a) a multi-scale investigation of the enzymatic mechanisms driving SARS-CoV-2 genome replication [2] and b) a combined cryoEM-computational study of the SIRT6 protein removal of acetylation marks on histone proteins in the context of DNA compaction regulation.

References:

- [1] Baek, M., McHugh, R., Anishchenko, I., Jiang, H., Baker, D., & DiMaio, F. (2024). Accurate prediction of protein–nucleic acid complexes using RoseTTAFoldNA. *Nature methods*, 21(1), 117-121.
- [2] Bignon, E., & Monari, A. (2022). Modeling the Enzymatic Mechanism of the SARS-CoV-2 RNA-Dependent RNA Polymerase by DFT/MM-MD: An Unusual Active Site Leading to High Replication Rates. *Journal of Chemical Information and Modeling*, 62(17), 4261-4269.
- [3] Smirnova, E., Bignon, E., Schultz, P., Papai, G., & Ben Shem, A. B. (2024). Binding to nucleosome poises human SIRT6 for histone H3 deacetylation. *Elife*, 12, RP87989.

PL4 - PORPHYRINS AT WORK: FROM MOLECULAR RECOGNITION TO LIGHT-ACTIVATED THERAPY

Valérie Heitz,

Laboratoire de Synthèse des Assemblages Moléculaires Multifonctionnels, Institut de Chimie de Strasbourg, CNRS/UMR 7177, Université de Strasbourg, email: v.heitz@unistra.fr.

Keywords: supramolecular chemistry, switchable receptor, antimicrobial photodynamic therapy, porphyrin.

Owing to their coordination capabilities and electronic and photophysical properties, metalloporphyrins have been integrated into various architectures for molecular recognition and chemical transformation. The incorporation of additional chemical, redox, or photoresponsive units enables fine-tuning of the properties of porphyrin-based hosts, including guest uptake and release as well as catalytic activity.^[1] Moreover, owing to their low toxicity, strong light absorption and generation of singlet oxygen, porphyrins are well suited as photosensitiser for photodynamic therapy (PDT). PDT enables the treatment of localised tumors with high selectivity and minimal side effects while triggering immune-stimulatory responses. PDT is also effective in eradicating pathogenic bacteria making this treatment attractive in light of the growing resistance of bacteria to even the latest class of antibiotics.^[2]

This lecture will present examples of porphyrin-incorporating supramolecular systems with stimuli-responsive units. Molecular cages (Figure 1a) and molecular tweezers enabling the control of guest binding using chemical or redox signals will be discussed.^[3] For light-induced therapeutic applications, π -extended porphyrin conjugates with targeting units were designed for selective treatment within the optical therapeutic window (Figure 1b).^[4]

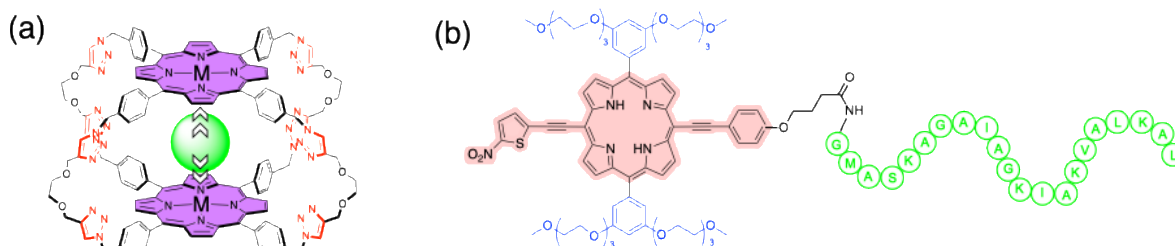


Fig. 1 (a). A molecular cage receptor. (b) Porphyrin conjugate for near-infrared light-activated therapy.

References:

- [1] S. Durot, J. Taesch, V. Heitz, *Chem. Rev.* **2014**, *114*, 8542; S. H. A. M. Leenders, R. Gramage-Doria, B. de Bruin, J. N. H. Reek, *Chem. Soc. Rev.* **2015**, *44*, 433. A. Blanco-Gómez, P. Cortón, L. Barravecchia, I. Neira, E. Pazos, C. Peinador, M. D. García, *Chem. Soc. Rev.* **2020**, *49*, 3834–3862.
- [2] H. Hamblin, *Curr. Opin. Microbiol.* **2016**, *33*, 67.
- [3] R. Djemili, L. Kocher, S. Durot, A. Peuronen, K. Rissanen, V. Heitz, *Chem. Eur. J.* **2019**, *25*, 1481; L. Zanetti-Polzi, R. Djemili, S. Durot, V. Heitz, I. Daidone, B. Ventura, *Chem. Eur. J.* **2020**, *26*, 17514; L. Schoepff, L. Monnerneau, S. Durot, S. Jenni, C. Gourlaouen, V. Heitz, *ChemCatChem* **2020**, *12*, 5826; R. Djemili, S. Adrouche, S. Durot, V. Heitz, *J. Org. Chem.* **2023**, *88*, 14760; A. Edo-Osagie, D. Serillon, F. Ruani, X. Barril, C. Gourlaouen, N. Armaroli, B. Ventura, H.-P. Jacquot de Rouville, V. Heitz *J. Am. Chem. Soc.* **2023**, *145*, 10691; F. Ruani, D. Veciani, D. Sanchez-Resa, A. Edo-Osagie, G. Creste, A. Barbieri, V. Heitz, H.-P. Jacquot de Rouville, N. Armaroli, B. Ventura, *Chem. Eur. J.*, **2025**, e02604.
- [4] S. Jenni, A. Sour, F. Bolze, B. Ventura, V. Heitz *Org. Biomol. Chem.*, **2019**, *17*, 6585. Jenni, F. Bolze, C.S. Bonnet, A. Pallier, A. Sour, E. Tóth, B. Ventura, V. Heitz, *Inorg. Chem.*, **2020**, *59*, 14389S. Boumati, A. Sour, V. Heitz, J. Seguin, G. Beitz, Y. Kaga, M. Jakubaszek, J. Karges, N. Mignet, G. Gasser, B.-T. Doan, *ACS Appl. Bio Mater.* **2023**, *6*, 11, 4791. C. Gourlot, A. Gosset, E. Glattard, C. Aisenbrey, S. Rangasamy, M. Rabineau, T-S Ouk, V. Sol, P. Lavalle, C. Gourlaouen, B. Ventura, B. Bechinger, V. Heitz, *ACS Infect. Dis.* **2022**, *8*, 8, 1509.

PL5 - FROM THE SEARCH FOR STRUCTURAL CHEMODIVERSITY TO APPLICATIONS IN MEDICINAL CHEMISTRY

Stéphane Gérard

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Keywords: Organic synthesis, Heterocyclic scaffold, Medicinal chemistry, Hit-to-lead strategy

Summary:

For several years our laboratory was specialized in the development of innovative methodologies for the preparation of new heterocyclic scaffolds possessing therapeutic applications.[1] The presentation will describe some examples of this search of structural diversity and the complementary development of “hit to lead” strategies for the preparation of molecule of therapeutic interest.

References:

[1] *Eur. J. Med. Chem.* **2019**, 175, 40–48.
RCS Med. Chem. **2021**, 12, 584–592.
Current Res. Biotech. **2025**, 10, 100332.
WO 066973 A1 20160506.

Conférences Invitées

Conférenciers en séance invitée



Pierre ADAM

CNRS Research Director – UMR 7177 (CNRS-UniStra)

Institute of Chemistry, University of Strasbourg (Strasbourg)

Exploring archaeological organic substances: molecular, isotopic and radiocarbon-dating approaches

Geochemistry, Analytical Chemistry



Jean-Bernard BEHR

Professor – UMR 7312 (CNRS-URCA)

Institute of Molecular Chemistry, University of Reims Champagne Ardenne (Reims)

Some examples of carbohydrate-templated chemical tools for biological purpose

Chemobiology, Organic Chemistry



Frédéric CHÉRIOUX

CNRS Research Director – UMR 6174 (CNRS-UMLP)

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On-surface synthesis: the role of halogen bonding

Nanosciences, Supramolecular Chemistry



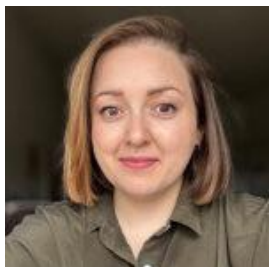
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Complex mixtures analysis by ViscY NMR experiments: at the limit of NOE

NMR Screening, Analysis



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From molecules to aggregates: in silico rationalization of optoelectronic properties of conductive materials

Molecular modeling, Complex Systems



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From surface chemistry to biomimetic nanozymes: multi-scale engineering of catalytic nanomaterials for biomass valorization

Nanocatalyst, Biosensing



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RECONFIGURABLE AND PROGRAMMABLE MATERIALS FOR LIGHT-INDUCED 3D & 4D PRINTING

Photochemistry 3D & 4D Printing

IL1 - ENGINEERING SURFACE-ACTIVE NANOMATERIALS FOR SELECTIVE CATALYSIS AND EMERGING NANOZYME APPLICATIONS

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Keywords: (Heterogeneous catalysis; Surface and interface engineering; photocatalysis; Nanozymes)

Summary: Surface-active nanomaterials play a key role in controlling activity and selectivity in heterogeneous catalysis. This contribution focuses on surface and interface engineering approaches applied to metal-based and hybrid nanocatalysts for the selective transformation of biomass-derived platform molecules, with a forward-looking perspective toward nanozyme-inspired photoactive catalytic systems. Precise control of surface composition, metal–support interactions, and support acidity allows efficient tuning of oxidation and hydrogenation reactions

Plasmonic gold nanoparticles coated with manganese oxide enable light-assisted oxidation of 5-hydroxymethylfurfural, where interfacial redox sites and photothermal effects contribute to enhanced catalytic performance ^[1]. Low-loading PdPt catalysts further demonstrate how bimetallic interactions can improve furfural hydrogenation selectivity under mild conditions ^[2]. In addition, iridium nanoparticles supported on silica with tuned acidity underscore the critical role of acid-modified supports in controlling hydrogenation pathways and improving catalytic performance ^[3].

Building on these established platforms, surface-engineered photoactive nanomaterials are introduced as prospective catalysts exhibiting enzyme-like behavior under light irradiation. From a catalysis perspective, these materials can be regarded as heterogeneous catalysts with tailored active sites, defects, and interfaces, offering a conceptual extension toward nanozyme-inspired catalytic systems. Overall, this work emphasizes a unified surface and interface engineering strategy for the rational design of selective nanocatalysts across thermally and light-assisted catalytic processes.

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IL2 - ON-SURFACE SYNTHESIS: THE ROLE OF HALOGEN BONDING

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Keywords: Halogen Bond, on-surface synthesis, supramolecular, STM

Summary: Over the past two decades, on-surface synthesis of organic nanostructures has been extensively investigated with the aim of fabricating molecular electronic components and functional nanomaterials. This growing interest is largely driven by the capabilities of scanning probe microscopy, which enable direct monitoring of reaction pathways with atomic-scale precision.¹ Here, we present two examples of on-surface chemistry directed by halogen bonding.^{2,3} Using scanning tunneling microscopy, we observe the formation of novel supramolecular phases and demonstrate that this supramolecular organization promotes the subsequent formation of well-defined one-dimensional covalent networks upon thermal annealing. These 1D covalent networks exhibit a high degree of order and are nearly defect-free, owing to the geometry of the initial supramolecular network, which facilitates controlled polymerization at relatively low temperatures and limits excessive precursor diffusion. These results highlight the potential of supramolecular templating to control surface-confined polymerization and to achieve defect-free conjugated nanostructures. Ongoing work focuses on optimizing the polymerization conditions to obtain longer polymer chains.

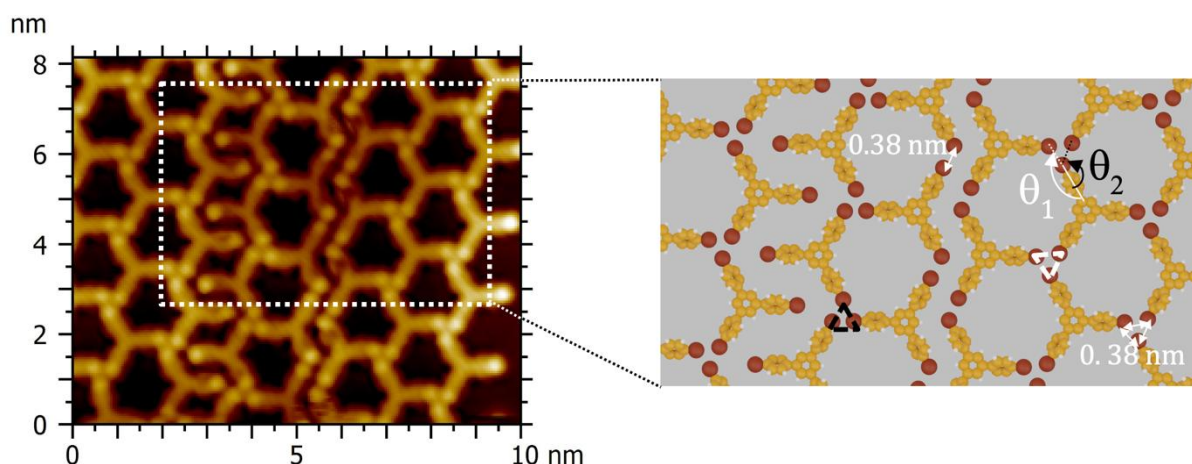


Fig. 1: STM image ($10 \times 8 \text{ nm}^2$, $V_s = -0.01 \text{ V}$, $I_t = 440 \text{ pA}$, 10 K) of the TBB/Au(111) interface. The porous network is formed by three TBB molecules that interact through three halogen bonds in a X_3 -synthon geometry, as highlighted by the dashed white triangle. The grain boundaries are stabilized by two halogen bonds between two TBB molecules (white arrows). The distance between bromine atoms involved in all Halogen bonds is $0.38 \pm 0.04 \text{ nm}$. The two enantiomeric X_3 -synthons are depicted, respectively with white and black dashed triangle.

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IL3 - FROM MOLECULES TO AGGREGATES: *IN SILICO* RATIONALIZATION OF OPTOELECTRONIC PROPERTIES OF CONDUCTIVE MATERIALS

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Keywords: (π -conjugated molecules, optoelectronic, TD-DFT, Molecular Dynamics)

Summary: π -Conjugated diimide-based materials constitute a versatile platform for the design of high-performance n-type organic semiconductors. However, subtle structural variations such as regioisomerism, heteroannulation and π -core extension strongly influence their optoelectronic properties and supramolecular organization, making their rational design challenging [1-4]. This presentation highlights the role of *in silico* approaches in bridging molecular-scale electronic structure and aggregate-level properties. The use of molecular dynamics simulations allows the description of aggregation processes, highlighting noteworthy assemblies. DFT and TD-DFT calculations are then used to rationalize structure-optoelectronic properties relationship and pave the way for the improvement of properties and later on of devices.

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IL4 - RECONFIGURABLE AND PROGRAMMABLE MATERIALS FOR LIGHT-INDUCED 3D & 4D PRINTING

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Keywords: One and Two Photopolymerization, 3D & 4D printing, Reconfigurable & Programmable materials, Controlled radical polymerization, Liquid crystal elastomers.

Summary: 4D printing concept appears in 2013 with the idea to facilitate the assembling of macroscopic objects [1]. The fourth dimension refers not only to the ability for material objects to change form after they are produced, but also to their ability to change function after they are printed [2-4]. At the microscale, 3D direct laser writing (3D DLW) based on multiphoton polymerization has become the gold standard for submicrometer additive manufacturing. Various stimuli-responsive materials have been employed to manufacture advanced microactuators. In particular, liquid crystal elastomers (LCEs) have attracted considerable attention due to their reversible, large shape-morphing and their fast response towards temperature or light stimuli. However, their processability by 3D DLW is not easy and the resulting objects rarely exhibit controlled and predictable deformation. In order to increase the complexity of deformation and thus to fulfil the requirements of nanorobotics, new programming strategies must be implemented. Besides, most of the printed objects present fixed properties. The possibility to reconfigure their properties on demand would definitively be a key parameter for many applications.

In this talk, we propose alternative strategies to reconfigure or program the shape and the surface properties of 3D printed micro-object. Firstly, the employ of controlled radical polymerization to confer to the object a living character will be introduced. Secondly, a new approach to perform the alignment of LCEs in a precise manner will be discussed. By playing both on the orientation strategy and the fabrication parameters, different deformations (curling, bending, twisting...) can be programmed starting from a single CAD model. A collection of building block is first demonstrated, then assembly of these building block is achieved, leading to 3D micro-objects presenting sophisticated behaviour (**Fig.1**). This work opens up new prospects for moving from a programmable material to a functional 3D-printed device.

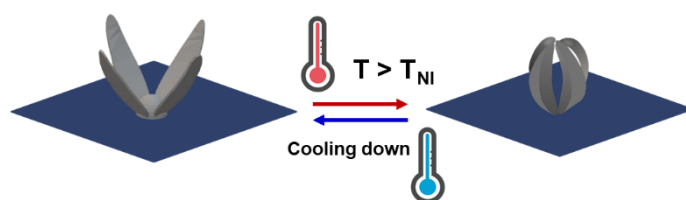


Fig. 1 : Schematic view of a liquid crystal based thermo-actuator made by two-photon polymerization

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IL5 - SOME EXAMPLES OF CARBOHYDRATE-TEMPLATED CHEMICAL TOOLS FOR BIOLOGICAL PURPOSES

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Keywords: carbohydrates, glycochemistry, enzyme inhibition, click reactions

Summary: Carbohydrates and their conjugates play key roles in many vital functions. They not only represent chemical scaffolds for biopolymers such as nucleic acids or structuring glycans (cellulose, chitin) but they also display peculiar roles in biological processes relating to immunology, virology, antibiotic action, cancer, and several life-threatening diseases.¹ Hence, great efforts have been made over the years on developing chemical access, including click processes, to specific sugar-based molecules.² Carbohydrate building blocks or target molecules are also of interest in terms of sustainable chemistry. Indeed, carbohydrates are available and renewable raw materials, the use of which eases the development of environmentally friendly processes.³ We will present recent findings on the use of carbohydrates in the synthesis of bioactive compounds and their conjugation through a new bioorthogonal click reaction.^{4,5}

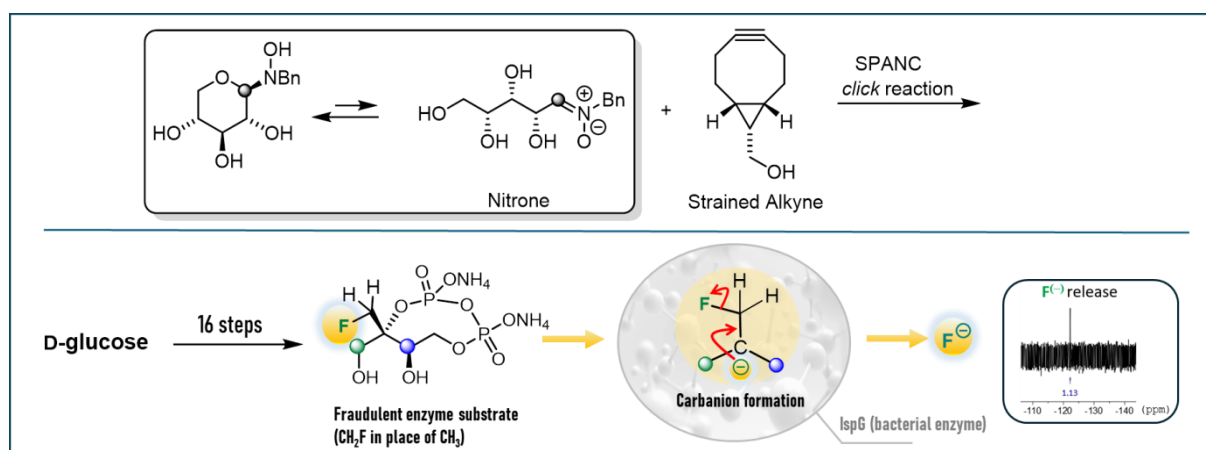


Fig. 1 : carbohydrate-based click reaction and synthesis of enzyme inhibitors

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IL6 - COMPLEX MIXTURES ANALYSIS BY VISCY NMR EXPERIMENTS: AT THE LIMIT OF NOE

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Summary:

The identification of organic molecules in a mixture is a crucial issue in the vast majority of human activities related to chemistry (healthcare, energy, materials, etc.). Transformation processes that lead from natural resources, whether from the fossil carbon industry or biomass exploitation, to low-value products in large quantities or to high-value speciality products, including pharmaceutical and cosmetic active ingredients, rarely produce chemically pure compounds. In the current state of knowledge, mixture analysis remains a necessity, and effective means to carry it out remain to be developed.

In this context, the ViscY (Viscosity enhancement spectroscopy) NMR experiments¹⁻¹⁰ were implemented to provide academic and industrial actors in organic synthetic and natural product chemistry with innovative and promising analytical methods based on the spin-diffusion phenomenon and dedicated to the mixture analysis of small molecules by liquid-state NMR, without resorting to any physical separation of mixture components.

The use of viscous solvents slows down the molecular tumbling rate in solution. As a result, the molecules display a negative nOe regime, and their resonances can be sorted according to their ability to exchange magnetisation through intramolecular spin diffusion. The 2D 1H-1H NOESY spectrum of a mixture reveals correlations between all 1H resonances of each analyte when recorded in spin diffusion conditions, thus giving access to the individual 1H NMR spectrum of every mixture component.

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IL7 - EXPLORING ARCHAEOLOGICAL ORGANIC SUBSTANCES: MOLECULAR, ISOTOPIC AND RADIOCARBON-DATING APPROACHES

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Keywords: Molecular archaeology, stable carbon isotopes, radiocarbon

Summary: Organic substances found in various archaeological contexts often contain valuable information about past ways of life, including cultural practices, dietary habits, technical know-how, exchange networks, and ritual activities. These substances notably include coatings, adhesives, balms, cosmetics or residues and food remains preserved in ceramic vessels. In addition, archaeological anthropised soils may also contain organic compounds derived from past activities from the sites, like agricultural practices, land use, food storage,

Molecular analysis of these organic substances—known as *molecular archaeology*—has developed considerably in recent years. This discipline is largely based on the identification of molecules whose structure is sufficiently characteristic to trace them back to precursor lipids of plant or animal origin, despite transformations related to their preparation (heating, reactions between ingredients) or ageing (biodegradation, oxidation, water washing). Such molecular signatures make it possible to identify the natural products used, to reconstruct manufacturing processes and uses, and to determine the geographical origin of the substances studied. Molecular archaeology has also been enriched by isotopic approaches, such as the measurement of $^{13}\text{C}/^{12}\text{C}$ ratios at the molecular scale, allowing more accurate attributions of biological or geographical sources. It also benefits from recent advances in radiocarbon (^{14}C) dating by AMS, which now allow age measurements on a few micrograms of organic carbon, opening the way to the dating of isolated individual compounds. In addition, innovative approaches based on experimental archaeology are sometimes used to better understand the different factors governing the selective preservation/degradation of organic substances over time.

Several examples of molecular, stable carbon isotopic, and radiocarbon dating studies will be presented. These will notably focus on the molecular characterization of a previously unknown resin-producing plant belonging to the genus *Commiphora*, which germinated from a 1026–1202 cal CE old seed recovered at an archaeological site and is a strong candidate for the ancient 'balm of Gilead' [1]. The presentation will also include the study of organic matter from soil infilling structures (silos and latrines) from an archaeological site in Obernai (Alsace), extending from the Bronze to the Roman Age [2] and the molecular investigation of amber jewellery from the Bronze Age aimed at determining its geographical source(s) in order to reconstruct past commercial routes throughout Europe. Finally, the advantages of combining molecular studies involving experimental archaeology and an isotopic approach for the investigation of food residues in archaeological ceramics will be presented.

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Communications Orales

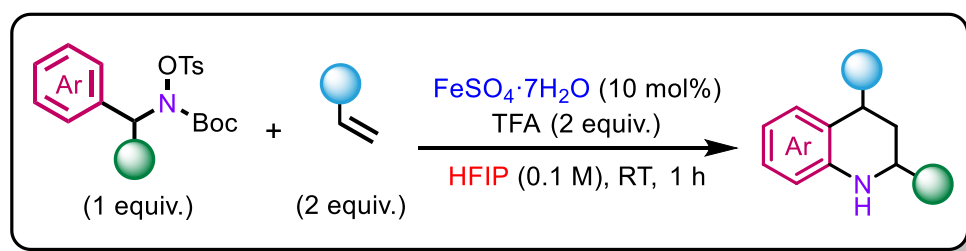
A POVAROV-TYPE REACTION TO ACCESS TETRAHYDROQUINOLINES FROM *N*-BENZYLHYDROXYL AMINES AND ALKENES IN HFIP

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Keywords: *N*-centered radicals, HFIP, Povarov reaction, electron poor alkenes

Summary: Although the importance of solvent effects has long been recognized as a critical factor in the development of new transformations, modern research groups often continue to consider solvent choice as a simple parameter among others (e.g., additives, catalysts, ligands etc.). Our research over the past 14 years has demonstrated that fundamentally new reactivity can be unlocked and unexplored chemical space accessed when the specific solvent effects of hexafluoroisopropanol (HFIP) are explicitly taken into account.¹ Our initial efforts focused on exploiting the unique properties of HFIP to investigate the reactivity of highly destabilized carbocations bearing electron-withdrawing groups. The main objective of my PhD work was to extend the reactivity of electronically deactivated substrates in HFIP, this time involving radical reactions.^{2,3} In this talk, I will disclose the synthesis of tetrahydroquinolines from newly developed *N*-benzylhydroxylamine reagents and alkenes using HFIP as the solvent. Notably, this transformation is applicable to highly electronically deactivated styrenes and aliphatic alkenes that were unreactive in previous iterations of the classical Povarov reaction, thereby expanding the accessible chemical space of this transformation due to the unique properties of HFIP.⁴

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TOWARDS LSPR-BASED DETECTION OF LIPOPOLYSACCHARIDES USING GOLD NANORODS

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Keywords: gold nanorods ; LSPR ; LPS ; biosensor

Summary: Lipopolysaccharides (LPS), major components of the outer membrane of Gram-negative bacteria, represent a significant safety concern in pharmaceutical and biomedical products, making therefore their detection critical. Currently, the gold standard for LPS detection is the Limulus Amebocyte Lysate (LAL) assay, which relies on hemolymph collected from horseshoe crabs – the latter being neither sustainable nor ethical. With horseshoe crab populations already endangered and the cost of LAL reagents escalating[1-2], there is an urgent need for alternative, robust, and ethical LPS detection strategies. To address the LPS detection, we introduce a localized surface plasmon resonance (LSPR)-based sensing platform utilizing gold nanorods (AuNRs), selected for their high sensitivity to local dielectric variations, which produce measurable shifts in their longitudinal surface plasmon resonance within UV–Vis spectra[3]. Initial investigations into spherical gold nanoparticle–graphene oxide assemblies, synthesized *via* covalent esterification, revealed valuable structural insights through Raman spectroscopy. However, their minimal plasmonic shifts in UV–Vis measurements limited their utility for LSPR sensing, prompting a shift towards AuNRs-based systems. By functionalizing AuNRs with mixed ligand shells combining short and long ligands, we simultaneously maintain the electromagnetic field sensitivity (*via* a thin and mainly short-ligand layer) and colloidal stability (through steric stabilization by long ligands). The adsorption of graphene oxide onto these AuNRs induced a measurable shift in their longitudinal plasmon resonance. Additionally, graphene oxide acted as a probe for evaluating ligand shell quality, particularly for the effective thickness of the ligand layer[4]. In parallel, a biological strategy was developed to identify suitable LPS-binding ligands. Sepharose-based affinity columns, functionalized with candidate ligands, were designed to capture the lipid A moiety of LPS *via* electrostatic interactions. To accommodate the structural diversity of LPS, a non-specific binding approach was employed to avoid highly specific antibodies which would be unsuitable for overall LPS quantification. These columns enabled the selection of the most promising LPS-binding ligand to assemble onto AuNRs, thus paving the way for further development of plasmonic sensing platforms.

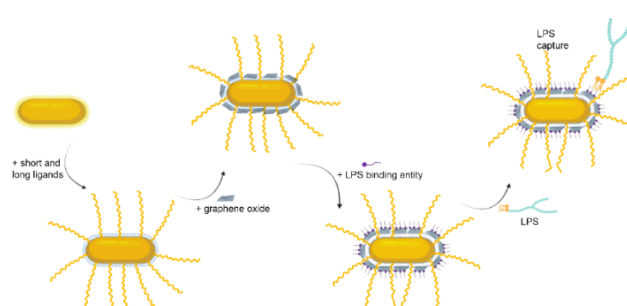


Fig. 1 : Design of the LSPR sensing platform for LPS detection.

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BUILDING MOLECULAR COMPLEXITY: CATALYTIC ACCESS TO CHIRAL POLYCYCLES WITH QUATERNARY CENTERS

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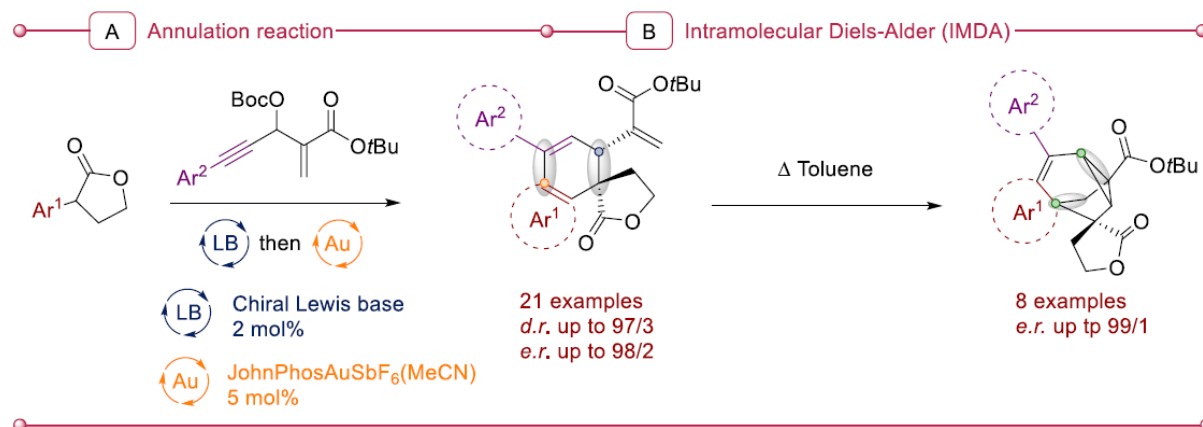
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Keywords: Cascade reaction, enantioselective organocatalysis, gold(I) catalysis, Friedel-Crafts reaction, Intramolecular Diels-Alder reaction

Summary: Merging organo- and gold-catalysis by sequential catalysis is a highly valuable approach for the synthesis of chiral complex molecules. [1] We will disclose a route to functionalized chiral heteroatomic polycyclic compounds leveraging these two unfriendly catalytic cycles in a one-pot sequential process. α -Heteroaromatic- γ -butyrolactones have been engaged in a highly stereoselective Lewis base asymmetric allylic alkylation with alkyne functionalized Morita-Baylis-Hillman carbonates. Gratefully to the low Lewis base catalyst loading, subsequent gold catalyzed Friedel-Crafts alkylation, entailing the formation of fused polycyclic compounds, can proceed efficiently leading to structurally complex products in high enantiomeric ratio (Scheme 1.A). [2]

These chiral polycyclic skeletons enable the Intramolecular Diels-Alder (IMDA) reaction, which provides a straightforward approach towards interesting tricyclo[3.2.1.0^{2,7}]octene [3] scaffolds containing five stereocenters, including two quaternary (Scheme 1 B).



Scheme 1. Catalytic synthesis of highly functionalized chiral polycyclic compounds bearing quaternary stereocenters.

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PhD Thesis Award from the SCF Lorraine

LOW-FIELD NMR RELAXOMETRY METHODS FOR STUDYING AND DESIGNING SUPERPARAMAGNETIC IRON OXIDE CONTRAST AGENTS

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Summary:

Iron oxide nanoparticles at a critical size of approximately 20 nm exhibit a unique size-dependent magnetic property known as superparamagnetism. This feature makes them highly valuable in various fields, particularly in biomedicine. Their applications range from therapeutics, such as the targeted heating of cancer cells, to diagnosis, including their use as contrast agents (CAs) in magnetic resonance imaging (MRI). SPIONs enhance image contrast in MRI by shortening the relaxation times of surrounding water protons. Herein, they were synthesized using an optimized coprecipitation-assisted microwave approach, which is fast, reliable, and reproducible. Their efficiency or relaxivity was studied by an in-depth analysis of NMR Dispersion (NMRD) profiles acquired with the Fast Field-Cycling methodology. Several other characterization techniques (TEM, DLS, Magnetometry, XRD, TGA) were also used to support and validate the NMRD approach. This work investigates the effects of solvents on SPIONs synthesis and redispersion, as well as the impact of different surface coatings on particles with the same core size. Finally, a new generation of SPIONs functionalized with phosphate and amine groups has been developed, offering high relaxivity and confirmed biocompatibility through biological testing.

Communications Orales

OC01 - COLLOIDAL SYNTHESIS OF TWISTED GOLD NANOPARTICLES

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Keywords: gold nanoparticles, chirality, circular dichroism

Summary: Chirality is a chemical phenomenon widely present in nature, in various forms such as DNA, amino acids, and snail shells. For example, amino acids that constitute proteins exist exclusively in the L form (levorotatory), whereas sugars predominantly adopt the D form (dextrorotatory). This phenomenon has attracted increasing interest within the scientific community, as it allows the modulation of electrical and optical properties of studied systems. In optical spectroscopy, chirality manifests itself through an absorption that depends on the circular polarization of the incident light, a phenomenon known as circular dichroism. Its counterpart in vibrational spectroscopy, vibrational circular dichroism, results in differences in Raman scattering intensities depending on whether the incident circular polarization is right- or left-handed [1]. These differences are, however, extremely weak and therefore require highly precise measurements to be detected. Coupling chirality with plasmonic particles, particularly gold nanoparticles, opens new avenues for applications, notably through the enhancement of vibrational circular dichroism [2]. The synthesis of these chiral nanoparticles begins with the formation of gold nanorods using the so-called seed-growth method. This synthetic approach allows the production of nanomaterials with excellent crystallinity, which is a key factor for inducing strong chirality. The nanorods are then transformed into quasi-spherical nanoparticles. To induce chirality, a ligand exhibiting optical activity is subsequently introduced; depending on the nature of its optical rotation, the resulting nanoparticles display a preferential right- or left-handed orientation. Finally, the synthesized nanoparticles were characterized using various physicochemical techniques, such as transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), and UV-Visible spectroscopy, in order to establish the relationships between nanostructure and properties at each stage of the synthesis. Circular dichroism measurements were also carried out to identify the synthesis parameters that allow the highest possible chirality to be achieved.

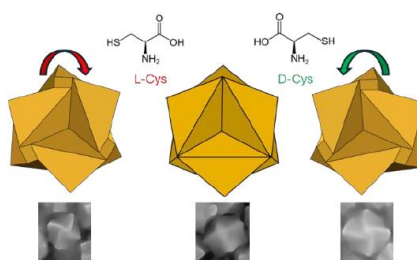


Fig. 1: Diagram of twisted gold nanoparticles depending on the enantiomeric nature of the ligand (either with L-cysteine or with D-cysteine), accompanied by an image of these nanoparticles under a SEM

References:

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OC02 - ENGINEERING ASSEMBLIES OF VIOLOGENS

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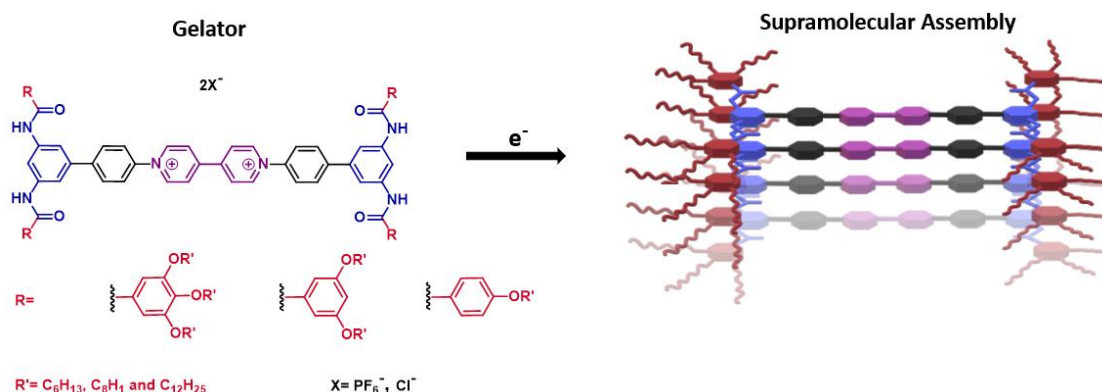
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Keywords: viologen, noncovalent interactions, spectro-electrochemistry

Summary: Structurally controlled self-assembly of redox active building blocks comprising aromatic cores remains a challenge.^{1,2} Among redox active π -conjugated aromatic cores, viologens, with their low-energy LUMO and unique redox activity, are an interesting class of compounds and may provide the opportunity of studying electronic conduction in fibrils if adequately functionalized.³ Previous work in our group showed that aryl viologens bearing four alkyl chains form organized structures in both the solid state and on an HOPG surface via van der Waals interactions.⁴ However, in solution this molecule formed aggregates that precluded in-depth studies in the liquid state. To overcome this limitation, a new target molecule was designed to incorporate hydrogen-bonding sites in a functionalized viologen scaffold. The building blocks designed in this work are represented in Figure 1 and incorporate three different noncovalent interactions: **electrostatic interactions** (from the viologen core), **hydrogen bonding** (via four amide groups), and **van der Waals interactions** (using long alkyl chains). To establish the self-assembly behaviour of these viologen architectures, complementary analytical techniques were employed. Atomic force microscopy (AFM) reveals that the dicationic state forms extended organized networks on HOPG, whereas spectro-electrochemical characterisation demonstrates an attractive interaction between radical cation species and the formation of π -dimers. These structurally defined assemblies highlight the potential of such systems for constructing complex



three-dimensional electronic nanomaterials and nanodevices.²

Fig. 1: Target molecule and envisioned supramolecular assembly upon reduction.

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OC03 - ALTERNATIVE METHODOLOGICAL APPROACHES FOR TAYLOR DISPERSION ANALYSIS - APPLICATION TO AUNP-PROTEIN INTERACTIONS

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Keywords: Taylor Dispersion Analysis ; Methodology ; Nanoparticle ; Lectin

Summary: Taylor dispersion analysis (TDA) is a technique used to determine the diffusion coefficient (D) of a species, whether organic or inorganic [1, 2]. One of the modes used is the Pulse mode, in which the sample is introduced into a capillary and mobilized under laminar flow, causing the sample band to widen. A Gaussian fit of the signal is then required to determine D. Building on previous work by our team [3], we present an alternative adjustment method for the Pulse mode called 'Dual-Erf' (see fig.1 A). This method enables a larger injection volume (>1% of the capillary volume) to be used, thus extending the application of the Pulse mode to low-concentration samples. We carried out a demonstration on measuring D for various molecules of different sizes down to the nm scale (e.g. caffeine, reduced glutathione, insulin, albumin and citrate-stabilized gold nanoparticles AuNPs see fig.1 B). The theoretical and methodological aspects are described, showing good correlation with values in the literature and results obtained from another TDA mode (Frontal). This methodology improves sensitivity by a factor of 20 (with injection volumes representing up to 30% of the capillary volume). It is also proposed for analyzing the formation of protein corona around AuNPs, providing a useful means of determining the interaction mechanisms between lectins and nanoparticles. The focus is on preserving the recognition capabilities of lectins towards carbohydrate functions, particularly after binding to AuNPs [4].

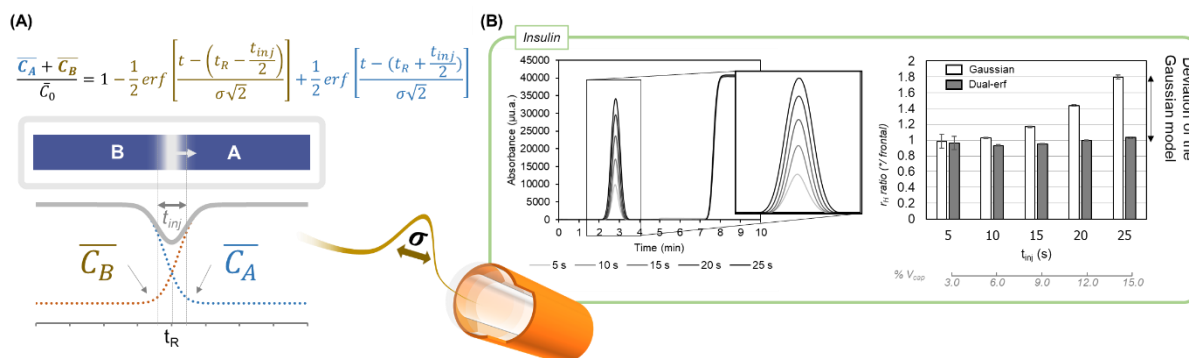


Fig. 1 : (A) Mathematical approach proposed for “dual-erf” TDA and (B) demonstration with insulin as model.

References:

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OC04 - ION EXCHANGE ON COLLOIDAL MG/AL LDH NANOPARTICLES: WHEN KINETICS LEADS TO THERMODYNAMICS IRREVERSIBILITY

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Keywords: LDH, colloid, nanoparticles, chromate, irreversibility

Summary: Chromium (Cr) serves as an exemplary case study of heavy metal contamination challenges. This element demonstrates extensive industrial utility due to its distinctive properties, with widespread applications across multiple sectors. Layered double hydroxides (LDH) are a class of materials that exhibit significant potential as inorganic scavengers. One of their notable attributes is their ability to achieve a high anion exchange capacity. This motivated a comprehensive study of the potentialities of Mg/Al LDH nanoparticles with chromate ion[1]

This study specifically investigates the mechanisms underlying anionic exchange in layered double hydroxides (LDHs) for hexavalent chromium (Cr(VI)) removal and recovery from aqueous solutions. Mg/Al-NO₃ LDH nanoparticles were synthesized via fast coprecipitation followed by hydrothermal treatment and subsequently saturated with Cr(VI)[1]. Ultrafiltration experiments [2] quantitatively evaluated the Cr(VI) recovery efficiency of various competing anions, establishing a clear selectivity hierarchy: HPO₄²⁻ > SO₄²⁻ > CO₃²⁻ >> Cl⁻ > NO₂⁻ ≥ NO₃⁻. Carbonate is unable to remove 100% of chromate from the LDH.

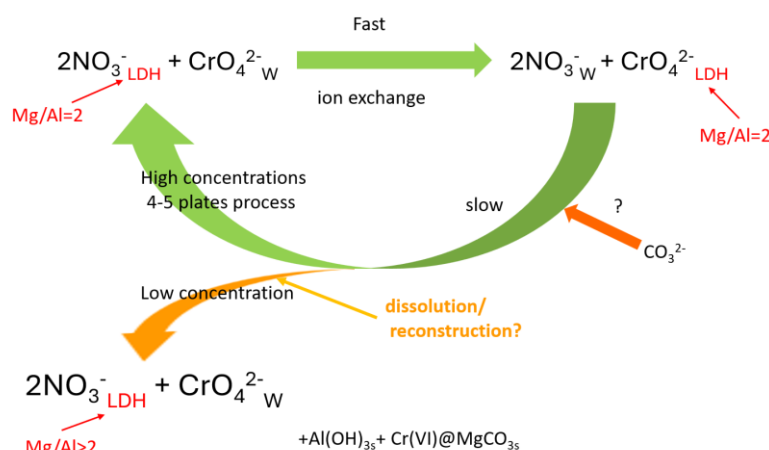


Fig. 1 : Scheme of the forward and back exchange of nitrate and chromate on LDH nanoparticles

Considering NO₃⁻/CrO₄²⁻ exchange, the determined equilibrium constants for the forward and back reaction indicate a non reversibility of the ion exchange process. Kinetic investigations and multiple plateaus experiments together allowed to show that the fast uptake nitrate-chromate reaction is only ion exchange whereas the slower recovery of chromate from the LDH in presence of nitrate occurs through a non topotactic process.

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OC05 - DEVELOPMENT OF RECOVERY PROCESSES FOR GADOLINIUM PRESENT IN HOSPITAL EFFLUENTS USING MODIFIED AND/OR ECO-DESIGNED NATURAL BIOSORBENTS

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Keywords: biosorbents, metal cations (Cu^{2+} , Gd^{3+}), chitosan, extraction, green chemistry

Metal contamination in aquatic environments has become an emerging environmental issue, particularly with the increasing release of anthropogenic metals that resist conventional treatment processes. Among these, gadolinium originating from Magnetic Resonance Imaging (MRI) contrast agents [1] provides a striking example. Although the majority of administered gadolinium complexes are excreted by patients, they pass through hospital effluents and wastewater treatment plants largely unaltered, ultimately reaching natural waters. Their high stability, hydrophilicity, and persistence make them representative of a broader class of metal-based micropollutants with potential for bioaccumulation and ecotoxicological impact. This growing concern highlights the need for more efficient monitoring tools and the development of innovative strategies for metal detoxification in water systems.[2], [3]

To face this challenge, the objective of my thesis is to provide novel selective and eco-friendly biosorbents to capture metal ions and particularly Gadolinium from wastewater. The design of biosorbents currently under study is based on the modification of Chitosan (CS), biosourced polymer, [4] by functionalizing its amine groups with ligands known for their strong affinity for metal cations such as hydroxamates, catecholates, or polydentate chelators (e.g., EDTA, DTPA). This presentation will cover the synthesis and the characterization of CS functionalized, and the sorption experiments of these materials for Cu^{2+} as a model cation and ultimately Gd^{3+} .

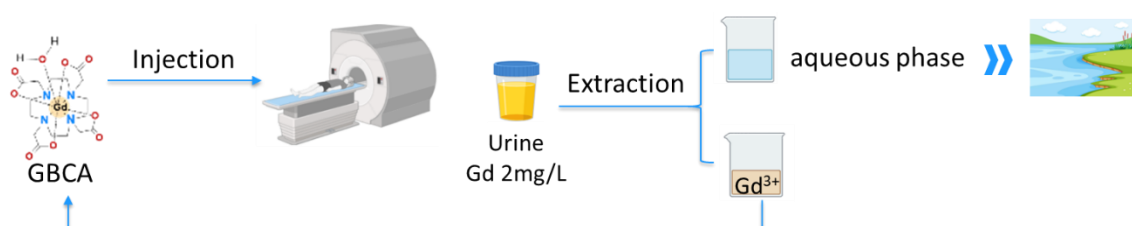


Fig. 1: Overall schematic diagram

References:

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- [3] *Environ. Pollut.* 1994, 85 (3), 345–350.
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OC06 - NEW L-PROLINE-BASED DEEP EUTECTIC SOLVENTS IN HETEROCYCLIC SYNTHESSES

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Keywords: Deep Eutectic Solvent, Heterocycles, Green chemistry

Summary:

The synthesis of most organic compounds still uses nowadays harmful reagents, volatile solvents, hard conditions and/or difficult purifications. It is estimated that ca 28 million tons of solvents are used annually with about 5 million tons used by the European solvents industry alone. Moreover, similar quantities are emitted to the environment [1]. In this context, many efforts are devoted to the search of greener and safer solvents. Particularly, deep eutectic solvents (DES) are considered as a promising emerging class of green solvents [2] since their first description by Abbott in 2003 [3].

The most common DES used in organic synthesis are based on choline chloride (CC) but a wide variety of other DES are also discussed in literature depending on the individual components chosen [4]. In our lab, we are particularly interested in L-proline-based DES and we showed that those DES are sometimes more powerful than the ones based on choline chloride. Especially we recently described a zero-VOC strategy for Knoevenagel reaction where (hetero)aromatic aldehydes were successfully condensed with rhodanine, thiazolidine-2,4-dione or barbituric acid under mild conditions in L-Proline:Glycerol (1:2) [5]. In other projects, L-Proline:Ethylene Glycol DES gave better results and for example, thiazolo[5,4-*d*]thiazoles (TzTz) were synthesized in satisfying yields under safe and eco-friendly conditions in a mixture of L-proline and ethylene glycol (1:50) (Fig. 1) [6].

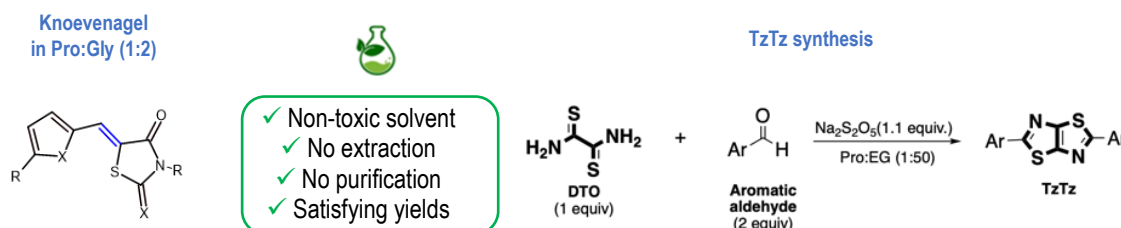


Fig. 1 : Two examples of heterocyclic synthesis in L-Proline-based DES

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OC07 - ISOTHIAZOLONES: HETEROCYCLIC COMPOUNDS OF THERAPEUTIC INTEREST

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Keywords: Isothiazolone, pharmacomodulation, Suzuki-Miyaura

Summary:

For several years now, a new heterocyclic scaffold has attracted growing interest: the isothiazolones. These five-membered heterocycles are distinguished by their broad spectrum of biological activities and their ability to interact with numerous molecular targets. Their structure contains several pharmacomodulation sites, allowing fine-tuning of their properties and enabling the synthesis of a wide variety of derived compounds. Thanks to this structural and functional versatility, isothiazolones now represent a promising scaffold for the development of new bioactive entities. This presentation therefore aims to highlight the synthesis of the various compounds obtained by the Therapeutic Chemistry Laboratory of the Faculty of Pharmacy in Reims.

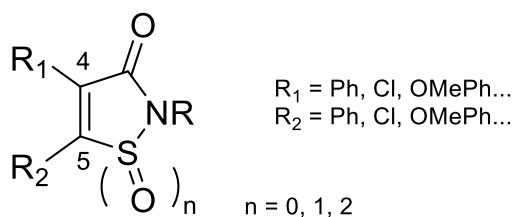


Figure 1: Isothiazolone general structure

References:

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- [3] *J. Org. Chem.* **2012**, 77, 482–489.

OC08 - THE VIRIDIUM-ACRIDINIUM CONJUGATE: A MULTI-RESPONSIVE MOLECULE

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Keywords: Acridinium | Viridium | Photochemistry | Electrochemical and Chemochromic Properties

Summary: The acridinium core is an appealing molecular building block since it has multi-responsive properties (chemo-, photo-, electrochromic properties) which can be exploited in supramolecular chemistry.^[1] Additionally, when functionalized with a 2-pyridyl moiety at their 9- position, an atypical intramolecular photocyclo-dehydrogenation reaction occurs under mild, clean, and efficient light-mediated conditions to afford a thermodynamically stable radical.^[2] Coined as the viridium radical cation, this open shell species exhibits uncommon amphoteric redox and π -dimerization properties.

In the present work, the combination of the acridinium and viridium building blocks is targeted in order to reach new chemical, optical and redox properties. Using the pyrazine bis-acridinium as the precursor, a viridium-acridinium conjugate was synthesized under light-mediated conditions. In addition to possessing the physicochemical properties of acridinium and viridium, this molecule also has new halochromic and optical properties.

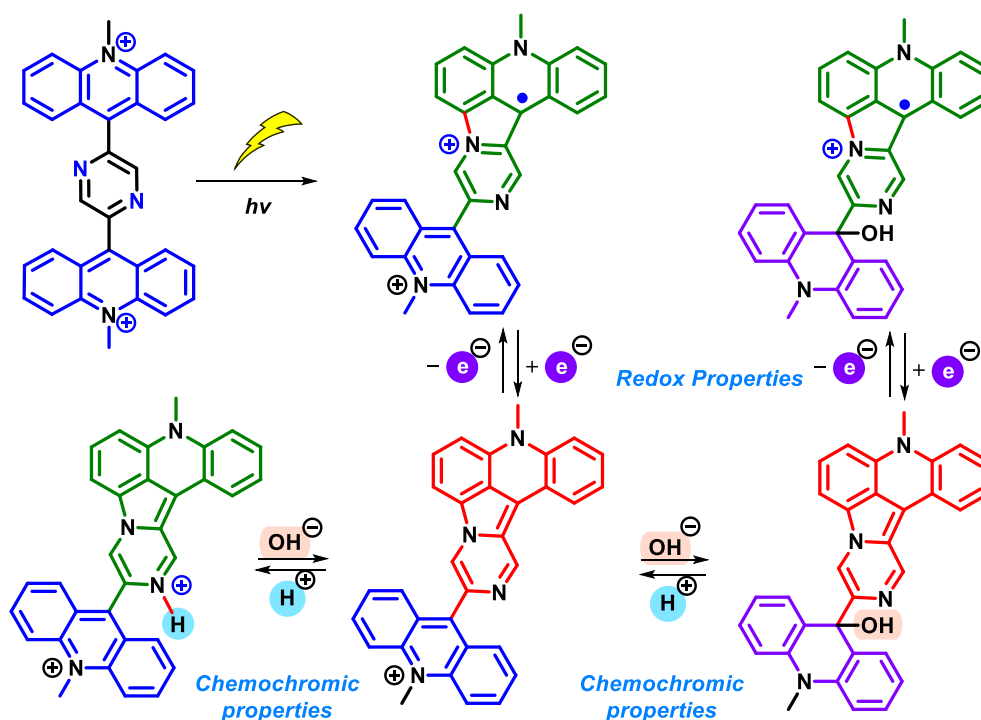


Fig. 1 : Photochemical reaction leading to viridium and their π -dimerization equilibrium

References:

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OC09 - TOWARDS SUSTAINABLE CHEMISTRY: PLASMONIC CATALYSIS FOR BIOMASS-DERIVED HMF OXIDATION

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Keywords: Nanoparticles, Biomass, Valorization, Plasmonic, Catalysis

Summary:

Background: Since 2005, 5-hydroxymethylfurfural (HMF) has emerged as a central biomass-derived intermediate, with its oxidation product, 2,5-furandicarboxylic acid (FDCA), serving as a key building block for sustainable polymers and fine chemicals [1]. Plasmonic catalysis, exploiting localized surface plasmon resonance (LSPR) in metallic nanoparticles, offers a promising approach for selective photocatalytic transformations [2]. Plasmonic catalysis, which utilises localized surface plasmon resonance (LSPR) in metallic nanoparticles (NPs), offers a promising approach for selective photocatalytic transformations. This study investigates the selective photocatalytic oxidation of HMF to FDCA, evaluating the synergetic effects of MnO₂ shell thickness (3.5–10 nm) [3] on gold nanoparticles (AuNPs), different irradiation wavelengths, support material and base addition based on product selectivity in liquid phase reaction.

Results and Discussion: The study presents and compares results from a series of control experiments conducted under varying conditions, including reactions performed in the absence of catalyst, NaOH, and light, as well as under different illumination wavelengths. The findings demonstrate that the addition of NaOH markedly enhances the overall catalytic performance across all tested conditions, underscoring the synergistic effect between the base and the catalyst. In contrast, neither light nor base alone produced significant conversion, confirming the necessity of both components for efficient oxidation.

Thermal catalytic experiments achieved a maximum HMF conversion of 30% with a carbon balance of approximately 72%, suggesting partial substrate degradation. Under these conditions, only HMFCa was detected as the main product when using the most active catalyst (Au@MnO₂, 10 nm). Under photochemical conditions at 365 nm, the reaction exhibited the highest overall activity, likely due to the overlap between the MnO₂ absorption edge and the UV emission spectrum, which facilitates more effective photoexcitation of the catalyst. However, this enhanced activity was accompanied by reduced selectivity and carbon balance.

The MnO₂ shell thickness was found to correlate with increased catalytic activity. At 365 nm, significant formation of HMFCa and FFCA was observed, along with minor amounts of DFF and FDCA. In contrast, irradiation at 450 nm primarily produced HMFCa with trace levels of FFCA and FDCA. These observations clearly demonstrate the influence of irradiation wavelength on the reaction pathway and product selectivity, emphasizing the potential of Au@MnO₂ nanostructures as tunable platforms for light-driven chemical transformations.

References:

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OC10 - SYNTHESIS AND BIOEVALUATION OF N-HETEROCYCLIC/M-M BONDED COMPLEXES

Isabelle Jourdain,¹ Méline Wang,^{1,2} Tobias Schrimpf,³ Michael Knorr,¹ Mohamed Othman,² Jalloul Bouajila,⁴ Agathe Figarol,⁵ Carsten Strohmann,³ Vincent Humblot⁵

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Keywords: (metallo drugs, biological activity, metal-metal bond, alkyne, N-heterocycles)

Summary: Many metals are essential to biological functions (Fe, Co, Zn...) and the use of a metal to develop metallo drugs for the treatment of diseases has attracted considerable interest since the discovery of the chemotherapeutic agent cisplatin in the 1960s. The development of new metal therapeutic complexes remains crucial to overcoming both side effects and drug resistance which are major clinical problems. To provide alternative metallo drugs, diverse strategies have been employed [1]. Among these, combining a biologically organic framework with an organometallic fragment offers great potential [2]. Isoindole-based scaffolds, derived from both natural and synthetic sources, have emerged as versatile scaffolds for the design of pharmaceutical and bioactive compounds [3]. An additional potential is offered by bimetallic complexes which combine the properties of different metal fragments to improve biological activity via synergistic effects. Most of the reported compounds involve a bridging ligand to connect the metals, including homo- and heterobimetallic systems [4]. In contrast, metal-metal bonded homobimetallic complexes are less explored as potential metallo drugs and heterobimetallics not at all.

In this study, we report on the synthesis, characterization, and biological evaluation of metal-metal bonded bimetallic scaffolds (Co-Co, Pt-Pt, Fe-Pt) as well as Pt(0) complexes incorporating an isoindole moiety. These organometallic species were prepared using alkyne-functionalized isoindole ligands, characterized by IR, multinuclear NMR spectroscopy, and single-crystal X-ray diffraction. Biological assays were also conducted to evaluate their cytotoxic, anti-Alzheimer, and anti-diabetic activities.

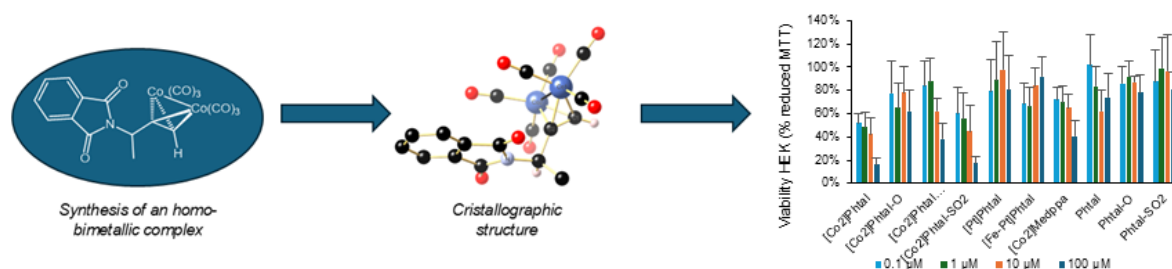


Fig. 1 : Crystal structure of a homobimetallic dicobalt tetrahedrane complex and cytotoxicity studies on HEK293 cell line.

References:

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OC11 - DEVELOPMENT OF A HARD CARBON/TIN COMPOSITE NEGATIVE ELECTRODE FOR SODIUM-ION BATTERIES VIA ELECTRODEPOSITION

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Keywords: Sodium-ion batteries; Hard carbon; Tin; Electrodeposition; Morphology

Summary: The energy transition relies on the electrification of society and the electrochemical storage of energy. However, an exclusive dependence on lithium raises major concerns. Indeed, approximately 87% of the lithium extracted is used for the manufacture of rechargeable batteries, corresponding to about 210,000 tons in 2024 [1]. In addition to its limited availability (0.0017% of the Earth's crust) and its uneven geographical distribution, which is a source of geopolitical tensions, other key elements of lithium-ion batteries, such as nickel (Ni), copper (Cu), cobalt (Co), manganese (Mn), and graphite (C), are scarce, expensive, and/or toxic [2]. In this context, sodium-ion batteries (SIBs) appear as a promising alternative, either as substitutes for or complements to lithium-ion technologies [3]. They stand out due to the abundance of sodium (2.27% of the Earth's crust) and its significantly lower cost, approximately 50 times lower than that of lithium. Nevertheless, several technological challenges remain, particularly a lower energy density. In this study, the objective is the development of a high-performance negative electrode for SIBs by combining hard carbon, the reference anode material with a theoretical specific capacity of approximately 300 mAh g⁻¹, with metallic tin, whose theoretical specific capacity reaches 847 mAh g⁻¹ [4–5]. This combination aims to take advantage of the high capacity of tin while mitigating its large volume variations (~420%) during sodation/desodation processes through the buffering effect of the carbon matrix, thereby improving electrochemical stability and cycling performance. This work therefore focuses on the controlled fabrication of composite electrodes by electrodeposition of tin onto hard-carbon-based electrodes coated onto a current collector. Electrodeposition offers the advantage of precisely controlling the amount, distribution, and morphology of the deposited tin by adjusting electrochemical parameters. The morphology of tin deposits (particle-like, dendritic, or tubular) plays a significant role in the electrochemical behavior of the electrodes, as it influences the active surface area, sodium-ion diffusion pathways, mechanical stress management, and the stability of the electrode/electrolyte interface during cycling. Potentiostatic electrodeposition of tin is carried out from an aqueous electrolyte bath based on sodium oxalate containing Sn²⁺ ions. Hard carbon electrodes are prepared by coating a conductive ink composed of hard carbon as the active material, poly-vinylidene fluoride as a polymeric binder ensuring mechanical cohesion and adhesion to the substrate, and carbon black as a conductive additive intended to enhance electronic transport properties. This ink is deposited onto various substrates prior to the electrodeposition step.

The first results enabled the investigation of interactions between the electrolyte bath and different substrates, such as aluminum, copper, and Papyex®. Several limitations related to the chemical and electrochemical stability of these substrates were identified, including cementation reactions between aluminum and tin and copper oxidation at the copper/hard carbon ink interface. These limitations led to the optimization of ink formulations by adjusting the proportions of the different components in order to improve adhesion and interfacial stability. These approaches showed promising results in terms of stability in the electrolyte bath and enabled the fabrication of electrodes compatible with coin-cell-type batteries. The electrochemical performances obtained during cycling highlight a synergistic effect between tin and hard carbon, with a specific capacity of 324 mAh g⁻¹ at the 20th cycle, associated with a coulombic efficiency of approximately 98%.

References:

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OC12 - SOLVOTHERMAL ELABORATION OF TRIDIMENSIONAL NITROGEN AND IRON CO-DOPED GRAPHENIC MATERIALS: TOWARDS PLATINUM FREE ORR CATALYSIS IN PEMFC

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Keywords: graphene; single-atom; doping

Summary: Climate change is nowadays one of the most challenging issues of our society, making it a major axis of research divided in three principal fields: energy production, industry, and transport. In transport, fuel cells, and more specifically the proton exchange membrane fuel cells (PEMFC), are particularly interesting non pollutant alternatives to our current thermal engines, that convert H₂ and O₂ reaction in electricity. However, despite their huge potential, they are not globally accessible yet for different reasons and notably their cost due to the presence of platinum nanoparticles supported on carbon black in the catalytic layer necessary for the oxygen reduction reaction (ORR) at the cathode. So, the idea is to develop a new platinum-free catalyst for this application, and a very promising more affordable structure with catalytic properties almost as good as platinum has been recently very studied: "single-atom". It is composed of a metallic atom, usually a transition metal, surrounded by heteroatoms, directly incorporated inside the structure of the carbon material [1]. The carbon material used here is a tridimensional graphenic structure elaborated via a solvothermal reaction between an alcohol and sodium followed by a pyrolysis and acid washing. This material, previously studied by the team, is notable for its exceptionally high surface area reaching up to 2 200 m².g⁻¹. A previous study focused on doping this inherently non-catalytic material with heteroatoms, such as nitrogen, by adding a nitrogen precursor during the solvothermal step. This doping process led to a partial redistribution of electric charges within the material, which demonstrated promising electrochemical performance in complete fuel cell with a current density over 30 mA.cm⁻², and a power density of 3.2 mW.cm⁻² [2]. In this new study, an iron precursor (FeAc) was moreover added either in the pyrolysis step at 850 °C, or directly in the solvothermal reaction, with the aim of promoting the formation of the "single-atom" iron structure. The obtained materials were then characterized by Transmission Electron Microscopy (TEM) (Fig. 1a), and Mössbauer spectroscopy and X-ray diffraction to look for the forms of the iron (Fig. 1b). Also, by Raman spectroscopy in order to investigate the carbon material's structure, N₂ adsorption to characterize the porosity of the materials, X-ray Photoelectron Spectroscopy (XPS) to see what is accessible on the surface, and finally linear sweep cyclic voltammetry in half fuel cell with impedance spectra to measure their catalytic properties.

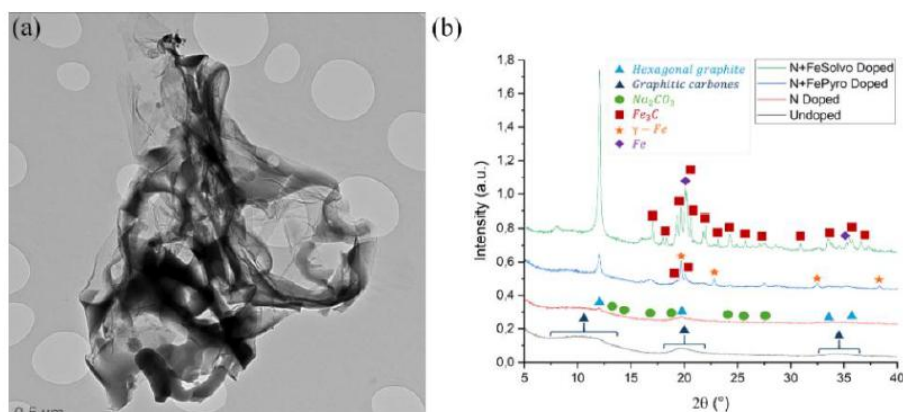


Fig. 1 : (a) TEM view of N+FePyro Doped material, (b) X ray diffractograms of materials with different doping

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OC13 - VARIATIONS AROUND THE CoNiFeMnCr EQUIMOLAR COMPOSITION: HIGH TEMPERATURE PROPERTIES OF SOME HEA OR MEA DERIVED FROM THE CANTOR'S ALLOY

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Keywords: Cantor's Alloy; Cast derivatives; Microstructures; High Temperature; HT properties

Summary: At the end of the 1990's a new family of metallic materials was born: the high entropy alloys (HEAs). Among the early first specimen of HEA there is the famous Cantor's alloy [1], quinary and equimolar, involving cobalt, nickel, iron, manganese and chromium. During the two past decades many studies have been devoted to the investigation of the properties at various temperatures of this type of alloy, particularly between cryogenic ones and several hundred °C more than ambient [2]. The present work deals with the exploration of the mechanical and chemical behavior at high temperatures (up to 1100°C) of a foundry version of the Cantor's alloy and of several derivatives resulting from *in situ* formation of MC carbides [3,4], Mn content decrease [5,6] or Ti addition [7]. It appeared that 1/the presence of TaC or HfC carbides reinforces mechanically the alloy [4], 1/the decrease in Mn [5] – or its total removal [6] – improves creep-resistance and hot oxidation behavior, and 3/Ti addition [7] induces mechanical strengthening and promotes an external oxide layer probably preventing the re-oxidation of the protective chromia scale losing a part as gaseous species.

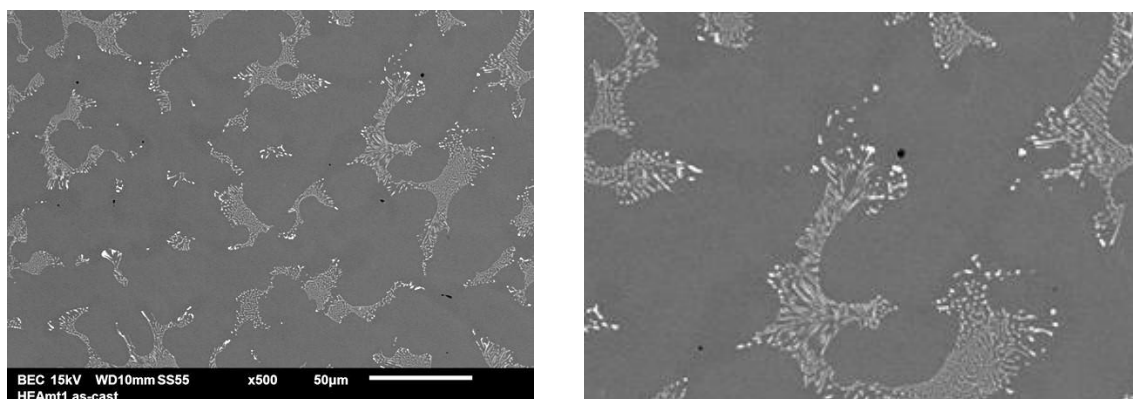


Fig. 1 : Microstructure of a Cantor-based HEA strengthened by eutectic TaC obtained by addition of 0.4C and 6Ta (wt.%); left: general view, right: the same but 2 × zoomed for more details

Acknowledgments to: Pauline Spaeter, Nassima Chenikha, Corentin Gay, Romin Chevalme, Lyna Amrouche, Siouare Hammi, Yasmina El Hadad, Lionel Aranda

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OC14 - OPTICAL IMAGING ELECTROCHEMICAL REACTIVITY THROUGH AN ELECTROCHROMIC COUNTER ELECTRODE

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Keywords: Electrochromism, Counter electrode, PEDOT, Modelisation, Reactivity

Summary:

Optical imaging has a long history for looking at surfaces at microscale. In the electrochemistry community, enormous effort has been made to visualize electrochemical reactions, usually by focusing on the optical change of the working electrode induced by e.g., surface plasmon resonance, electrochemiluminescence and fluorescence. This allows studying the heterogeneity of electrochemical reactivity of electrodes, which may offer better understanding of ca. electrocatalysis. However, this is limited to specific materials and reactions, as not all the reactions can be directly “seen” or labeled.

This presentation aims to present a new approach based on projecting the heterogeneity of working electrode (WE, the sample) to the color map of an electrochromic counter electrode (CE, the cover glass). By setting up the quantitative link between the optical change of CE with the potential and current, we may analyze the reactivity of WE from the experimentally measured optical signals from CE. The qualitative proof-of-concept was firstly done with WO₃ as the electrochromic film [1].

Here, we push forward the concept by developing poly(3,4-ethylenedioxythiophene) (PEDOT) based electrochromic counter electrode, for the sake of improving the color switching speed. The preparation and calibration protocols for PEDOT films are established. Furthermore, we focus on the theoretical and modelling aspect for guiding the experimental conditions by considering a model system with oxygen evolution reaction (OER). The first step is to simulate the oxidation and reduction of PEDOT on CE from known kinetics of OER on the WE while considering the geometry and mass transport of H⁺. The second step is to revert the process, that is, to convert experimental data of the color map of CE with time to the electrochemical reactivity map of the sample. This will be achieved by Python programming or COMSOL.

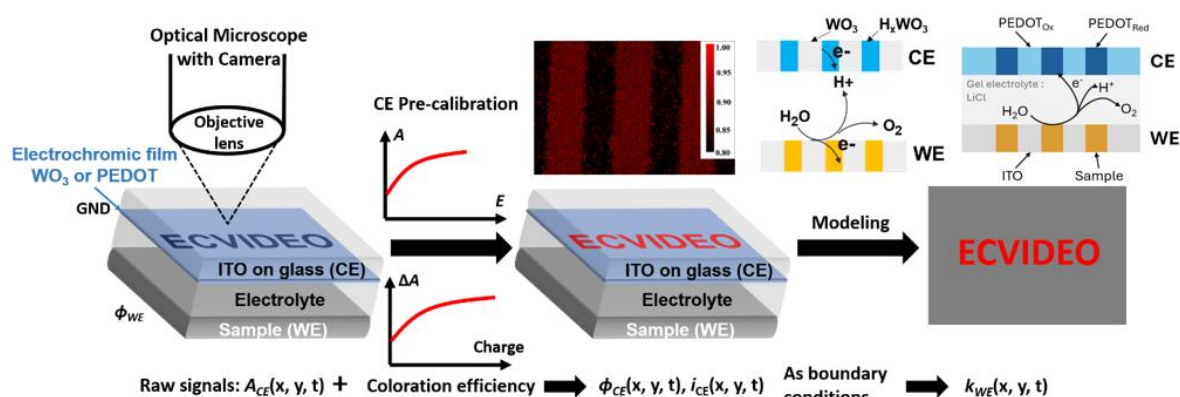


Fig. 1 : Schematic diagram of the project

Acknowledgment :

The authors acknowledge the financial support from LCPME and ANR (ECVIDEO, ANR-23-CE50-0020).

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OC15 - AZAULLAZINE MEETS IRON: ORBITAL DESIGN UNLOCKING LONG-LIVED EMISSION IN Fe(II) COMPLEXES

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Keywords: Iron(II) complexes, azaullazine, conjugation, HOMO-inversion, fluorescence

Summary: The search for earth-abundant alternatives to ruthenium photosensitizers has positioned iron complexes as highly attractive candidates in photophysical applications. Recent advances have shown that replacing classical polypyridyl ligands with pyridyl-based N-heterocyclic carbenes (NHCs) can significantly enhance Fe(II) photoactivity, yielding excited-state lifetimes of several tens of picoseconds. [1] Yet, achieving efficient solar-energy conversion demands not only longer-lived excited states but also broad, intense, and ideally panchromatic absorption. Strategies such as extended π -conjugation and HOMO inversion have recently proven effective in expanding spectral coverage. [2] In this work, we introduce a new ligand platform based on azaullazine, a fused and highly conjugated heterocycle which synthetic access has been developed by our team. [3] By substituting the central pyridine ring of pyridyl-NHC ligands with azaullazine, we sought to reshape the frontier orbitals of Fe(II) complexes and unlock new photophysical behavior. This design allowed us to synthesize the **C2** complex exhibiting one of the broadest absorption spectrum reported for Fe(II) systems, effectively achieving panchromatic light harvesting (Fig. 1A). [4] A combination of transient-absorption spectroscopy, spectroelectrochemistry, DFT calculations and photoluminescence studies reveals how the extended conjugation enables frontier-orbital engineering. Most remarkably, complex **C2** exhibits an unprecedented, long-lived emissive excited state, with an average lifetime of 3.5 ns, and a high fluorescence quantum yield, arising from a mixed MLCT / ILCT singlet state (Fig. 1B). This behavior, not observed in the analogous complexes **C0** and **C1**, is enabled by the distinctive azaullazine-based ligand framework. Overall, this work demonstrates how rational frontier-orbital design, enabled by azaullazine ligands, can overturn long-standing limitations of iron photophysics and pave the way toward next-generation Fe(II) photosensitizers with performance approaching that of precious metals.

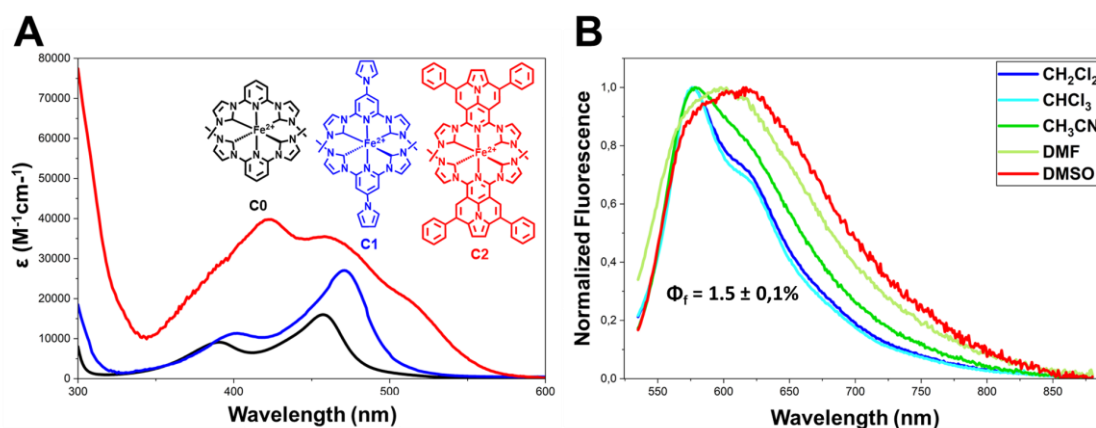


Fig. 1: (A) UV-VIS absorption spectra of complexes **C0**, **C1** and **C2** in acetonitrile. (B) Normalized emission spectra of **C2** Fe(II) complex in solvents of various polarity (λ_{exc} 520 nm).

References:

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OC16 - DESIGN AND SYNTHESIS OF NEW IRON COMPLEXES FOR PHOTOPHYSICAL APPLICATIONS

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Keywords: Iron complexes, *N*-heterocyclic carbenes

Summary: The development of photoactive iron complexes as sustainable alternatives to ruthenium-based systems has gained significant momentum in recent years. To match the properties of ruthenium complexes, they must meet specific photophysical requirements, including broad and intense absorption bands in the visible region and MLCT long-lived excited states to enable electron-transfer processes. In that context, our recent research has demonstrated their great potential of Fe(II) complexes for applications as new sensitizers in dye-sensitized solar cells.^{[1],[2]}

The pioneering work of Wärnmark's group, as well as our own, has led to the development of iron(II) complexes showing extended MLCT lifetimes and broadened spectral coverage through careful ligand design. All these complexes feature pyridine-bis(NHC) ligands, whose π -acceptor and σ -donor properties play a key role in increasing the MLCT lifetime, reaching up to tens of picoseconds for the best candidates.^{[3],[4]}

Among the structural modifications explored to date, the absorption spectra of the complexes bearing a pyrrole **C1** or a thiophene **C2** scaffold in the 4-position^[4] display a bathochromic shift compared to the Wärnmark's **C0** reference complex^[3] (figure 1A). To further enhance this effect, we investigated the impact of introducing conjugated motifs, such as thienyl units at the C3- and C5-positions of the pyridinyl ring ligand, molecular design that was not explored to date.

My presentation will highlight on the different strategies we explored and the synthetic challenges encountered. Especially, the functionalization of the 3- and 5-positions of the central pyridine ring via Suzuki cross-coupling required substantial optimization. thanks to these efforts, we successfully prepared the targeted ligands and the expected complex **C3**. Ongoing work on the **C4** complex is especially promising, although its Fe(II) structure has not yet been fully elucidated, offering exciting opportunities for further investigations.

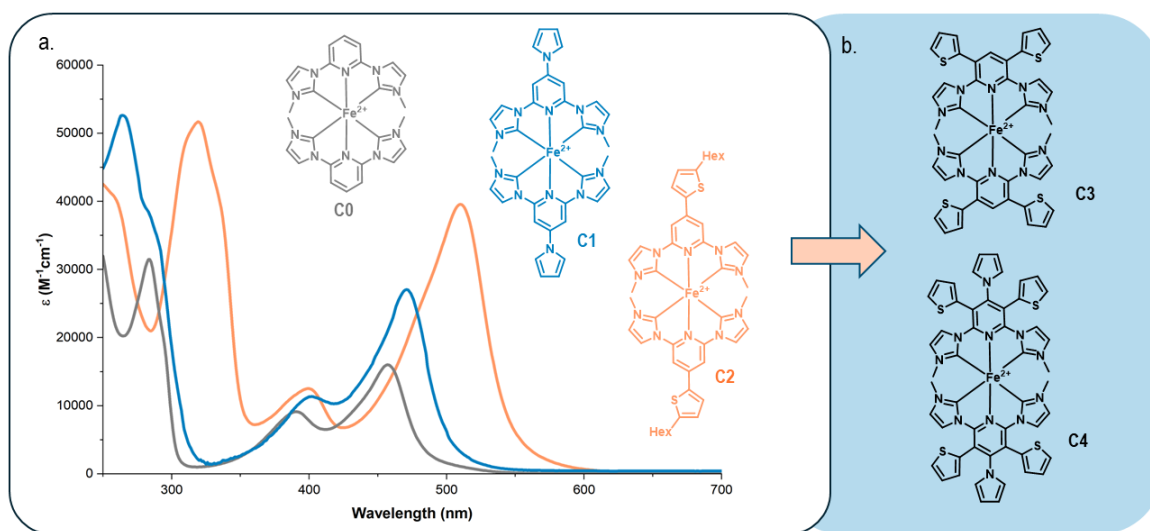


Fig. 1: a. UV-vis spectrum of Fe(II) complexes. b. Targeted structures

References:

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OC17 - INTEGRATED ABSORPTION-EMISSION SPECTROSCOPY UNDER ONE- AND TWO-PHOTON EXCITATION FOR ACCURATE PHOTOCHEMICAL PROFILING OF STYRYL-SUBSTITUTED CYCLIC ENONES

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Keywords: Photoswitches, Z/E Isomerization, Quantum Yields, Two-Photon Absorption

Summary:

Light-responsive molecular tools that enable precise, non-invasive control of biological structures represent a frontier in chemical and biomedical research. Amphiphilic photoswitches and photoswitchable lipids (photolipids) allow reversible modulation of membrane organization and function with high spatiotemporal precision.^[1] Developing such platforms require chromophores that combine efficient photoisomerization with optical activity in spectral regions suitable for deep-tissue penetration. We focused on styryl-substituted cyclic enones, cyclocurcumin-inspired chromophores which undergo reversible E/Z photoisomerization under UV irradiation (250–400 nm).^[2–3] Molecular dynamics simulations predict that these chromophores can also be efficiently excited in the biological NIR-I window (650–900 nm) via two-photon absorption (2PA), enabling deeper tissue penetration while minimizing photodamage.^[4]

To enable rational photolipids design, we developed an integrated experimental setup dedicated to the spectrophotometric monitoring of photoinduced reactions, simultaneously tracking absorption and emission. Using this approach, we demonstrate efficient two-photon-induced isomerization of our styryl-substituted cyclic enones and investigate switching fatigue under both one- and two-photon excitation. The simultaneous measurement of absorption and emission allows accurate determination of both photoisomerization and fluorescence quantum yields for each isomer. By linking molecular structure, optical response, and photochemical performance, our work provides a framework for designing next-generation photolipids for deep-tissue optical control with reduced phototoxicity.

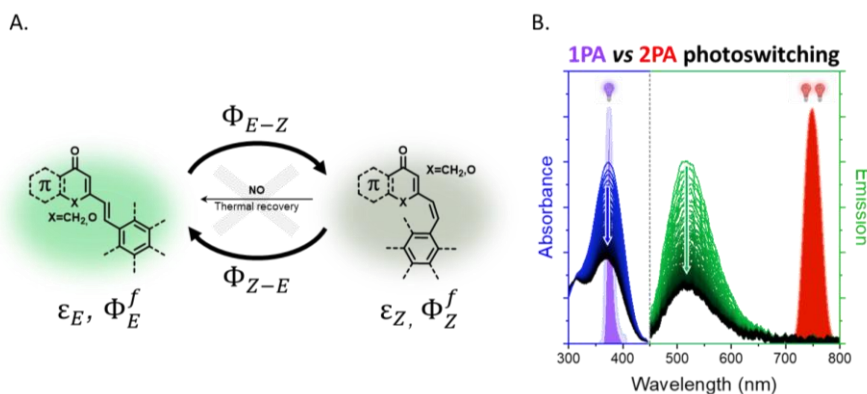


Fig. 1 : (A) Schematic representation of the photochemical and photophysical properties of styryl-substituted cyclic enones . (B) Isomerization induced by one-photon (1PA) or two-photon (2PA) activation, with simultaneous monitoring of absorption and emission.

References:

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OC18 - ENGINEERING NIR-ACTIVE PHOTOSENSITIZERS FROM SUPRAMOLECULAR NHC PLATFORMS FOR PHOTODYNAMIC THERAPY

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Keywords: bis-heterocycles, macrocycles, photophysical properties, biological evaluation, X-ray structures

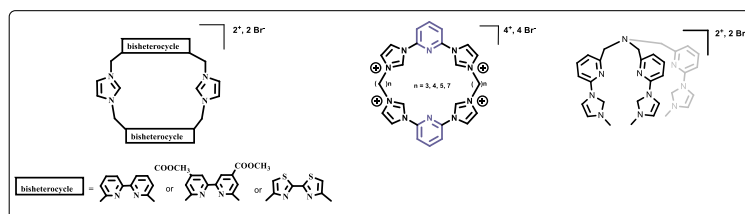
Summary: The overall objective of this work is the design of new photosensitizers based on near-infrared (NIR) light activation of original proligands, including hemicages and cages, for applications in photodynamic therapy (PDT). Particular emphasis is placed on their complexation with earth-abundant metals in order to enhance their photophysical properties (UV-vis absorption, fluorescence, and singlet oxygen (¹O₂) generation) as well as their biological activity.

First, we report the synthesis, via different synthetic pathways, of new symmetrical and asymmetrical macro-bis-heterocyclic bis-imidazolium ligands (L1–L6) as *N*-heterocyclic carbene (NHC) precursors, together with related pincer ligands (L1'–L3') [1]. Some of these compounds, either free or assembled into silver supramolecular architectures, exhibit notable intrinsic photophysical and biological properties. In particular, efficient ¹O₂ generation upon light irradiation (λ = 290 nm) was observed, with quantum yields reaching up to 84% in D₂O for certain macrocycles, highlighting their potential for PDT applications.

Secondly, we describe a rapid two-step synthetic route to a new family of symmetric tetra-imidazolium bis-heterocycles (C1–C7). Among them, compound C7 [2] was extensively investigated for its photophysical properties with a view toward theranostic applications based on fluorescence. C7, both in its free form and as iron complexes, was evaluated for biological activity against clinically relevant viral, fungal, and bacterial human pathogens. A possible inhibitory mechanism targeting bacterial cell wall synthesis was proposed, supported by electron microscopy observations and molecular docking studies.

Finally, this work also focuses on the multistep synthesis of novel supramolecular assemblies, namely hemicages and cages, constructed from tripodal ligands bearing pyridine-NHC or bipyridine coordination motifs. These architectures are designed to optimize metal-to-ligand charge transfer (MLCT) excited states, particularly in iron(II) complexes, by increasing structural rigidity and suppressing undesired metal-centered (MC) deactivation pathways. The chelating units are anchored to a central amine platform. The pyridine-NHC-based ligand shows promising coordination behavior, while parallel efforts led to the synthesis of a bipyridine-based hemicage and its corresponding iron(II) complex.

Overall, these systems aim to stabilize photoactive complexes of earth-abundant metals, paving the way toward more efficient, sustainable, and biologically relevant photosensitizers for photodynamic therapy



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OC19 - SIRT6–NUCLEOSOME INTERACTIONS: C-TERMINAL DOMAIN BINDING MODES THAT MODULATE DNA UNWRAPPING

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Keywords: SIRT6, nucleosome core particle, molecular dynamic, histone deacetylation, C-terminal domain

Summary:

In prokaryotes and eukaryotes, Sirtuins are a class of NAD-dependent histone deacetylases that regulate important biological pathways. This enzyme family comprises seven members, named SIRT1 to SIRT7. Among them, Sirtuin 6 (SIRT6) is a human sirtuin that deacetylates histone H3 and plays a key role in DNA repair, telomere maintenance, carbohydrate and lipid metabolism, and lifespan. SIRT6 consists of a zinc finger domain, a Rossmann fold domain containing the NAD⁺ binding site, a disordered N-terminal and a disordered C-terminal domain (CTD), figure 1. CTD has been found to influence the interaction between SIRT6 and the nucleosome, the first level of DNA compaction, composed of DNA wrapped around histone proteins. However, the specific role of the CTD on SIRT6 interaction with nucleosomes for histone deacetylation remains unclear. Here, we run molecular dynamics simulations of full-length SIRT6 bound to the nucleosome with different initial positions of CTD to uncover its dynamical behaviour. We found that CTD preferentially interacts with DNA at the entry/exit point of the nucleosome side near the enzyme's binding site. In specific cases, CTD participates in the promotion of DNA unwrapping. Additionally, we observed that CTD modulates the accessibility of lysine sites near the H3 histone core, facilitating their binding to SIRT6's active site. This work reveals the dynamic binding behaviour of full-length SIRT6 to the nucleosome, providing structural insights into its role in DNA unwrapping and lysine accessibility. [2]

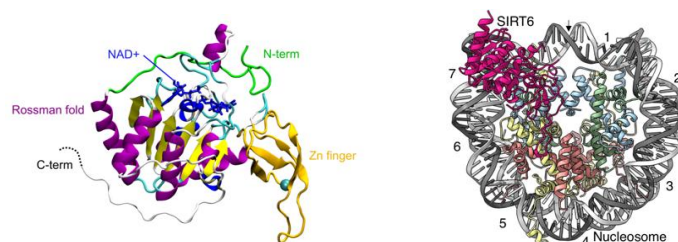


Fig. 1 : *Left*: SIRT6 structure, a catalytic domain structured as a Rossmann fold (purple) that harbors the NAD⁺ cofactor (blue), a Zinc-finger domain (yellow), and a N-terminal (green) and a C-terminal domain (gray); *Right*: SIRT6 (magenta) in complex with the nucleosome (H3 in blue, H4 in green, H2A in yellow, H2B in orange and DNA in gray) [1].

References:

[1] *eLife*. **2024**, 12:RP87989

[2] *J. Phys. Chem. B*. **2025**, 129, 9855-9861

OC20 - SYNTHESIS AND FUNCTIONALIZATION OF CYANINE-7 DYES FOR THERANOSTIC APPLICATIONS

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Keywords: cyanine-7, fluorescence, photoacoustic imaging, Photothermal therapy.

Summary:

Heptamethine cyanine (cyanine-7) dyes possess attractive photophysical properties,¹ notably their strong absorption in the near-infrared (NIR) region and their ability to generate fluorescence (radiative relaxation) and photoacoustic signals (non-radiative relaxation).² Their efficient light-to-heat conversion also makes them suitable for photothermal therapy (Figure 1).² The combination of imaging and therapeutic functions provides valuable complementary information for diagnosis and treatment monitoring.⁴

In this work, we report the synthesis and functionalization of cyanine-7 dyes starting from the commercially available IR-780 (X = Cl), chosen for its stability and selective reactivity at the meso position of the cyclohexene ring. Structural modulation at this position, through the introduction of different heteroatoms (N, S), allows access derivatives with fine-tuning photophysical properties. In addition, a series of cyanine-7 dimers bearing various linkers and heteroatoms at the meso position was developed (Figure 2). Optical and photothermal studies highlight the potential of these cyanine-7 derivatives as theranostic platforms for image-guided phototherapy.³

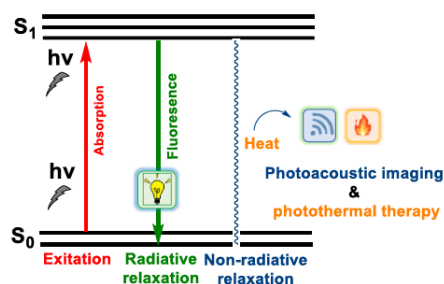


Figure 1: Jablonski diagram

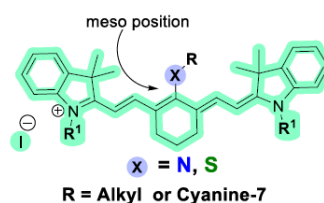


Figure 2: cyanine-7 derivative

References:

- [1] Org. Biomol. Chem., 2020, 18, 9385–9397
- [2] WO Patent WO2025210124, 2025
- [3] Dyes Pigm., 2024, 223, 111995
- [4] Bioact. Mater., 2021, 6, 794

OC21 - NEAR INFRARED PHOTODYNAMIC THERAPY FOR PANCREATIC CANCER: DESIGN OF PORPHYRIN-BASED PHOTSENSITIZERS

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Keywords: Photodynamic therapy, near-infrared porphyrin photosensitizer, pancreatic cancer

Summary:

Pancreatic ductal adenocarcinoma (PDAC) remains one of the deadliest cancers, with a five-year survival rate of 5% and is projected to become the second leading cause of cancer-related mortality by 2040. The limited efficacy of current treatments is largely due to the aggressive biology of the disease and the lack of tumor-selective therapeutic strategies. Photodynamic therapy (PDT) represents an attractive, minimally invasive approach that can be combined with existing PDAC treatments. This method relies on light-triggered activation of a photosensitizer, leading to the generation of reactive oxygen species (ROS) inducing cancer cells destruction. However, the clinical translation of PDT in PDAC is still hindered by the limitations of currently approved photosensitizers, mostly based on porphyrin scaffolds, including suboptimal tumor selectivity, poor solubility, and prolonged off-target photosensitivity.^[1] Building on the successful application of our own design of porphyrin-based photosensitizers in cancer and anti-bacterial PDT,^[2] we are now extending this approach to PDAC. In this context, we focus on the development of next-generation porphyrin-based photosensitizers specifically designed and targeted for PDAC. These compounds combine improved aqueous solubility, activation in the near-infrared (NIR) region to enhance tissue penetration, and conjugation to tumor-targeting peptides to promote selective accumulation within pancreatic tumors.

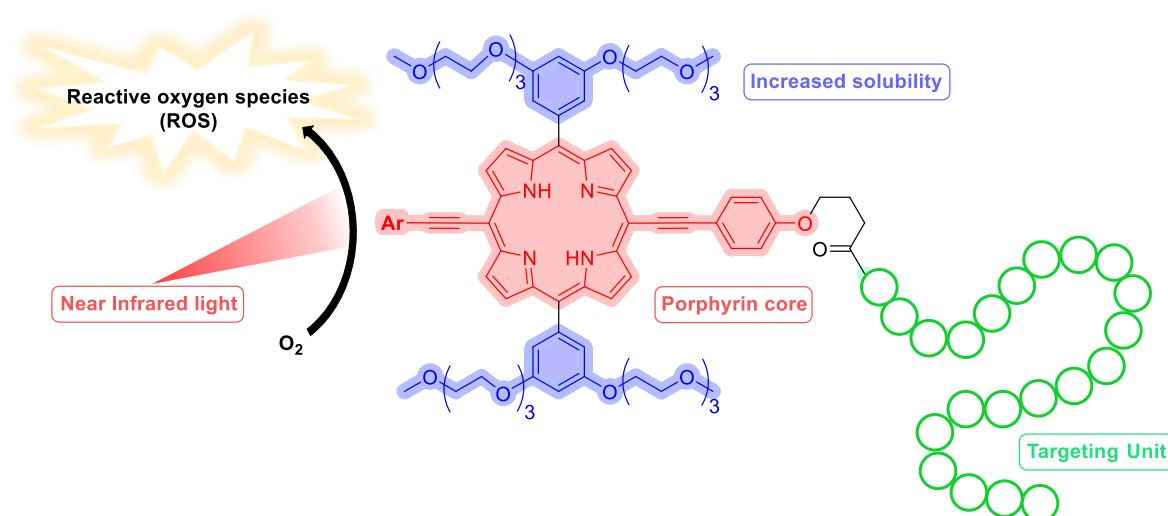


Fig. 1: Structure of the targeted near-infrared photosensitizer for pancreatic cancer cells destruction via ROS generation.

References:

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- [2] a) S. Jenny, A. Sour, F. Bolze, B. Ventura, V. Heitz, *Org. Biomol. Chem.*, **2019**, 17, 6585; b) C. Gourlot, A. Gosset, E. Glattard, C. Aisenbrey, S. Rangasamy, M. Rabineau, T.-S. Ouk, P. Lavalle, C. Gourlaouen, B. Ventura, B. Bechinger, V. Heitz, *ACS Infect. Dis.* **2022**, 8, 1509.

OC22 - ISCRIMINATION OF RACEMIC AND ENANTIOPURE PHENYLALANINE CRYSTALS BY LOW FREQUENCY POLARIZED RAMAN SPECTROSCOPY

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Keywords: Low-frequency Raman spectroscopy, 2D correlation, polarization, racemic, enantiomer

Summary: The discrimination between enantiopure and racemic species is essential due to their distinct physicochemical and biological properties. Conventional methods include X-ray diffraction for the discrimination of solid crystals and chromatographic separation for liquid mixtures of enantiomers. We propose here to investigate low-frequency polarized Raman spectroscopy (LFRS) as a spectroscopic alternative to discriminate between racemic and enantiopure crystals.

LFRS is a powerful technique to study collective vibrational modes in molecular systems, especially those involving global structural deformations. These modes, typically below 200 cm^{-1} , are highly sensitive to weak intermolecular forces such as hydrogen bonding and van der Waals interactions, which influence both frequency and intensity of Raman signals. In molecular crystals, small changes in packing or orientation can cause noticeable spectral shifts, making LFRS useful to detect polymorphism, impurities, and differences between racemic and enantiopure crystals.

However, interpretation of LFRS spectra is complicated by molecular polarizability anisotropy, as orientation relative to laser polarization affects intensity. Polarization-resolved Raman spectroscopy helps revealing molecular orientation and symmetry. However, broad low-frequency bands and peak overlap can obscure details, even with polarization analysis. To address this, chemometric methods like two-dimensional correlation spectroscopy (2D-COS) improve resolution by analyzing correlations under controlled perturbations.

This work integrates polarized LFRS with 2DCOS to investigate phenylalanine crystals, focusing on pure D-enantiomer powders and DL racemic mixtures. The combined approach enables the discrimination of characteristic low-frequency vibrational modes specific to each crystalline form. Leveraging these spectral markers in Raman mapping reveals localized racemic DL inclusions within nominally pure D samples. This methodology provides a spatially resolved probe of racemization phenomena in enantiopure systems, offering significant implications for pharmaceutical manufacturing and quality control.

Posters

P01 - IMPACT OF IONIC STRENGTH ON *IN SITU* ELECTROCHEMICAL PH MODULATION

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Keywords: Electrochemical pH control; In situ detection; Lead (Pb^{2+}); Microelectrodes; Environmental water analysis

Summary: *In situ* detection of trace metals, such as lead (Pb^{2+}), in environmental waters remains a major analytical challenge. One key challenge is the non-optimal pH of waters (pH 6–8), which contrasts with the acidic conditions required for effective electrochemical detection. Conventional laboratory protocols rely on the addition of strong acids or buffer solutions to adjust the optimal pH, however, this approach is not suited for on-site applications due to risks of sample contamination, and the need for reagent treatment.

Our previously published work* focuses on the electrochemical modulation of pH as a reagent-free alternative for sample conditioning. We developed an electrochemical cell integrating two working electrodes: a gold screen-printed electrode for Pb^{2+} sensing and a platinum grid acting as a local acidifier. By applying an oxidative potential to the platinum electrode, water electrolysis is performed, leading to the *in situ* generation of protons. This process enables a controlled and localized acidification to adjust the pH near the sensing electrode without the addition of chemical additives to the sample. The design and operating parameters were optimized to achieve the optimal local acidification for Pb^{2+} detection. Under these conditions, lead was detected at concentrations below the World Health Organization guideline value for drinking water, proving the suitability of this approach for on-site analysis.

Another additional challenge for *in situ* Pb^{2+} detection relates to the low ionic strength and poor conductivity of water samples. Ongoing work aims to address these constraints by the use of microelectrodes architectures. The integration of homemade fabricated microelectrode is expected to enhance mass transport, minimize ohmic drop effects, and ensure stable potential control in low-conductivity media. The synergy between microelectrodes and electrochemical pH modulation offers a promising route toward reliable, reagent-free *in situ* detection of trace metals in real environmental water samples.

References:

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P02 - ELECTRODEPOSITION OF GOLD AT LIQUID-LIQUID INTERFACE

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Keywords: Charge transfer, liquid-liquid interface, gold, electrodeposition, SERS substrate

Summary: Electrochemistry can be used to synthesize (nano)materials, for instance by reduction of noble metallic species. Electrodeposition at the Interface between Two Immiscible Electrolyte Solutions (ITIES) is an alternative route to promote the nucleation and growth of metal deposits and avoid surface defects when using a solid | liquid interface. Electrons are in that case supplied by a reducing agent present in the organic phase, instead of the working electrode in classical electrochemistry, while the metallic species are dissolved in the aqueous phase. This technique was applied here to reduced gold species. It enabled a gold film deposition at the interface between an organic phase (TFT) and an aqueous phase containing tetrachloroaurate anion (AuCl_4^-). In spite of its conceptual simplicity, the reaction mechanism remains relatively unknown. The reduction of gold (III) by the organic reducing agent, DecamethylFerrocene (DcFc) was therefore studied using in situ UV-visible spectroscopy, scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and Raman scattering spectroscopy. Characterization analyses revealed an accelerated degradation of the organic reagents during synthesis, as well as the exaltation of the Raman scattering properties of the obtained film.

P03 - DEVELOPMENT OF AN ELECTROCHEMILUMINESCENT SENSOR BASED ON TRIS(2,2'-BIPYRIDYL)RUTHENIUM(II) IMMOBILIZED IN ORIENTED MESOPOROUS SILICA FILMS

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Keywords: Electrochemiluminescence - Tris(2,2'-bipyridyl)ruthenium(II) - Mesoporous silica films - Click chemistry - Sensor

Summary:

Electrochemiluminescence (ECL) is an analytical technique based on light emission generated by an electrogenerated chemical reaction involving a luminophore and, most often, a sacrificial co-reactant [1]. When the analyte of interest acts as the co-reactant, the light intensity produced after electrochemical stimulation is proportional to its concentration. Among the luminophores commonly used, the tris(2,2'-bipyridine)ruthenium(II) complex, $[\text{Ru}(\text{bpy})_3]^{2+}$, stands out due to its high redox stability, highly reproducible signal, and well-defined optical properties [2]. Conventionally, the luminophore is adsorbed onto a solid support (electrode, polymer, or gold nanoparticles) to create sensitive and selective analytical platforms [3]. However, these immobilization strategies do not ensure long-term sensor stability. In this work, we explore an approach based on the durable immobilization of this complex within thin films of oriented mesoporous silica deposited on the electrode surface (Fig. 1) [4]. These films, prepared using the Electrochemically Assisted Self-Assembly (EASA) method, exhibit a hexagonal structure with pores oriented perpendicular to the electrode surface, thereby promoting analyte diffusion toward the active surface and significantly enhancing electrode sensitivity [5]. Unlike simple impregnation with the $[\text{Ru}(\text{bpy})_3]^{2+}$ reagent, covalent immobilization via click chemistry onto the silica walls ensures the stability of the luminophore within the mesochannels and prevents its release into solution. This guarantees sensor durability and reduces risks associated with luminophore toxicity. The developed devices were tested and compared using a glycine-derived pesticide, glyphosate, as the co-reactant.

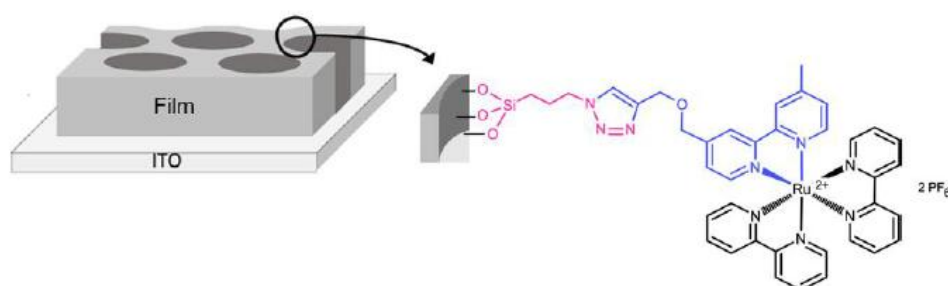


Fig. 1: Schematic representation of the silica film functionalized with the ruthenium (II) complex.

References:

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- [2] Anal. Chim. Acta 1999, 378, 1–41.
- [3] IntechOpen, 2021, Chapter 75769.
- [4] Microporous Mesoporous Mater. 2025, 113524.
- [5] Acc. Chem. Res. 2021, 54, 3563–3575.

P04 - INTERCALATION OF PHOTSENSITIZERS IN Zn₂Al-LAYERED DOUBLE HYDROXIDE FOR WATER REMEDIATION

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Keywords: LDH – Hybrids – Intercalation – Photosensitizers

Summary:

Layered double hydroxides (LDHs), also known as anionic clays, have the general chemical formula $[M^{II}_{1-x}M^{III}_x(OH)_2]^{x+}[(A^{n-})_{x/n} \cdot yH_2O]^{x-}$. They consist of positively charged metal hydroxide sheets where cations are located at the center of octahedra formed by hydroxides. Solvated anions (A^{n-}) are intercalated between these sheets. The compositional tunability of LDHs, enabled by the flexible selection of cations and intercalated anions (organic or inorganic), makes them highly versatile for various applications, with particular interest in water remediation [1]. In this context, the use of 2D systems, such as films formed either by *in situ* method or by particle deposition, is attractive as the materials can be recycled and reused. According to the literature, certain organic anions (benzoate, isophthalate, trimesate, etc.) intercalated into Zn₂Al-LDH through direct synthesis have been used as supramolecular photosensitizers, exhibiting photocatalytic properties in the near-infrared region [2]. These could allow the formation of highly reactive singlet oxygen ¹O₂, to initiate the degradation of organic pollutants by oxidation mechanisms [3].

In this work, we investigated the intercalation of various anions (benzoate, phthalate, isophthalate, terephthalate, trimesate, trimellitate and pyromellitate) into Zn₂Al-LDH in two systems: films and suspensions. The hybrid organic-inorganic LDHs were synthesized using direct coprecipitation, anion exchange, and reconstruction. The arrangement of anions in the interlayer space was investigated as a function of (1) the synthesis method and (2) the system (whether particles were immobilised on a substrate or not) considering that the dynamic of the interlayer space may be constrained in the case of films [4]. The intercalation of organic anions in LDH materials was characterized by vibrational spectroscopies (Raman, IR), scanning electron microscopy (SEM) and X-ray diffraction (XRD). First, the successful intercalation of organic molecules was confirmed. Then, we demonstrated that the synthesis method influenced the microscopic structure of the materials (**Fig. 1**). Finally, the anion stability in the interlayer space was studied in carbonate and chloride solutions to evaluate their exchange properties. The photocatalytic properties of the materials will be assessed in future studies.

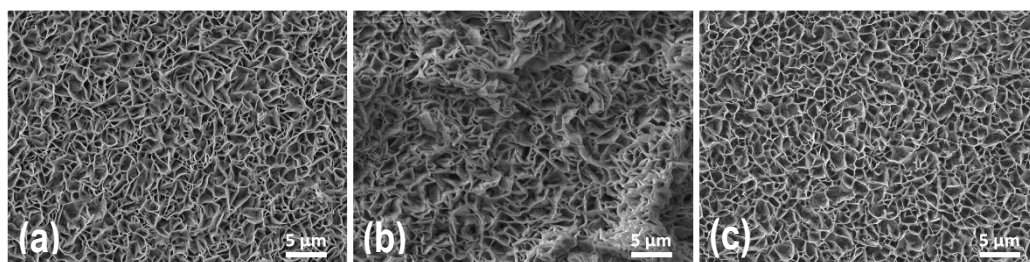


Fig. 1 : SEM images of (a) Zn₂Al-NO₃ LDH, (b) Zn₂Al-Benzoate LDH synthesized by exchange and (c) Zn₂Al-Benzoate LDH synthesized by reconstruction.

References:

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- [2] *Nat. Commun.*, **2018**, 9, 2798.
- [3] *ChemPhotoChem.*, **2018**, 7, 535-547.
- [4] *Mater. Today Chem.* **2024**, 35, 101897.

P05 - ON-SURFACE SYNTHESIS AND CHARACTERIZATION OF KAGOME GRAPHENE

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Keywords: Kagome graphene, on-surface synthesis, AFM, STM

Summary:

Kagome graphene (KG),^{1–3} a two-dimensional (2D) arrangement of corner-sharing graphene triangles, is long regarded as an ideal candidate for strongly correlated electron phenomena and frustrated magnetism. Flat bands in Kagome graphene might host strong electron correlations and frustrated magnetism upon electronic doping. However, the porous nature of Kagome graphene opens a semiconducting gap due to quantum confinement, preventing its fine-tuning by electrostatic gates. Here we induce zero-energy states into a semiconducting Kagome graphene by inserting π - radicals at selected locations. We utilize the on-surface reaction of tribromotrioxazatriangulene molecules to synthesize carbonyl- functionalized Kagome graphene on Au(111), thereafter modified in situ by exposure to atomic hydrogen. Atomic force microscopy and tunneling spectroscopy unveil the stepwise chemical transformation of the carbonyl groups into radicals, which creates local magnetic defects of spin state $S = 1/2$ and zero-energy states as confirmed by density functional theory. The ability to imprint local magnetic moments opens up prospects to study the interplay between topology, magnetism, and electron correlation in Kagome graphene.

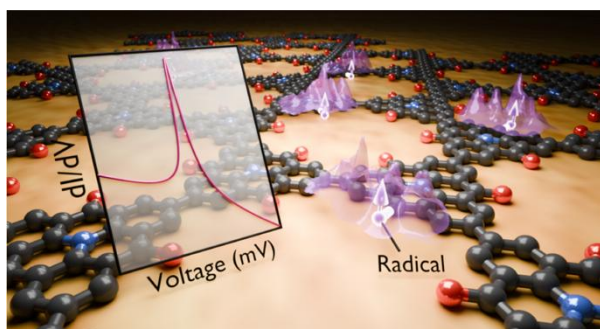


Fig. 1: Artistic representation of Kagome graphene obtained by on-surface synthesis

References:

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- [2] Pawlak, R.; Anindya, K. N.; Chahib, O.; Liu, J.-C.; Hiret, P.; Marot, L.; Luzet, V.; Palmino, F.; Chérioux, F.; Rochefort, A.; Meyer, E. *ACS Nano* **2025**, 19, 4768-4777

P06 - TROUBLES IN THE SOLIDIFICATION PROCESS OF 15%Al-CONTAINING COBALT ALLOYS VERY RICH IN TAC CARBIDES

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Keywords: High frequency induction melting; Co(Al) alloys; High TaC fraction; TaC local accumulation

Summary: Tantalum carbides are hard particles especially efficient to strengthen on long times superalloys at elevated temperature and allowing them resisting mechanical stresses and creep deformation [1,2]. Their effect is expected to be enhanced for higher TaC fractions, but enriching too much the alloys with carbon and tantalum may influence the development of the microstructure during solidification. In the present work Ta and C are progressively added – by respecting their atomic equivalence – to a cobalt-aluminum base, elaborated at a small scale (40g–weighing ingots). From the less {Ta,C}–alloyed to the most alloyed one, i.e. from 0.4C-6Ta to 1.0C-15Ta (wt.%), the obtained TaC fraction increases but an increasing part of this phase moves to the periphery of ingot. Consequently the core of the ingot becomes effectively richer in TaC, eutectic and pre-eutectic, but an increasing part of TaC has migrated to the periphery and bottom of the ingots (under the effects of the electromagnetic stirring and of the high density of the TaC phase by comparison with the density of the whole liquid alloy). This phenomenon, earlier encountered for a cobalt-chromium with 1.0C-15Ta too [3], makes that a significant part of the costly element Ta is lost. These observations made here in the case of small ingots (40g) let expecting much greater lost at an industrial scale (several tons of liquid alloy).

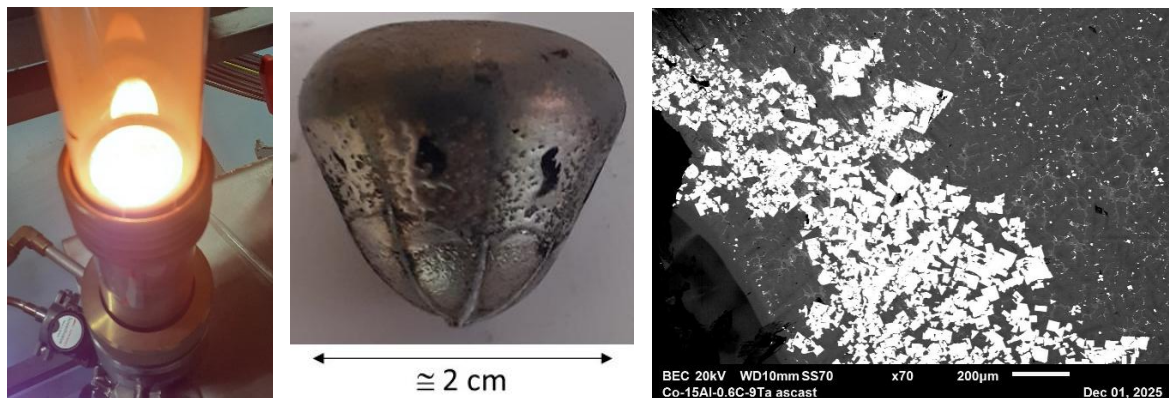


Fig. 1 : Small scale high frequency induction melting (left), obtained ingot (middle) and TaC cluster observed in ingot periphery (right)

References:

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P07 - SELECTIVE LEACHING OF ZINC IN ELECTRIC ARC FURNACE DUST

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Keywords: zinc, EAFD, leaching, nitriloacetate, design of experiments

Summary:

Electric arc furnace dusts (EAFD) are a major by-product of the steelmaking industry containing heavy metals such as zinc and lead. In order to reintroduce the iron oxides they contain into the steelmaking process, these hazardous wastes [1] must be processed to extract and recycle zinc. Also present in the soluble form ZnO, zinc in ferrite form (ZnFe_2O_4) is hardly dissolved by reagents that provide selective leaching and leave iron in its solid form [2]. It is therefore important to determine the proportion of each before a hydrometallurgical treatment.

This work aimed to study the composition of three dusts (one resulting from the fusion of stainless steel, two from the fusion of carbon steel) and to conduct zinc speciation with the use of ammonium acetate and hydrochloric acid [3]. The second part of this study aimed to model the influence of temperature and molar ratio on the leaching yield of zinc in the ZnO form by the nitriloacetate ion with the use of design of experiments and to determine the influence of time with kinetic monitoring.

The first results showed that the nature of the scrap metal impacts the dusts composition and confirmed that iron and zinc are the major elements composing the EAFD studied. Zinc speciation showed that it is mostly present as ZnO (between 53,7 and 72,8 wt%). Results of the leaching using trisodium nitriloacetate at pH 8 confirmed the selectivity of the reagent regarding iron and showed that a 100 % yield could be obtained at 60 °C after 4 hours of reaction with a molar ratio of 6. For a reaction time of 30 minutes, the impact of temperature on the yield is 1,81 times higher than that of molar ratio. Kinetic monitoring showed that the reaction starts fast (70 % yield at 10 min, 60 °C, molar ratio = 6) and that a plateau is observed after 40 to 50 min in each case but a kinetic study using the shrinking core model would be suitable for this type of reaction. [4, 5]

The authors acknowledge the ANR – FRANCE (French National Research Agency) for its financial support of the MICAMEL project n°ANR-24-CE04-6837 and the Bourse Orion program for funding.

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- [5] *Hydrometallurgy*. **2004**, 71 (3), 435–446

P08 - SUSTAINABLE AND DIRECT UPCYCLING OF WASTE GRAPHITE ANODES VIA DEEP EUTECTIC SOLVENTS

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Keywords: Waste graphite; Deep eutectic solvents; Sustainable and direct upcycling; Phosphate-rich interfacial film

Summary:

Lithium-ion batteries (LIBs) have flourished in power and energy storage, followed by a huge amount of waste batteries that pours into the market. In our work, a deep eutectic solvent (DES), with low melting point, low cost, and natural environmental protection, has been applied as a green reagent to realize the sustainable and direct upcycling of waste graphite. Substances in DES existing as ionic structures and charged P-containing groups are more likely to attack defect-rich graphite and realize in situ phosphorus doping. Consequently, doped phosphorus participates in construction of Li_3PO_4 -rich solid electrolyte interphase (SEI). Due to the reconstruction of phosphate-rich interfacial film, the capacity of regenerated graphite maintains as high as 365 mAh/g at 0.5C with a capacity retention rate of 95.5%, which is much higher than that of waste graphite, and even commercial graphite. In addition, the low melting point of DES makes the regeneration temperature significantly lower, which is part of a reduction in energy consumption and in the CO_2 emission. More importantly, the environment and economy have been optimized, which is conducive to its large-scale promotion in the industry. This provides solutions for next-generation technologies with more sustainable materials.

References:

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P09 - INTERCOMPARISON STUDY OF DGT DEVICES WITH DIHYDROXAMATE-BASED BINDING GELS FOR URANIUM(VI) SAMPLING IN FRESHWATER

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Keywords: DGT, dihydroxamic acids, uranyl binding, chelating resins

Summary: Uranium is released into the environment through mining activities, production and use of nuclear fuel (~65 kt/year), reprocessing of spent fuel and storage of nuclear waste, coal burning, and spreading of phosphate fertilizers. Once discharged, uranium may migrate across various environmental compartments, ultimately leading to the contamination of trophic chains [1]. Monitoring such contamination, particularly in aquatic systems, calls for innovative analytical techniques capable of assessing both the distribution and bioavailability of actinides. In that respect, Diffusive Gradients in Thin Films (DGT) is one of the most promising techniques for determining the concentration of labile metal species in aquatic environments, including wetlands and sediments. Unfortunately, the most widely used and commercially available binding gels for uranium, namely the Chelex-100® ion-exchange resin and the TiO₂-based Metsorb® adsorbing material, are known to underperform in hard, carbonate-rich freshwater and seawater [2,3].

To overcome these shortcomings, we designed a pincer-like UO₂²⁺ chelator bearing two terminal hydroxamate bidentate groups able to coordinate the uranyl cation in its equatorial plane [4]. Potentiometric studies revealed a high binding affinity towards UO₂²⁺ and an excellent selectivity with respect to Ca²⁺ and Mg²⁺ ions. According to PHREEQC speciation calculations, uranium(VI) is efficiently chelated between pH 4 and 8 even in the presence of major competing ions such as Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, SO₄²⁻, and HCO₃⁻. Hence, the dihydroxamic acid was covalently grafted by amide bond formation onto a hydrophilic organic resin, Sephadex CM-25®, and the resulting extracting material embedded in a binding gel made of agarose. The uranium(VI) uptake performances of the new DGT samplers made thereof were assessed under controlled laboratory conditions, using both mineral waters and synthetic seawater spiked with 20 µg/L of UO₂²⁺. Accordingly, uranium prevails as [M_xUO₂(CO₃)₃]^{(4-2x)-} triscarbonato species (M = Mg, x = 1; M = Ca, x = 0-2) in each medium. Results were benchmarked against commercial Chelex-100® and Metsorb® samplers, highlighting the superiority of the hydroxamic acid based extracting resin

This work was supported by ASNR (formerly IRSN), CNRS, the "Agence Nationale de la Recherche" (grant n° ANR-17-CE08-0053 - PLUTON project), and the French program NEEDS (NEPTUNE project). The Conseil Regional de Bourgogne Franche-Comté (T.F.), the Conseil Regional de Bourgogne (O.F.), and the EU program FEDER are acknowledged for granting PhD fellowships.

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P10 - ULTRASONICATION-DRIVEN ADVANCES IN MnO_2 NANOMATERIALS: UNLOCKING NEW HORIZONS FOR CANCER TREATMENT

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Keywords: MnO_2 , ultrasonication, oncology, cytotoxicity, colloidal stability

Summary: We report a controllable ultrasonication-driven remodeling of MnO_2 nanosheets into progressively exfoliated sheets and nanofibers, enabling fine tuning of morphology, crystallographic fingerprints, surface redox state, porosity, hydrodynamic size, and colloidal behavior. This structure–property trajectory is established by complementary TEM/XRD/Raman/XPS/DLS/BET analyses, and directly informs biomedical formulation constraints, showing improved dispersion in water but reduced stability under physiologically relevant ionic strength (0.15 M NaCl, PBS). In vitro viability assays (MTS) performed on cancer (TSA, 4T1) and healthy (NIH3T3) cell lines reveal dose-dependent effects, with nanofibers exhibiting stronger cytotoxicity on tumor cells than the parent nanosheets. By linking sonication-controlled nanoform evolution to interfacial area, surface chemistry, and bioresponse, this work provides practical design rules for MnO_2 -based oncology nanoplateforms that aim to exploit tumor-microenvironment reactivity (e.g., hypoxia relief and redox modulation) and to support imaging/therapy combinations such as MRI guidance and radiotherapy enhancement. [1]

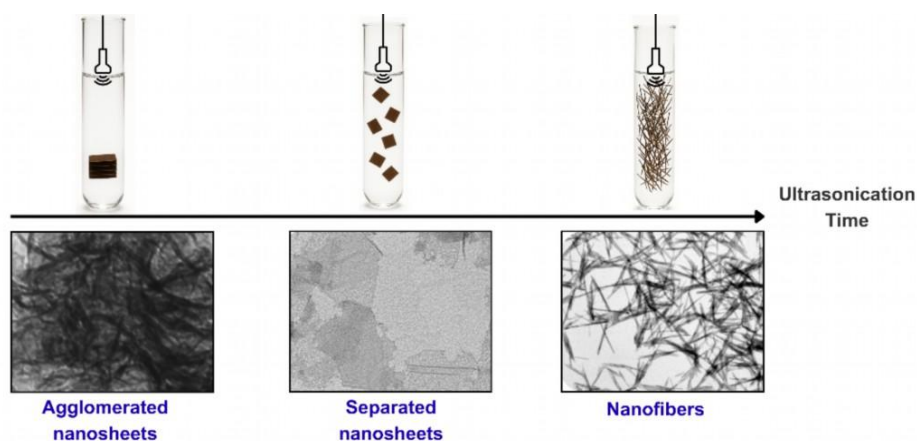


Fig. 1: Time-dependent ultrasonication-induced evolution: agglomerated nanosheets → exfoliated nanosheets → nanofibers

References:

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P11 - BIOSENSORS BASED ON GOLD NANOPARTICLES ENCAPSULED BY GRAPHENE OXIDE SHEETS FOR THE DETECTION OF LIPOPOLYSACCHARIDES

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Keywords: AuNPs ; LSPR ; LPS ; biosensor

Summary: Lipopolysaccharides (LPS) are major structural components of the outer membrane of Gram-negative bacteria. It has long been known that if these molecules access to the blood stream of mammals, violent inflammatory responses may occur. The Limulus Amebocyte Lysate (LAL) test [1] is to date the most widely used method for testing traces of LPS in injectable pharmaceuticals or surgical devices. However, with a population decline of the limulus, new approaches to LPS detection need to be developed. Our attention focused on LSPR-type biosensors out of all alternatives because of their high sensitivity. To go further on the sensibility of this sensor, layers of graphene oxide (GO) were coated on the surface of gold nanoparticles (GNPs). The “Turkevich method” [2], the modified “Jana et al. method” [3], and the “seed in situ method” [4] are used to create spherical GNPs with various charge surfaces and shapes. A modified version of “Hummer’s method” is used to create graphene oxides, which are then exfoliated and chosen to provide tiny sheets [5]. Covalent bonds and electrostatic attraction enable the assembly of GNPs and GO. LPS-binding peptides and anti-LPS aptamers interact with the GO coat via covalent binding. Multiple characterizations are performed for both the assembled GNPs-GO and NPs alone. We have two types of 15 nm spherical GNPs with zeta potentials of -45 mV and 55 mV at pH 6.5. We obtained a sheet thickness of around 1.2 nm for GO, a zeta potential of approximately -45 mV, and an O/C ratio of approximately 0.38. The GO: Au ratio for the completed GRNPs-GO platform is around 15 nm² GO/NP. GO-coated GNPs might be a straightforward and promising way to improve LSPR, and new developments will be realized such as evaluations of the local electromagnetic field intensity of GNPs with and without GO coat.

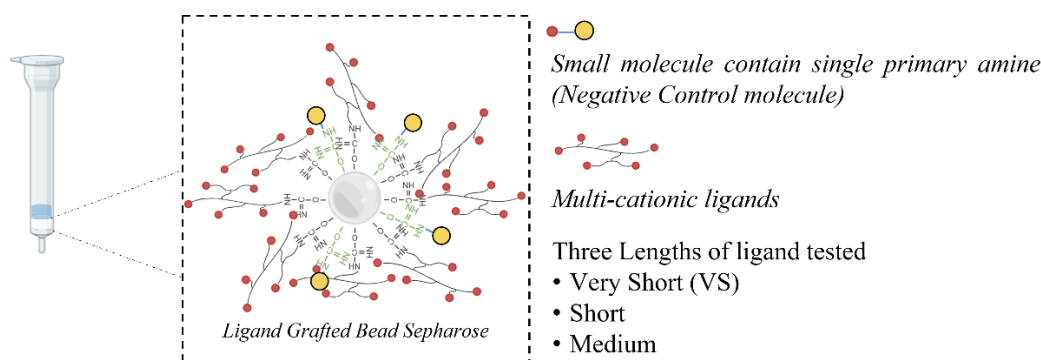


Fig. 1 : Principle of ligand screening using a Sepharose-based affinity column for LPS detection.

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P12 - BIMETALLIC MG/LI COMPLEXES: EFFICIENT TOOLS FOR THE SYNTHESIS OF FUSED (HETERO)ARYL LACTONES

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Keywords: bimetallic, organomagnesiates, metallation, phthalides, azaphthalides.

Summary:

Phthalides and derivatives are widespread in biologically active compounds and natural products. These heterocycles can also serve as versatile building blocks for the synthesis of natural and pharmaceutically-important products. Their preparation is widely documented in the literature even though many of their synthetic routes are non-convergent and relied on intramolecular cyclization, requiring relatively complex syntheses of the starting materials in order to bring diversity to the final phthalides. Moreover, fused heteroaryl-lactones (pyridinyl and benzothienyl-) are poorly exemplified in the literature. [1,2,3,4]

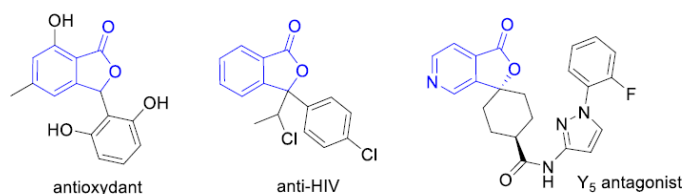


Fig. 1: Example of bioactive phthalides and pyridinic analogs.

In the past few years, our laboratory has been focusing on developing chemistry using bimetallic ate complexes composed of a polar organometallic and a “soft” organometallic in metal halogen exchange (MHE) reaction. Based on that expertise, we decided to start a research program with the aim of exploring the reactivity of organomagnesiates for the synthesis of substituted phthalides, azaphthalides and also fused benzothienyl-lactones. Thereby, we showed that BIPHEN or BINOL-based monobutylmagnesiates ((rac)-BIPHENBuMgLi or (rac)-BINOLBuMgLi) can efficiently promote the MHE of easily available 2-iodobenzoate derivatives, followed by the addition of an aldehyde or a ketone, which leads to an intramolecular cyclisation and the formation of a series of new, diversely substituted phthalide derivatives in moderate to good yields. [2,3,4]

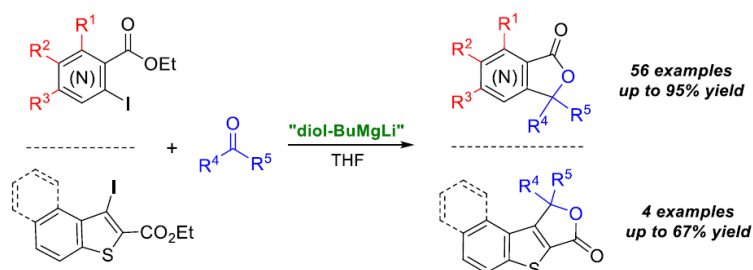


Fig. 2: Synthesis of fused (hetero)aryl lactones.

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P13 - SYNTHESIS OF BIOINSPIRED COMPLEX POLYCYCLIC MOTIFS SUPPORTED BY DFT MECHANISTIC STUDIES

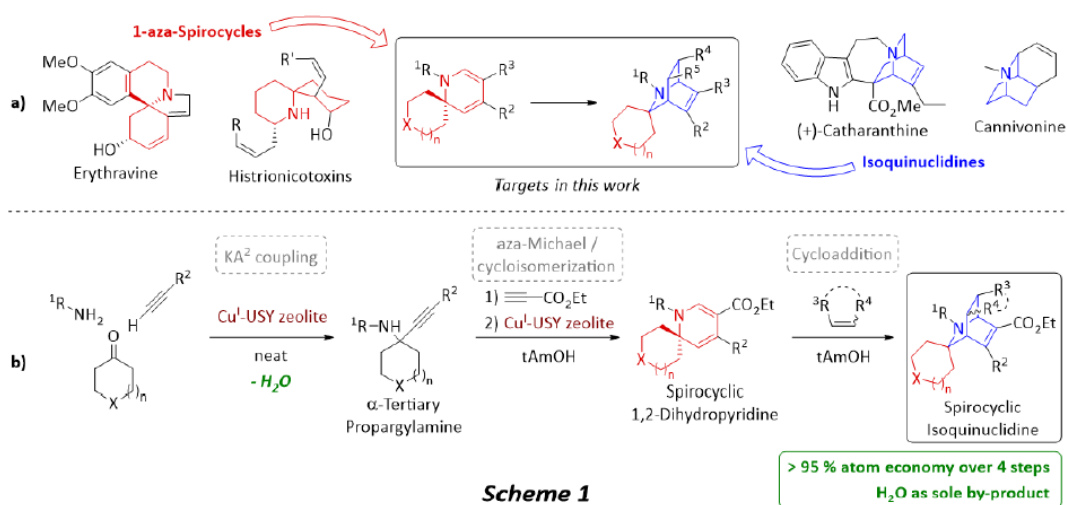
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Keywords: organic synthesis – green chemistry – catalysis – DFT calculations – zeolite chemistry

Summary: Constructing 3D aza-polycyclic architectures remains a big challenge in organic synthesis. In particular, much synthetic efforts have been devoted to **1-azaspirocyclic** and **isoquinuclidine** ring systems, due to their presence in many natural products of biological relevance (**Scheme 1a**).^{1,2} Our goal is to go further in 3D structural complexity by accessing to unprecedented architectures merging these two aza-cyclic systems of high relevance.



Herein, we wish to report our synthetic approach towards this complex aza-spiro/isoquinuclidine hybrid skeleton from simple starting materials (Scheme 1b). Our approach starts with a 3-step sequence, including 2 steps under Cu^I-zeolite catalysis (*i.e.*, KA² coupling and enyne cycloisomerization reactions)^{3,4}, that first furnishes **1-azaspirocyclic** systems featuring a 1,2-dihydropyridine motif. The potential of the resulting 1,2-dihydropyridine motif as diene is finally exploited to construct the additional **isoquinuclidine** ring system *via* a formal cycloaddition process.^{5,6} DFT calculations are conducted in parallel to rationalize the reaction mechanism and energetic pathway of the cycloaddition process. Noteworthy is that this methodology is highly atom and step economical, with water as sole by-product during the whole 4-step sequence.

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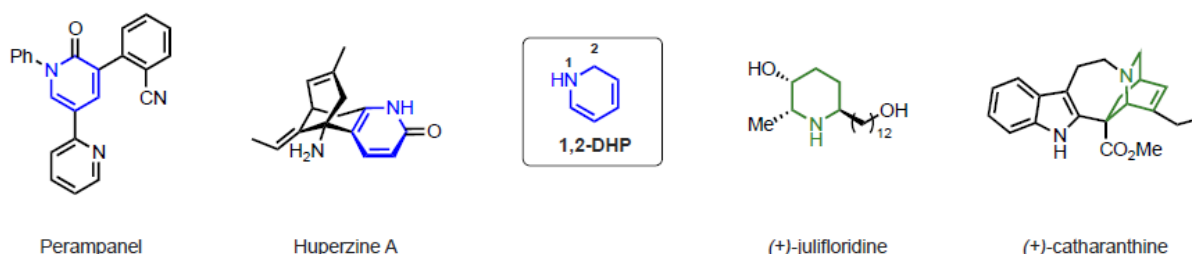
P14 - DEVELOPMENT OF NEW METHODS FOR THE SYNTHESIS OF NITROGEN-CONTAINING HETEROCYCLES CATALYZED BY GOLD(I)-POLYOXOMETALATES COMPLEXES

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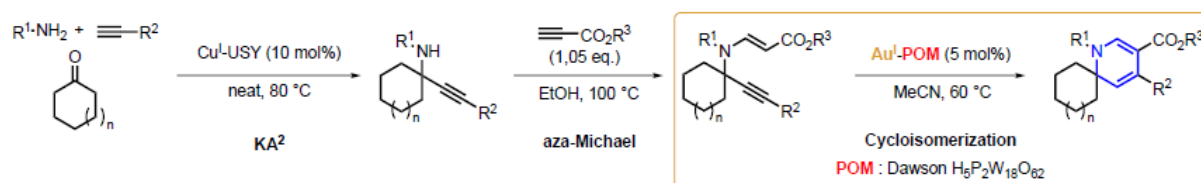
Keywords: organic synthesis – catalysis – green chemistry – polyoxometalate chemistry

Summary: Nitrogen-containing heterocycles have always attracted considerable interest in organic synthesis and medicinal chemistry due to their wide range of biological activities. Currently, approximately 60 % of drugs are based on nitrogen-containing heterocycles, highlighting their importance in the design of new drugs.¹ Among these structures, **1,2-dihydropyridines**, although rare, exhibit interesting biological activities, notably on the nervous system.² These molecules also serve as key intermediates in synthesizing **piperidines** and **isoquinuclidines**, scaffolds found in natural alkaloids.³ (Scheme 1).



Scheme 1

Therefore, accessing the **1,2-dihydropyridine** framework has been the subject of significant research. Among the various approaches reported, the cycloisomerization of aza-1,5-enynes has emerged as an attractive tool due to its excellent atom economy. In our laboratory, we developed a route to highly functionalized **spiro-1,2-dihydropyridines** using heterogeneous copper(I)-doped zeolite catalysis (Cu^I-USY Ultra-Stable Y).⁴ To address the limitations of the zeolite-catalyzed version, this project proposes using gold(I)-based heterogeneous catalysts supported on **polyoxometalates** (POMs).⁵ In addition to being generally inexpensive, easy to prepare, and straightforward to recover/recycle, our supported catalysts have proven highly efficient for various significant organic transformations, allowing access to key molecular "building blocks" for the chemical and pharmaceutical industries under "green" conditions.



Scheme 2

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P15 - SYNTHESIS AND BIOLOGICAL EVALUATION OF NEW INDOLO[2,3-*b*]QUINOLINE DERIVATIVES AND MUSHROOM EXTRACTS AS POTENTIAL ANTIBIOFILM CANDIDATES

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Keywords: Indolo-[2,3-*b*]-quinolines, Radical cascade, Antibiofilm, Bones infection

Summary:

Antibiotic resistance is a major global public health concern. It has been shown that nearly 80% of bacterial infections involve the formation of biofilms. This microbial communities that exhibit a high level of tolerance to antimicrobial agents. In this context, it is essential to develop new therapeutic approaches specifically targeting biofilm-associated infections.

The Therapeutic Chemistry Laboratory (ICMR UMR CNRS 7312) has developed a scaffold of new indoloquinolines, prepared via an innovative radical pathway. These compounds have demonstrated antibiofilm activity against *Pseudomonas aeruginosa*.

In parallel, the BIOS laboratory have developed an in vitro model designed to reproduce the main factors of the bone environment likely to influence biofilm formation and structure during osteoarticular infections (OAI), particularly those associated with prosthetic devices.

This poster present the preliminary studies for the screening of various antibiofilm strategies on *Staphylococcus aureus* strains, notably through the evaluation of natural extracts.

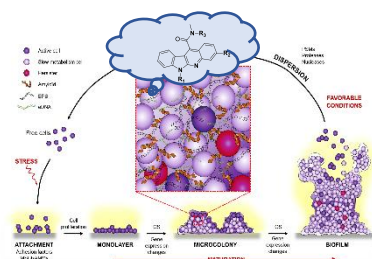


Fig. 1 : Indoloquinoline's antibiofilm strategies

References:

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P16 - A UNIFIED STRATEGY TOWARDS BIS-INDOLE ALKALOIDS: TOTAL SYNTHESIS OF (±)-STREMPELIOPIDINE

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Keywords: Total synthesis, unified synthesis, hydroformylation, bis-indole alkaloid

Summary: Bis-indole alkaloids of the Apocynacea family featuring both aspidosperma and eburnane core units are showing promising activities against certain types of cancer.^[1] However, only a few syntheses of such compounds are yet reported.^[2] In the context of accessing new scaffolds and new molecular diversity, our laboratory has been successfully using homogeneous catalysis. Through the hydroformylation reaction, we are currently focusing on synthesizing highly functionalized structures such as indole alkaloids from easily synthesizable or commercially available olefins.^[3] The objectives of this project are 1) to develop a synthesis of a common intermediate via the hydroformylation reaction and 2) perform a quick and efficient unified synthesis of original bis-indole alkaloids and their analogs.

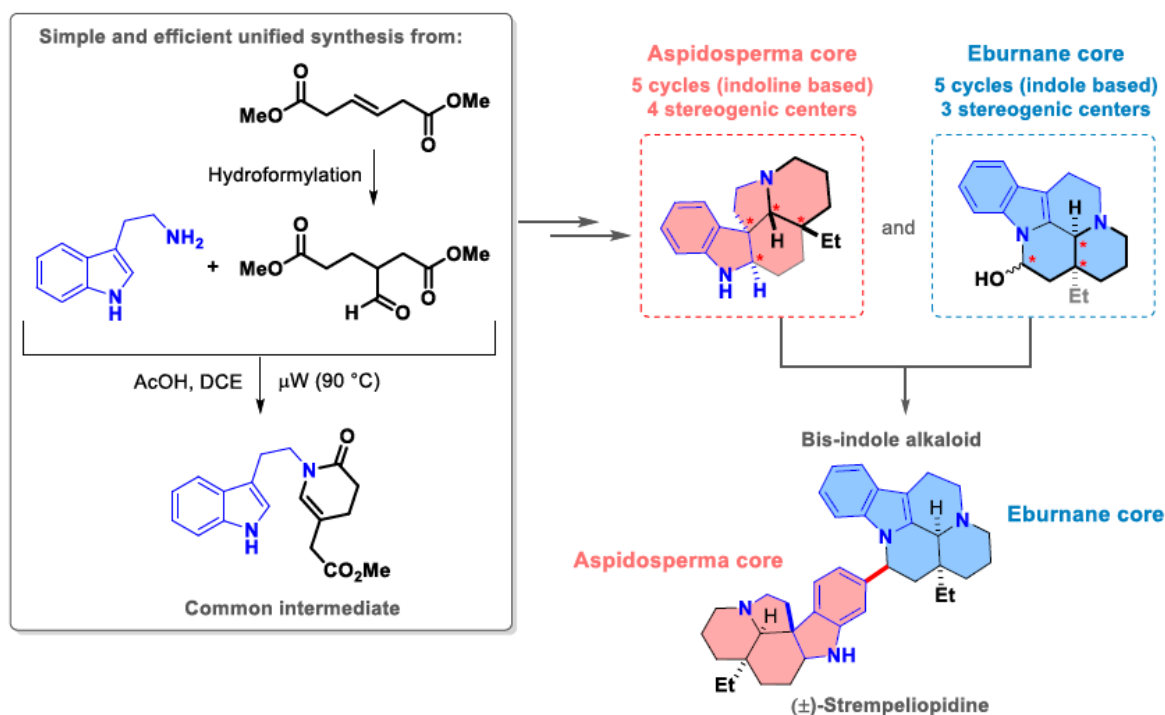


Fig. 1: Synthesis of aspidosperma and eburnane cores via a common intermediate towards the bis-indole alkaloid strempelepidine

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P17 - DEVELOPMENT AND CHARACTERIZATION OF DIHYDROXAMIC LIGANDS FOR THE CHELATION OF URANIUM(VI)

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Keywords: hydroxamate, uranyl complex, enantiomers, chirality transfer, speciation

Summary: Highly radiotoxic actinides, such as uranium, have been used in a wide range of civilian industrial and military applications since the end of World War II. In addition, significant amounts of thorium and uranium occur naturally in the environment or have been released through human activities, including the processing and disposal of nuclear fuel-cycle wastes, nuclear weapons tests, nuclear power plant accidents, and the deterioration of storage facilities for nuclear materials.¹ Beyond their role of uranium and plutonium in nuclear energy production, the potential use of nuclear weapons and radiological dispersal devices ("dirty bombs") further increase the risk of environmental contamination and internal human exposure. Once internalized, these elements can trigger both radiological and chemical damages.

To prevent them, decorporation therapy based on chemical chelation is currently the only effective countermeasure for reducing the radiation dose to tissues or organs after accidental intake of radionuclides. This treatment involves the administration of high-affinity chelating agents able to displace contaminating metals from biological ligands or deposition sites within the body (e.g., liver, kidneys, or bones). These agents work by forming rapid, stable, and water-soluble complexes with the metals, thereby enhancing their removal from the bloodstream and organs and promoting their quick excretion in urine or feces. Currently, Pentetate® (DTPA salts) is the only drug approved worldwide by regulatory agencies for treating actinide intoxications but its therapeutic performance with plutonium, americium, and curium is modest.² Moreover, DTPA is ineffective and not recommended for uranium³ and neptunium.⁴

Therefore, there is an urgent need for devising effective *in vivo* decorporating agents of uranium(VI). We relied on a biomimetic approach for designing efficient pincer-like UO_2^{2+} chelators, like $(\text{L}^{\text{Cy,Pr}})^{2-}$, bearing two terminal hydroxamate bidentate groups able to coordinate the uranyl cation in its equatorial plane.⁵ In addition to speciation studies in aqueous media, the structural characterization of the couple of (*R,R*)- and (*S,S*)- $(\text{L}^{\text{Cy,Pr}})_2\text{H}_2$ enantiomers and their uranyl complexes were performed by NMR, ATR-FTIR, UV spectrophotometry, and electronic circular dichroism spectroscopies. The latter method highlights a chirality transfer from the ligand to the metal. Decorporation and toxicity tests are ongoing.

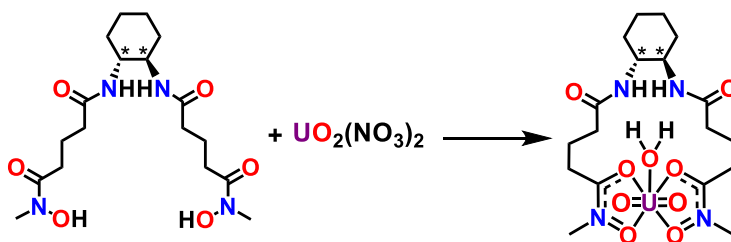


Fig. 1: Uranyl complexation reaction of our $\text{L}^{\text{Cy,Pr}}\text{H}_2$ ligand

The French Ministry of Research and Higher Education is acknowledged for funding the PhD grant of D.C. This study is supported by ANR (ActiDecorp project, grant n° ANR-23-CE18-0046).

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P18 - TRIGGERED PHOTOTHERMO-TRANSLOCATION IN ION AND WATER CHANNELS BY TWO-PHOTON ACTIVATED MOLECULAR TRANSDUCER

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Keywords: artificial channels, ion and water transport, push-pull dyes, photothermal effect, two-photo absorption

Summary:

Aqueous or ionic channels are transmembrane proteins essential for the proper functioning of cells. They ensure highly selective transport of various molecules, such as water, ions (e.g. Na⁺, K⁺, Cl⁻), and certain small solutes across cell membranes. Among these proteins some channels are known to be sensitive to stimuli, such as the thermosensitive ion channels TREK and TRPV proteins found in neurons. Acquired knowledge of the structure and function of these natural proteins paved the way for the design of artificial channels that mimic the properties of their biological counterparts. These synthetic channels hold significant potential in various scientific and technological fields, ranging from water desalination to biomedical applications. From them, light-gated artificial channel incorporating a photosensitive moiety are of great interest.

This project aims to develop photothermally activatable artificial water channels by integrating photothermal transducers directly within the channel architecture. To this end, we designed molecular building blocks that combine a chromophore unit for photothermal transduction, urea motifs to promote self-assembly into supramolecular channels, and transport units enabling selectively transport of water or ions. As the chromophore unit, we selected push-pull distilbene derivatives, that benefit from light-to-heat conversion capability and strong two-photon absorption properties, allowing two photon activations of the channel in the future work. Some of these molecular building blocks have been successfully synthesized, and their self-assembly and transport properties have been preliminary evaluated using membrane model systems (giant unilamellar vesicles, GUVs) and stop-flow and HPTS assay, respectively.

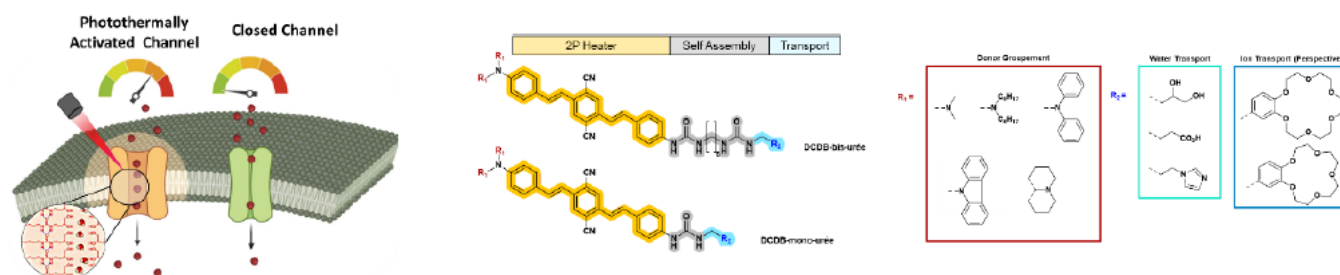


Fig. 1 : A) Mechanism of light-induced activation of artificial channels when irradiated with light, B) Targeted compound with the dicyanodistyrylbenzene chromophore with the different water transport and ion transport pattern

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P19 - NOVEL NANOHYBRIDS COATED WITH (CELL-PENETRATING) PEPTIDES TO CROSS THE HUMAN BLOOD-BRAIN BARRIER

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Given the increase in life expectancy, neurodegenerative diseases have become more prevalent, and their highly debilitating symptoms urge for new treatments.[1] Oxidative stress, mainly due to mitochondrial metabolism failure, plays a key role in neurodegenerative diseases physiopathological processes, notably in Alzheimer's disease representing 60-70% of dementia.[2]

We elaborated hybrid nanoparticles (HyNPs) aimed at crossing the human blood-brain barrier (BBB), targeting neuronal mitochondria and having an antioxidant activity. Our HyNP is made of superparamagnetic iron oxide nanoparticles (SPIONs) functionalized with cell-penetrating peptide (CPP) or with peptide targeting the transferrin receptor, that can cross the BBB, target mitochondria and reduce the oxidative stress owing to intrinsic antioxidant properties. HyNPs, peptide and CPPs were labeled with fluorescent probes to track them *in vitro* (see Fig).

In this presentation, we will focus on the new nanohybrid and particularly on i) each step of its synthesis with different characterizations to prove the effectiveness of each coupling, ii) the first biological and BBB crossing tests and iii) the prospects in targeting mitochondria and reducing oxidative stress in model systems.

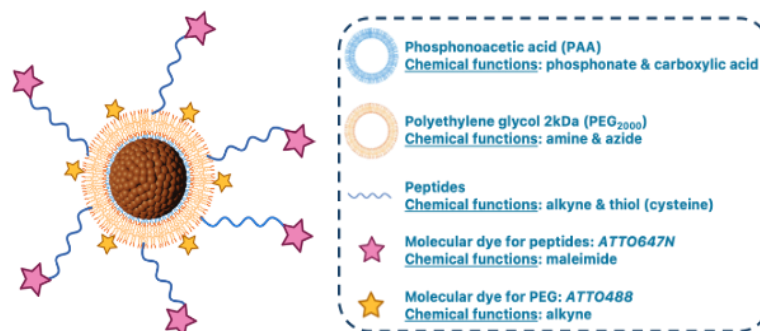


Fig: Scheme of the nanohybrid made of SPIONs pre-functionalized with a biocompatible polyethylene glycol (PEG) and functionalized with CPPs labelled with fluorophores.

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