Book of abstracts

March – June 2025

Réseau des Jeunes Chimistes
Société Chimique de France

Société Chimique de France
Section Bretagne-Pays de Loire

The program

March 19th	
12:00	**Dr. Benjamin Doistau** : "*Luminescence and chiroptic switches upon chromophore encapsulation*"
12:35	**Dr. Ana Velasco** : "*Green Chemistry Strategies for Flavonol Extraction from Onion: Exploring Natural Deep Eutectic*"
April 24th	
12:00	**Yoann Fréroux** : "*New antennae for photoswitchable luminescent lanthanide (III) complexes*"
12:20	**Prof. Thomas Just Sørensen** :" Beyond point charges, how Crystal Field Theory describes Nd(III) ions
May 21st	
12:00	**Prof. Jonathan Nitschke :** "*Molecules in metal boxes*"
12:35	**Thomas Defuentes :** "*Total Synthesis of Chaxalactins*"
June 18th	
12:00	**Dr Inderpal Yadav : "***Green & Sustainable Wacker-Type Oxidations Avoiding Palladium Catalysts* "
12 :25	**Colleen Mudau :**
12 :45	**Louis Hardoin :** *"Supramolecular assembly of electro- and photoactive π-functional foldamers"*

Luminescence and chiroptic switches upon chromophore encapsulation

Dr. Benjamin Doistau

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Implementing chirality in emissive complexes or organic molecules triggers circularly polarised luminescence (CPL) which received increasing interest due to its panel of prospective applications in CP-OLED technologies or bio-imaging. Switching, tuning and enhancing CPL properties is therefore an important challenge worth to overcome. Providing a supramolecular chiral environment around a chromophore offers an innovative bio-inspired approach to triggers CPL switch or ultimately raise CPL from achiral emitters or racemic mixtures. Encapsulation of emissive coordination complexes or organic dye in hexameric self-assembled resorcin[4]arene capsule will be presented as well as the outcoming luminescence et chiroptic properties switches.

Green Chemistry Strategies for Flavonol Extraction from Onion: Exploring Natural Deep Eutectic

Dr. Ana V. González-de-Peredo, Alicia Maroto, and Antony Memboeuf

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The study of bioactive compounds in vegetables and fruits has gained increasing significance in diverse fields such as nutrition, pharmaceuticals, and cosmetics, primarily due to the health-promoting properties these compounds exhibit. Among these compounds, flavonols stand out due to their antioxidant, anti-inflammatory, and anti-cancer properties, contributing to the growing interest in understanding their potential. Traditionally, extraction methods have relied on organic solvents like methanol or acetonitrile, which, although effective, pose significant environmental risks. In response to these challenges, natural deep eutectic solvents (NaDES) have emerged as a promising, more sustainable alternative that aligns with the principles of green chemistry. NaDES are biodegradable, non-toxic, and eco-friendly, making them a viable option for improving the sustainability of extraction processes. This study explores the use of choline chloride (ChCl)-based NaDES for the extraction of flavonols from onions, a widely consumed vegetable known for its numerous health benefits. Flavonols are key bioactive compounds in onions, contributing to their antioxidant properties and offering many health benefits. Given the growing recognition of the health benefits of flavonols, developing efficient and sustainable methods for their extraction has become essential. In this context, NaDES present a viable alternative not only due to their environmentally friendly nature but also because of their ability to effectively extract bioactive compounds. Moreover, the integration of ultrasound-assisted extraction, a cutting-edge green technology, has been shown to further enhance the efficiency of the extraction process, offering a combination of high yield and reduced extraction time. In this study, several NaDES formulations, including combinations of levulinic acid, tartaric acid, 1,3-propanediol, and urea, were tested in different molar ratios (1:1, 1:2, 1:3, 1:4, 2:1, and 2:3). Among these, the 1:2 choline chloride:levulinic acid was found to provide the highest ultrasound extraction efficiency for the five major flavonols in onions, as analyzed by liquid chromatography-mass spectrometry. To further evaluate the performance of NaDES, two Box-Behnken designs were employed—one for the methanol-based extraction and the other for the ChCl:levulinic acid mixture. The results showed that this NaDES not only yielded comparable or greater amounts of flavonols compared to methanol but also significantly reduced the extraction time (25 minutes for methanol vs. 12 minutes for NaDES). Under optimal conditions, the ultrasound-assisted extraction method exhibited excellent reproducibility (RSDs lower than 10%) and recovery (total amount of flavonols was $4.834 \pm 4.862 \times 10^{-2}$ mg g). These findings highlight the potential of NaDES as an efficient and environmentally friendly alternative for the extraction of bioactive compounds, marking a significant advancement in the development of sustainable extraction techniques.

Beyond point charges, how Crystal Field Theory describes Nd(III) ions

Prof. Thomas Just Sørensen

Department of Chemistry, University of Copenhagen.

For getting on 15 years we have been producing increasingly better experimental data on the electronic structure for lanthanide(III) ion. Although we are heavily centred on the experimental side, we have, with collaborators, dabbled in computational descriptions of the electronic structure of various lanthanide(III) complexes.

It is well-established that the orientation of the donor atoms around a lanthanide(III) center is important. Here, I will use the example of the Nd(III) ion (Figure 1) to show just how important the orientation of the donor atom orbitals are in determining the electronic structure of lanthanide(III) ions (Figure 2). We are not able to make the theoretical descriptions better, but we can provide as much benchmarking data as any theoretician can dream off, so please consider this a call to action. We are able to show where we need to improve the theory, and I will do so here.

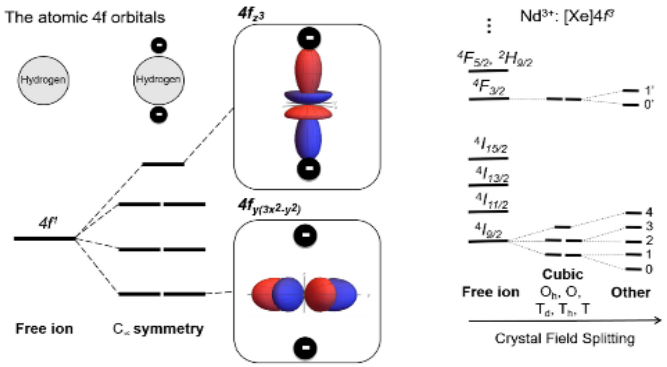

Figure 1. Left: Coordination polyhedron with lowest electrostatic repulsion for CN = 8, 9, and 10. Right: Generic electronic structure of neodymium(III) with the splitting of the ground state and emitting state in different symmetries.

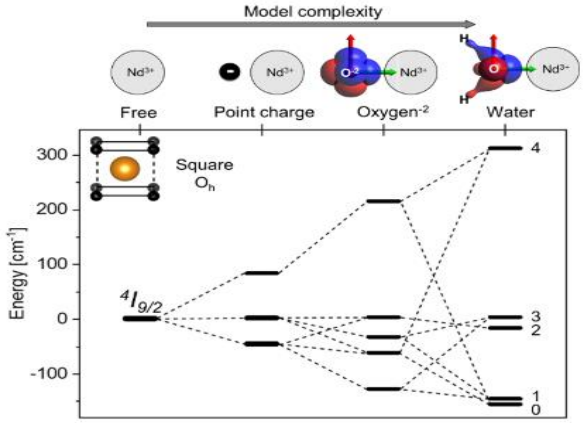

Figure 2. The electronic configuration of the $^4I_{9/2}$ of neodymium(III) calculated in four different ligand models of increasing complexity: free ion, point charges, oxygen ions, and water molecules, at the vertexes of the square polyhedron with neodymium(III) in the centre. The energy levels have been normalized to the barycentre of the multiplet.

New antennae for photoswitchable luminescent lanthanide (III) complexes

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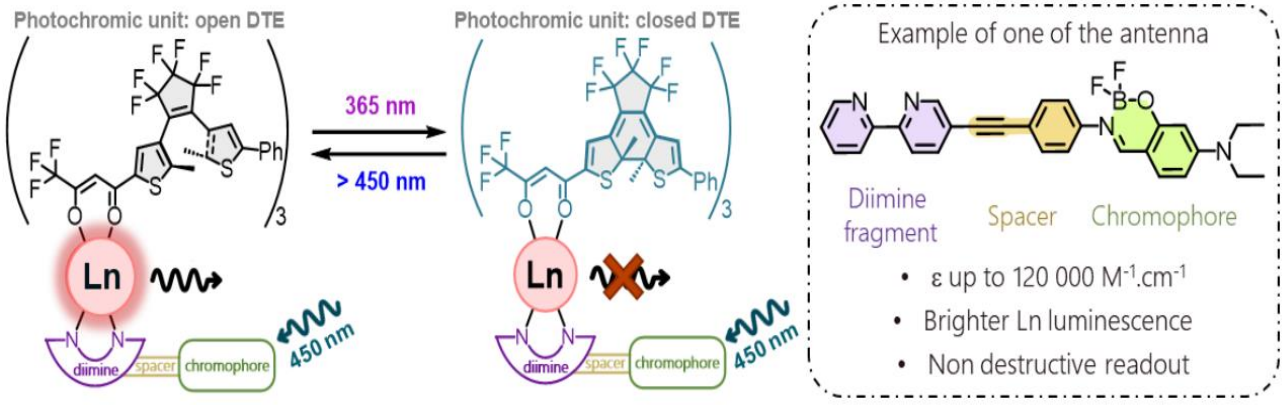
Counterfeiting is a global problem that challenges businesses, governments, and consumers. To develop novel anti-counterfeiting systems, lanthanide-based complexes are widely used due to their original emission features such as long lived and narrow bandwidth luminescence from the visible up to the near infrared spectral range.[1a-b] To obtain innovative signatures, the challenge is now to add new features to these complex luminescences. A goal of our research is to design lanthanide complexes which NIR luminescence can be turned on or off at will, with the use of an external photostimulation.[2] Light control is achieved with a dithienylethene (DTE) moiety, capable to quench the luminescence of the complex by energy transfer in only one of its two states,[3] even in the NIR range. Here, we present the synthesis of new boranil-based lanthanide complexes with a significant brightness, a high on/off intensity ratio and with an excitation wavelength located in the visible range in order to meet standards required for applications. In particular, the photophysical results shine light on these boranyl chromophore abilities to sensitize lanthanide ion displaying NIR emission (Ln = Yb, Er) and to provide a non-destructive readout.



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Molecules in metal boxes

Prof. Jonathan R. Nitschke

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Simple organic subcomponents can come together around metal-ion templates to produce intricate hollow capsules,[1] which can bind guest molecules selectively. This talk will describe the design and uses of some of these three-dimensional architectures, a few of which are shown in Figure 1 below, along with the use of the same construction principles to produce interlocked structures – catenanes[2] and knots[3] – and double-helical metallopolymers with potentially useful optoelectronic properties.[4]

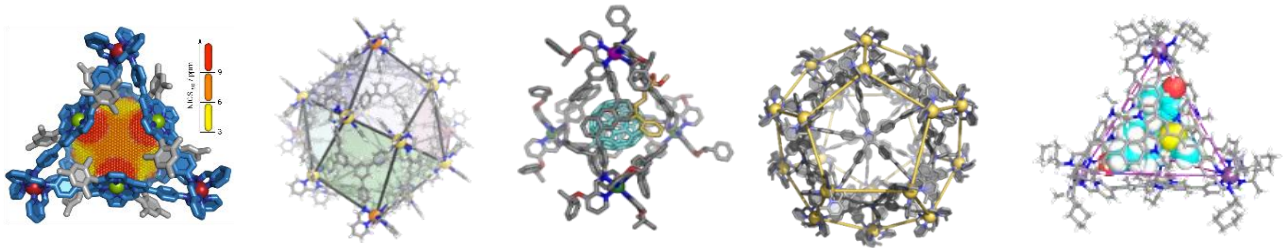

Figure 1. From left to right: an antiaromatic-walled cage;[5] a capsule isomorphous to a bacterioferritin;[6] a capsule capable of stereoselectively functionalizing fullerenes,[7] a dodecahedral capsule with enough interior volume to house a small protein,[8] and a capsule that discriminates between and selectively binds steroids.[9]

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Total Synthesis of Chaxalactins

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Chaxalactins A, B and C are 22-membered macrolactones isolated in 2011 from a strain called Streptomyces sp. C34, collected in hyper-arid Atacama Desert (Chili).[1] The complex structure of these molecules coupled with their interesting antibiotic and potential antitumoral activities make this family of molecules synthetically challenging important targets. Despite of their interest, no total synthesis of these compounds has been reported so far. The aim of our project is to synthesise for the first time chaxalactins A, B and C and their analogues. For now, we have been focusing our research on the synthesis of chaxalactins A and B, which differ by the position C14.

Chaxalactins could be obtained by a Suzuki coupling between the C1-C9 and C10-25 fragments, followed by a macrolactonization reaction. The C10-C25 fragment could be prepared from the C13-C25 fragment using a Marshall allenylation key step to introduce and control the C12 and C13 stereocenters. The C13-C25 fragment could in turn be obtained by a Stille coupling between the C13-C17 and C18-25 fragments. Retrosynthetic analysis of Chaxalactins A and B.

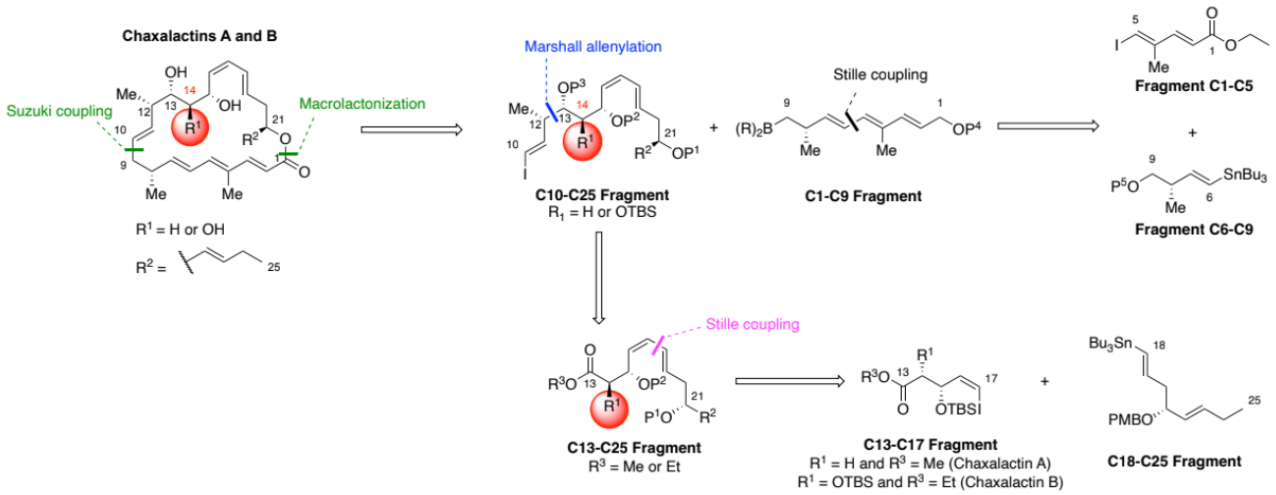

Figure 1. Retrosynthetic analysis of chaxalactins A and B.

In this communication, the synthesis of the chaxalactin B and the progress towards the synthesis of the chaxalactin A will be presented.

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