

# JOURNÉES DE L'ÉCOLE DOCTORALE 3M

## LE MANS 2021 ÉDITION VIRTUELLE



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# Santé

# Adsorption capacity of the corrosion products of nanoscale zerovalent iron for emerging contaminants

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Despite the extensive use of nanoscale zerovalent iron (NZVI) in water and soil remediation, no data exist on the reactivity of secondary iron minerals formed upon the NZVI corrosion. Herein, we investigated the oxidation kinetics of NZVI by monitoring the variations of pH, oxidation–reduction potential (ORP) and dissolved Fe(II) concentration, and then examined the reactivity of resulting oxidized particles for the adsorption of an emerging contaminant (nalidixic acid (NA)). NA adsorption was found the greatest on oxidized particles and negligible on the fresh NZVI. Interestingly, the formed secondary mineral phases exhibited an unusual pH adsorption curve with an unexpected great adsorption at alkaline pH values. X-ray photoelectron spectroscopy and high resolution-transmission electron microscopy revealed a gradual increase in the Fe(II) content at the surface of the magnetite phase over the reaction time. Additional experiments and surface complexation modeling showed that the enhanced adsorption of NA onto the secondary magnetite is due to the formation of surface bound Fe(II). Fe(II) is released into the solution because, for instance, of the presence of organic buffer molecules, decreased surface Fe(II) and NA adsorption at alkaline pH values. This work sheds light on an overseen aspect of the reactivity of secondary iron minerals resulting from NZVI passivation, which can bind co-existing emerging contaminants and then affect their fate in the environment.

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\*Intervenant



**Mots-Clés:** nanoscale zero valent iron, adsorption, contaminants, nalidixic acid

# CHEMICALLY MODIFIED ADENO-ASSOCIATED VIRUS FOR SELECTIVE GENE DELIVERY

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Adeno-associated virus (AAV) are highly efficient vectors for the transfer of therapeutic genes into different target human cells. It has been shown to be effective for the treatment of genetic diseases and more than one hundred clinical trials using AAV are in progress. Those clinical trials led to the commercialization of three drugs, Glybera, Luxturna and Zolgensma. However, despite these available treatments, the use of AAV as therapeutic vectors remains a real challenge. Indeed, a number of biological factors interfere with the delivery of the therapeutic gene. These two major parameters are: tropism of the vector which is not specific enough to a cell type, inducing a large bio-distribution in the organism; and recognition of AAV by neutralizing antibodies, leading to a decrease of the efficiency of the treatment. To solve these biological limitations several genetic engineering techniques are under study. In our case, to increase the therapeutic index of these particles, we have chosen to chemically modify the AAV *via* the coupling of ligands on its capsid. These ligands consist of a coupling function, allowing their bio-conjugation by chemical reaction on the capsid of the vector, and a recognition pattern for a specific receptor of a defined cell type. The functionalization of the virus *via* this type of ligand should allow a better tropism for the defined cell type, but should also decrease the recognition by the neutralizing antibodies. A first study showed the possible functionalization of the capsid of an AAV *via* ligands possessing a recognition pattern for the asialoglycoprotein receptor (ASGPR) on the surface of hepatocyte cells. These new vectors showed improved transduction for this cell type *in vitro* and better biological effects *in vivo*. The purpose of my thesis is to generate a new set of ligands with more affine recognition patterns for the ASGPR.

**Mots-Clés:** Bio, conjugaison, AAV, thérapie génique, interactions ligand, récepteur

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\*Intervenant

# Coupled effects of Mn(II), pH and anionic ligands on the reactivity of nanostructured birnessite

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While the oxidative capacity of nanostructured birnessite-type manganese oxide has been widely investigated, no comprehensive work exists on the combined effects of dissolved Mn(II), pH and inorganic anions on sorption and redox reactions of organic contaminants with MnO<sub>2</sub>. Herein, we have showed how molecular interactions with MnO<sub>2</sub> surfaces controlled on the removal kinetic behavior, which depended on contaminant type and co-existing anions. Competition between contaminant and Mn(II) for binding at the edge sites determined the initial kinetic step, while buildup of Mn(II) at both edge and vacancy sites continuously decreased adsorption and subsequent oxidation over time. Redox interactions of Mn(II) to MnO<sub>2</sub> surfaces was a pH dependent process, and high pH favored Mn(II) removal and comproportionation reaction, thus decreasing adsorption and oxidation processes. ATR-FTIR and XRD data showed that only high Mn(II)/MnO<sub>2</sub> ratio (2.3) and high pH ( $\geq 8$ ) enabled surface-catalyzed oxidation of Mn(II) by molecular oxygen and then formation of manganite ( $\gamma$ -MnIII(OH)). However at lower Mn(II)/MnO<sub>2</sub> ratio, MnO<sub>2</sub>, positively charged from the adsorption of Mn(II) ions, adsorbed more effectively anions such as phosphate or silicate and thus reducing interactions with organic compounds. These results highlight the combined suppressive effects of Mn(II), pH and naturally occurring anions on the reactivity of nanostructured birnessite, and have strong implications on the fate of organic contaminants in terrestrial and aquatic environments.

**Mots-Clés:** manganese oxides, contaminants, adsorption, oxidation

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\*Intervenant

# De l'effet Ouzo à la Chimiothérapie

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L'effet Ouzo est un phénomène d'émulsification spontanée permettant la formation de nanogouttelettes métastables, sans l'utilisation de tensioactif et sans agitation mécanique. Ce phénomène se produit lors du mélange ternaire d'une huile hydrophobe, d'un alcool miscible à l'eau et d'eau. Ainsi, l'huile sursaturée s'agrège en petites gouttelettes suspendues dans la phase continue. Ce phénomène a été utilisé principalement pour la formation de nanoparticules, de nanocapsules, et l'encapsulation de médicaments. Dans notre cas, nous avons élaboré un procédé simple et efficace d'encapsulation de principe actif hydrophobe basé sur l'effet Ouzo. Des nanocapsules hybrides, appelées Hybridosomes<sup>®</sup>, sont obtenues par émulsification spontanée dans un mélange THF/eau/hydroxytoluène butylé (BHT). Elles sont constituées d'une enveloppe de nanoparticules inorganiques NP (Oxyde de Fer, Au, QD, etc.) stabilisée par un polymère (PAA, PEG-PAA, etc.). Ces nanocapsules possèdent un volume interne permettant de charger à l'intérieur des nanocapsules jusqu'à 170 g.L<sup>-1</sup> ( $\sim$  0,35 M) de molécule hydrophobe. Leur taille moyenne est typiquement de 100 nm de diamètre. Nous avons cherché à nanoencapsuler des molécules chimiothérapeutiques telles que Sorafénib et Paclitaxel. Il existe un véritable enjeu en innovation thérapeutique à pouvoir développer des objets permettant d'appliquer simultanément chimio- et radio-thérapies.

**Mots-Clés:** Ouzo, nanoparticules, nanoprecipitation, nanoencapsulation, chimiothérapie

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\*Intervenant

# Double addition of propargylzinc reagents to acylcyanohydrins and cyanocarbonates

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Amines bearing a tertiary carbon (tertiary carbinamines) are present in various natural products and synthetic bioactive compounds such as alkaloids for instance. Usual accesses to these compounds are the Ritter reaction, the use of nitro compounds or the addition to imine derivatives, but these methods require several steps to afford the tertiary carbinamines. In this context, the double addition of organometallics to nitriles represents an attractive and convergent alternative. Indeed, this reaction is generally limited to a single nucleophilic addition which affords ketones after acidic hydrolysis. Our team already developed a methodology to master the double addition of Grignard or organozinc reagents onto acylcyanohydrins to obtain tertiary carbinamines. The topic of this communication deals with the development of an efficient and mild synthetic methodology of double addition of propargylzinc reagents onto acylcyanohydrins and cyanocarbonates. This synthetic tool will allow the straightforward preparation of functionalized  $\alpha,\alpha$ -disubstituted hydroxyamides and *N*-Boc-protected amino alcohols. The valorization of the so-obtained compounds will be highlighted by cobalt-catalyzed [2+2+2] cycloaddition reactions to provide functionalized pyridine derivatives.

**Mots-Clés:** amine, double addition, organometallic

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\*Intervenant

# Développement de radiopharmaceutiques à base de cyclam pour l'imagerie TEP au cuivre-64 et la thérapie des cancers

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Les radiométaux suscitent un fort intérêt dans le domaine de la médecine nucléaire notamment pour des applications en imagerie TEP (Tomographe par Emission de Positrons) de nombreuses pathologies. Le cuivre-64, qui est un émetteur  $\beta^+$ , est largement étudié grâce à son temps de demi-vie ( $t_{1/2}=12.7\text{h}$ ) suffisamment long pour être adapté à des applications biologiques. Les tétraazamacrocycles *N*-fonctionnalisés, tels que les dérivés du cyclam, sont des agents chélateurs très efficaces pour la complexation du Cu(II). Notre groupe a développé un cyclam monopicolinate, le TE1PA, qui est l'un des meilleurs chélateurs actuellement disponibles pour le Cu(II) formant un complexe très stable et inerte évitant les risques de dissociation ou de réduction en milieu biologique.

En collaboration avec l'entreprise sud-africaine NECSA (Nuclear Energy Corporation of South Africa) situé à Pretoria et spécialisée dans la production de radioisotopes, nous avons synthétisé des agents chélateurs trifonctionnels à base de cyclam pour l'imagerie TEP au cuivre-64. Les radioligands conçus, appelés **GluCAB** (**G**lucose-**C**helator **A**lbumin **B**ioconjugate), sont composés de trois parties ayant des rôles distincts : *i*) un dérivé du cyclam pour la coordination du cuivre, *ii*) un groupe maléimide capable de se lier *in vivo* à l'albumine pour un ciblage passif des tumeurs *via* l'effet EPR (Enhanced Permeability and Retention) et *iii*) une unité glucose pour un ciblage actif permettant d'affiner la sélectivité pour une meilleure accumulation du radiopharmaceutique au niveau de la tumeur.

**Mots-Clés:** cyclam, TE1PA, Imagerie TEP, albumine

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\*Intervenant

# Exploring Structural Perturbation of UnaG Fluorescent Protein Dynamics upon Mutations

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UnaG is a new class of fluorescence protein that belongs to the class of fatty-acid-binding protein. A highly specific and endogenous ligand namely bilirubin (BLR) is playing the role of chromophore. BLR is an end-product of the heme metabolism and is therefore a natural marker for liver function in hospital pathological laboratories and a key indicator for the prevalent childhood diseases of jaundice. Upon photoexcitation, holo-UnaG emits green light. It has been shown that a single mutation, substituting asparagine residue (N57) to alanine (N57A) or glutamine (N57Q) induces a decrease in the fluorescence quantum yield. However, mechanisms underpinning such behaviors remain elusive and were up to now related to BLR structural changes mainly due to the loss of direct hydrogen bonds to the endo-vinyl dipyrinone moiety inducing higher flexibility in the BLR increasing the rate of the non-radiative process. Long molecular dynamics (MD) simulations were carried out for the WT UnaG and both mutants (N57A and N57Q) to deeper investigate the structural impact onto the global structure. We show for the first time that such ligand structural modifications upon mutations are tightly related to the key structural changes in UnaG protein. Our results show that BLR in WT UnaG is rather rigid while when embedded into N57A or N57Q, dihedral angles between endo and Exo vinyl moieties and, particularly between A and B rings at the entrance of UnaG are strongly modified as well as the number of inter / intramolecular interactions and water molecules behaviors in the binding cavity. The present work suggests that, to understand the fluorescence properties of UnaG protein and its mutants, not only the interaction network between BLR and its neighboring residues should be investigated but also the global structure. 1.Kumagai, A. ; et al , Cell. 2013, 153 (7), 1602-11.

**Mots-Clés:** Molecular dynamics simulation, UnaG Protein, Bilirubin, fluorescence, interactions.

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# Photo-cross-linkable porous hydrogels for cell encapsulation

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Hydrogels are polymer networks that contain high amounts of water. Photo-cross-linkable hydrogel scaffold biomaterials attract attention because of their injectable ability before crosslinking and their suitable mechanical properties after irradiation. Here, I will present a biomimetic scaffold by mixing two incompatible polymers solutions, leading to a water-in-water (W/W) emulsion. A biocompatible PEG-based copolymer (tPEO) utilized as the continuous protection phase, and a biopolymer solution (dextran ou gelatin) is used as the dispersed phase in which cells are encapsulated. The microstructure of the emulsions was visualized using confocal laser scanning microscopy, and different morphologies can be obtained by varying the dispersed volume fraction. Preliminary results showed that the biphasic hydrogel could encapsulate plant cells (microalgae) and have high biocompatibility as well as good viability. They can also potentially encapsulate animal cells (liver stem cells, fibroblasts, etc.), making the gel a good candidate for tissue engineering.

**Mots-Clés:** hydrogel, dextran/gelatin, cell encapsulation

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\*Intervenant



# Suivi du remodelage d'implants osseux par tomographie à comptage de photons

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Les ciments phosphocalciques (CPCs) injectables sont des substituts osseux actuellement très utilisés en clinique pour combler des pertes osseuses, sachant qu'au bout de quelques mois ils sont graduellement remplacés de l'os naturel. Cependant aux rayons X, la majorité de ces produits ont des contrastes similaires à ceux de l'os naturel ce qui rend très difficile la visualisation de l'évolution de la zone implantée par scanner. L'utilisation conjointe d'un scanner spectral à comptage de photons (SPCCT) et l'incorporation de nanoparticules (NPs) de tri-fluorure de lanthanide (LnF<sub>3</sub>) dans un CPC en tant qu'agent de contraste, permettent de distinguer clairement le biomatériau de l'os environnant. L'objectif de ce travail est de préparer des formulations stables de CPC injectables incorporant comme agent de contraste SPCCT des nanoparticules de type LnF<sub>3</sub>, dans le but de suivre l'évolution du biomatériau implanté lorsqu'il est progressivement remplacé par de l'os. Des essais *in vitro* démontrent que lors de l'inclusion de ces NPs au sein d'une matrice cimentaire, celles-ci ne sont pas relarguées lors du processus de prise du CPC en solution saline. La visualisation par SPCCT d'un CPC incorporant des NPs est optimale à partir d'une concentration minimale de 3 mg de Ln/mL de CPC. L'implantation *in vivo* dans un défaut osseux critique induit chez 4 lapins (Néo-zélandais) et le suivi en imagerie SPCCT à 1, 3 puis 8 semaines, ont permis de mettre en évidence la visualisation spécifique de la zone implantée. Nous avons également montré que le revêtement de surface permettant de stabiliser les NPs de fluorure de terre rare et éviter leur agrégation est lessivé par le liquide durcisseur du CPC

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(solution aqueuse de phosphate disodique), ce qui nous a conduit à développer un revêtement de surface de deuxième génération qui permet de stabiliser les NPs dans ce milieu.

**Mots-Clés:** biomatériau, ciment phosphocalcique, nanoparticules, tri, fluorure de lanthanide, scanner spectral à comptage de photons

# Surfaces nanostructurées pour la détection et l'identification de polluants et pesticides

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Depuis des décennies l'homme rejette dans la nature des substances chimiques provenant de l'industrie, l'agriculture et autre. Aujourd'hui c'est environ 100 000 substances chimiques qui sont produites, importées et utilisées en Europe dont 5000 sont considérées comme dangereuses pour l'homme et l'environnement. Une partie de ces substances chimiques risque de polluer les sols et les eaux, comme les nappes phréatiques et les cours d'eau. Bien que la grande majorité de cette pollution provient d'anciens sites industriels, dépôts d'hydrocarbures ou de déchets, les jardins privés sont également une source de pollution par l'utilisation de produits phytosanitaires dans le non-respect des doses.

L'OMS et l'Union Européenne ont fixé des valeurs de tolérances dans les produits destinés à la consommation humaine et animale, allant jusqu'à moins d'un microgramme par litre. Malheureusement, des micropolluants ne sont pas inclus dans les réglementations, ils restent néanmoins dangereux pour la santé et l'environnement.

Il est nécessaire de développer des techniques permettant la détection et l'identification de substances chimiques à faibles doses dans un milieu donné. De nombreuses techniques sont actuellement utilisées ; bien que de plus en plus performantes elles ne permettent pas systématiquement d'identifier et de quantifier les espèces recherchées.

Dans ce contexte, nous développons un capteur ultrasensible reposant sur la détection et l'identification optique des composés chimiques. Ce capteur utilisera la Diffusion Raman Exaltée de Surface (DRES) grâce à des surfaces métalliques nanostructurées. Cette technique présente des avantages car elle est rapide, sensible et permet de détecter et d'identifier une ou plusieurs substances dans des mélanges même à très faibles concentrations (10-10 M). Nos recherches visent à optimiser des supports métalliques pour améliorer la sensibilité.

Quand nous pourrons détecter et identifier tous les polluants présents dans l'environnement, il sera alors plus simple de traiter ces pollutions pour une meilleure qualité de vie et protection de l'environnement.

**Mots-Clés:** Polluants, pesticides, détection et identification, Raman, Nanostructures

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# TOWARDS THE 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 (North of Chili). [1] The complex structure of these molecules coupled with their interesting antibiotic and potential antitumor activities makes this family of molecules synthetically challenging important targets. Despite their interest, no total synthesis of these compounds has been reported so far. The aim of this project is to synthesise for the first time chaxalactins A, B and C and related analogues in order to evaluate their biological activities. Chaxalactins could be obtained by a Suzuki coupling between the C1-C9 and C10-C25 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, C13 stereocenters. The C13-C25 fragment could in turn be obtained by a Stille coupling between the C13-C17 and C18-C25 fragments. In this communication, we will report our journey towards the synthesis of chaxalactins, especially the synthesis of the C1-C9 and C10-C25 fragments and the first cross-coupling attempts.

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**Mots-Clés:** chaxalactins, macrolactone, antibiotique, antitumeur, synthèse totale

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# Topochemical synthesis of new metastable rare earth oxysulfides materials

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Low-temperature synthesis is a developing field of solid-state chemistry, which provides access to metastable phases with new properties and characteristics. The topochemical intercalation of the transition metal such as copper in the material  $\text{La}_2\text{O}_2\text{S}_2$  leads to the synthesis of the known compound  $\text{La}_2\text{O}_2\text{Cu}_2\text{S}_2$  [1]. The oxysulfide  $\text{La}_2\text{O}_2\text{S}_2$  is formed by sulfur ( $\text{S}_2$ )<sup>2-</sup> dimers sandwiched between the  $[\text{La}_2\text{O}_2]^{2+}$  layers, thus copper donates electrons to the sulfur dimers which breaks them to form a two-dimensional layer in situ. However, when we use an alkali (Na, K, Rb) instead of copper, this one is not intercalated but take out one sulfur of  $\text{La}_2\text{O}_2\text{S}_2$  by topochemical pathway to form a metastable compound. This PhD work aims to explore the rich topochemistry of sulfur deintercalation from polychalcogenide compounds in order to synthesise new functional materials.

Keywords : Topochemical, deinsertion, sulfur, oxysulfide.

Sasaki, S., Driss, D., et al (2018). A Topochemical Approach to Synthesize Layered Materials Based on the Redox Reactivity of Anionic Chalcogen Dimers. *Angewandte Chemie International Edition*, 57(41), 13618-13623.

**Mots-Clés:** Topochemical, deinsertion, sulfur, oxysulfide.

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# Tyrosine selective bioconjugation using an electro-oxidative methodology for biomolecules labeling

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Development of innovative methodologies for simple and clean chemical protein engineering is of great importance in the field of pharmacology and biotechnology to access novel therapeutics, diagnostics and functional biomaterials tools. Targeting the less abundant surface exposed tyrosines (Y) residues is an increasingly promising strategy to i) achieve controlled and homogeneous protein modification, ii) offer an alternative for classical lysine and cysteine targeting methodologies.[1],[2] 4-phenyl-1,2,4-triazoline-3,5-dione (PTAD) was reported a decade ago as a tyrosine labeling agent, though requiring prior chemical oxidation from 4-phenylurazole (UrPh) anchor.[3] We recently developed the first electrochemical tyrosine-click methodology, termed eY-click, as a green and traceless alternative.[4] Using a conventional three electrodes system, UrPh electro-oxidation was achieved *in situ* in pure aqueous buffer by low potential chronocoulometry. In this study, the eY-click methodology was implemented to a range of anchors revealing 2-methyl-2,3-dihydrophthalazine-1,4-dione (NMeLum) as a highly efficient and more chemoselective Y-modifier under single-electron anodic oxidation. A range of polypeptides and proteins were successfully Y-tagged with increased kinetics, without any cross-coupling on other amino-acids bearing aromatic rings (His, Trp, Phe) and with analytical evidence of double Y-labeling capability. The tweaked methodology proved efficient with biologically relevant targets (proteins, enzymes, antibodies) with an azido-armed NMeLum anchor being further functionalized with strained cyclooctynes probes by SPAAC.

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2. J. C. Jewett, *et al.*, *Bioconjugate Chem.*, **2021**, *32*, 254-258
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4. S. Gouin, *et al.*, *J. Am. Chem. Soc.*, **2018**, *140*, 17120-17126

**Mots-Clés:** Bioconjugation, Tyrosine, Electro oxidative protocol, eY click

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# Élaboration et optimisation des cibles de gadolinium pour la production de terbium radioactif pour la médecine nucléaire

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L'approche théranostique est un nouveau paradigme de la médecine qui consiste à combiner le diagnostic et la thérapie pour personnaliser les traitements. En médecine nucléaire cette approche est possible en utilisant des isotopes d'un même élément chimique comme ceux du terbium :  $^{149}\text{Tb}$  ( $\alpha$ -thérapie),  $^{161}\text{Tb}$  ( $\beta$ -thérapie),  $^{152}\text{Tb}$  (tomographie par émission de positons) et  $^{155}\text{Tb}$  (tomographie par émission monophotonique). À part le  $^{161}\text{Tb}$ , les trois autres radionucléides sont produits par des réactions de spallation à haute énergie couplées à la séparation isotopique. Ce processus est cher et les installations pour le réaliser sont peu fréquentes ce qui limite la disponibilité de ces radio-isotopes. L'emploi de cibles de Gadolinium enrichi pour produire des  $^{149}\text{Tb}$ ,  $^{152}\text{Tb}$  et  $^{155}\text{Tb}$  à l'aide d'un cyclotron est l'une des méthodes possibles pour augmenter la disponibilité des Tb grâce aux réactions nucléaires suivantes:  $^{154}\text{Gd}(p,6n)^{149}\text{Tb}$ ,  $^{152}\text{Gd}(p,n)^{152}\text{Tb}$ ,  $^{155}\text{Gd}(p,n)^{155}\text{Tb}$ .

L'objectif de ma thèse est de développer des cibles de  $\text{Gd}_2\text{O}_3$ , forme sous laquelle se trouve le gadolinium enrichi. Nous sommes partis sur deux méthodes: la co-électrodéposition et le pastillage. La première méthode, qui consiste à piéger des particules de  $\text{Gd}_2\text{O}_3$  dans une matrice de nickel, est utilisée pour fabriquer des cibles fines pour les mesures de sections efficaces des réactions :  $^{154}\text{Gd}(p,6n)^{149}\text{Tb}$  et  $^{155}\text{Gd}(p,n)^{155}\text{Tb}$ . Ces mesures seront les premières données expérimentales disponibles et permettront d'évaluer les rendements de production. La seconde méthode permet de réaliser des cibles épaisses et est envisagée pour la production de masse d'isotopes du terbium.

Pour la co-électrodéposition, après avoir fait varier différents paramètres, nous avons obtenu des dépôts d'une épaisseur de  $20\ \mu\text{m}$ , contenant 5% de Gd. Cette teneur en Gd est suffisante pour les mesures de sections efficaces. Des pastilles compactes et uniformes d'une épaisseur d'environ  $0,5\ \text{mm}$  ont également été obtenues pour la production et sont en cours de caractérisation.

**Mots-Clés:** Terbium, Gadolinium, coélectrodéposition, pastillage, mesure de section efficace

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# Maison



# Caractérisation physico-chimique des poudres de phosphates de calcium utilisées comme additifs alimentaires

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Les surfaces importantes développées par les nanomatériaux leur confèrent un large panel d’applications mais peuvent aussi interroger sur leurs interactions avec les milieux biologiques. Le phosphate tricalcique (TCP), aussi référencé comme E341, est un additif alimentaire utilisé en particulier dans les formulations pour lait infantile pour son apport nutritionnel en phosphate et en calcium. Une étude américaine a identifié la présence de phosphate tricalcique nanométrique dans des préparations pour laits infantiles commercialisés aux Etats-Unis. En France, ce composé est absent du registre des nanomatériaux mais la mondialisation des marchandises laisse à penser que des formes nanométriques similaires pourraient circuler. Dans la mesure où la présence de nanomatériaux dans les produits alimentaires est une source de préoccupation sanitaire importante en France, notre travail a pour but de répondre à cette question. Une première partie de ce travail a consisté à caractériser cet additif (DRX, MET, RMN, Raman, FT-IR, mesures de potentiel zêta), d’une part pour identifier la présence de nanoparticules et les quantifier, et d’autre part pour connaître la nature des phases présentes ainsi que leur réactivité en solution aqueuse.

**Mots-Clés:** phosphates, calcium, additif alimentaire, caractérisation, hydroxyapatite, nanoparticules, nanomatériaux

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# Dégradation des PolyHydroxyAlcanoates : Analyse par Spectrométrie de Masse Multi-Étapes et DFT

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Les PolyHydroxyAlcanoates (PHA) sont des polymères biosourcés et biodégradables. Ils sont largement utilisés comme matériaux résorbables dans le domaine médical[1] ou comme agents d'emballage recyclables[2] et constituent une alternative viable aux plastiques obtenus du pétrole. Les PHA peuvent, en effet, être produits à partir de biomasse[3] ou par fermentation bactérienne.[4]

Le développement de méthodes d'analyse moléculaire fiables est essentiel afin de faire le lien avec les propriétés macroscopiques de ces matériaux, mais également afin de mieux caractériser les produits de dégradation de ces PHA et d'évaluer leur potentielle recyclabilité. L'analyse par électro-nébulisation (ESI) suivie de la spectrométrie de masse tandem (MS/MS) est réalisée en phase gaz avec la technique de dissociation par activation collisionnelle (CID). Elle nous permet d'obtenir des informations sur les structures moléculaires, mais également sur les mécanismes potentiels de dégradation et la nature des produits ( ~ pyrolyse).

Avec ce type d'approche, plusieurs mécanismes de fragmentation ont été décrits, en conditions basiques, conduisant à la perte d'un produit carboné et de CO<sub>2</sub>. [5] Nous avons mis en évidence la fragmentation des polymères en partant de l'extrémité  $\alpha$ -carboxylate suivant un processus SN<sub>2</sub> intramoléculaire (cyclisation d'une unité monomère sur elle-même). Pour valider ce nouveau mécanisme, la fragmentation de certains polymères a été étudiée par CID-MS<sub>n</sub> en mode négatif. Suivant la longueur de chaîne carbonée du monomère, les calculs de chimie quantique (DFT) indiquent des barrières énergétiques de cyclisation favorables, permettant la régénération des lactones (précurseurs de synthèse des PHA) sans perte d'atomes, suggérant une décomposition éco-compatible de ces polymères.

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**Mots-Clés:** PHA, biodégradable, fragmentation, cyclisation, DFT, MS, CID

# Extension du photovoltaïque au BIPV : synthèse et caractérisations de colorants du proche infrarouge pour le développement de dispositifs solaires hybrides transparents et incolores

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Dans un monde où les ressources fossiles s'amenuisent, et où les problèmes environnementaux liés à leur utilisation ne cessent de croître, le développement de nouvelles énergies, dites renouvelables, apparaît comme une nécessité. Le photovoltaïque apparaît comme une solution appropriée pour répondre à des besoins énergétiques toujours plus importants. Dans ce contexte, les cellules à base de silicium occupent une place importante mais possèdent des limitations telles que la dépendance de l'efficacité vis-à-vis de l'ensoleillement et la couleur reste figée au bleu foncé. Ainsi, pour étendre le champ d'applications du photovoltaïque, il convient de recourir à de nouveaux dispositifs. Parmi ceux-ci, les technologies solaires transparentes et incolores présentent des caractéristiques intéressantes car elles pourraient être appliquées au BIPV (Building Integrated Photovoltaics)<sup>1</sup>. Ce type d'architecture pourrait ainsi être facilement intégré, tel des vitres transparentes électrogènes, dans les maisons de demain.

Les cellules solaires à colorant (DSSC) possèdent de nombreuses caractéristiques clés pour répondre à ce défi<sup>2</sup>. Les DSSCs présentent potentiellement un faible coût de production et la couleur de ces cellules peut être modifiée à souhait par le choix du colorant. Ainsi, nous avons développé des photosensibilisateurs originaux qui absorbent non plus dans le domaine du visible mais sélectivement dans le proche infra-rouge (NIR). Pour ce faire, des composés de la famille des pyrrolopyrroles cyanines<sup>3</sup> ont été synthétisés, caractérisés, et les premiers résultats démontrent leur fort potentiel avec une efficacité finale proche de 4% pour une transparence supérieure à 65%.

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**Mots-Clés:** Photovoltaïque transparent, BIPV, DSSC, Pyrrolopyrrole cyanine

# Influence on photophysical properties of (de)protonation of phenol-substituted diazine chromophores: experimental and theoretical studies

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In recent years, lighting has become more and more energy consuming, now reaching around 20% of the global electricity consumption. Thus, there is need to properly design new environment friendly lighting devices and organic light emitting devices (OLEDs), in particular White OLEDs (WOLEDs), are more relevant than ever. The major issue is that obtaining white light is not an easy task, and is in most cases achieved by using multilayer devices or a combination of different emissive molecules. In this contribution, we present an innovative way of obtaining white light emission by modulating the protonation and deprotonation of organic fluorophores. To this end, a series of 8 push-pull phenol substituted hydroxystyryldiazines has been designed by varying the nature of the acceptor diazinic heterocycle to be protonated and of the linker moieties. The photophysical investigation of this series of compounds in solution showed a systematic redshift of the emission spectra compared to the neutral form, not only upon the protonation, but also after deprotonation. Extensive quantum chemistry calculations were performed to rationalize this behavior and understand the impact of (de)protonation on the different photophysical properties of this family of fluorophores. Furthermore, the influence of the modification of the chemical moieties in this series of compounds has been studied.

To the best of our knowledge, modulation of the emission by deprotonation has not yet been reported as an alternative strategy for obtaining WOLEDs. Our experimental and theoretical results on the phenol-substituted diazinic chromophores demonstrate that this approach proves successful, at least in solution. Thus, it opens a new route for the design of efficient WOLEDs and shall prompt further investigations up to device fabrication.

**Mots-Clés:** Quantum chemistry, Theoretical chemistry, photophysics, OLED, WOLED, chromophores

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# Le bon vin et les batteries Li-ion performantes pourraient-elles avoir en commun les polyphénols naturels ?

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<sup>2</sup>, Thomas Devic \*

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Les appareils portables sont omniprésents dans notre vie domestique (aspirateur sans fil, climatiseur rechargeable), cela est possible grâce au développement des systèmes de stockage électrochimique de l'énergie, notamment les batteries Li-ion. Une batterie est composée principalement de trois constituants : électrodes négative et positive imprégnées par un électrolyte organique. Ma thèse vise à améliorer les performances électrochimiques de l'électrode négative composé de silicium comme matériau actif. Ce matériau présente plusieurs avantages notamment sa capacité spécifique élevée (3579 mAh.g<sup>-1</sup>). Cependant, lors de sa lithiation, il subit une expansion volumique d'environ 280% qui induit de nombreux dommages : perte de la cohésion de l'électrode et de son adhésion au collecteur de courant[1]. Notre stratégie pour adresser cette problématique est de développer de nouveaux liants à base d'acide tannique, un polyphénol peu onéreux, présent dans les noix de Galle et aussi en quantité significative dans le vin rouge[2],[3]. Cet acide est capable de complexer les cations métalliques, notamment tétravalents (Zr<sup>4+</sup>, Ti<sup>4+</sup>) pour former des polymère de coordination[4] présentant de bonnes propriétés mécaniques, notamment d'autoréparation. Nous cherchons ici à tirer profit de ces avantages pour accommoder les variations de volume du Si.[5]

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**Mots-Clés:** Appareils portables, Batterie Li\_ion, électrode au silicium, polyphénols naturels



# Micro-supercondensateurs 3D tout solide à base de ionogel pour l'Internet des Objets

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L'Internet des Objets (IoT, Internet of Things) commence à faire partie de notre vie quotidienne avec des objets connectés tels que des caméras, des capteurs de mouvement, des assistants virtuels programmables, etc... La miniaturisation et l'autonomisation de ces objets sont les conditions nécessaires pour démocratiser et diversifier leur utilisation.

Ces objets de l'IoT auront des besoins en énergie et puissance pour fonctionner. Cela passe par l'utilisation d'un système de stockage de l'énergie, dont les micro-supercondensateurs (MSC), parmi les systèmes les plus prometteurs de par leur forte densité de puissance. Leur densité d'énergie, limitée par la miniaturisation des électrodes, et leur fiabilité, limitée par le type d'électrolyte utilisé, sont deux enjeux majeurs qui seront abordés dans le cadre de ma thèse.

Les performances d'un supercondensateur sont proportionnelles à la surface de ses électrodes. Pour une taille limitée, un moyen d'accroître la surface des électrodes, et donc les performances du MSC, est d'utiliser des électrodes 3D. La gravure de micro-piliers sur un wafer de silicium permet de multiplier la surface d'une électrode près de 45 fois.

Une autre manière d'améliorer la densité d'énergie d'un MSC, est l'utilisation de matériaux d'électrode pseudocapacitifs, tel que le dioxyde de manganèse (MnO<sub>2</sub>). Ces matériaux ont un comportement faradique, comme dans une batterie, avec l'adsorption et la désorption d'un cation de l'électrolyte, mais avec une cinétique très rapide, assimilable au comportement capacitif d'un supercondensateur.

La fiabilité et la sécurité du MSC dépend principalement de l'électrolyte. Les ionogels permettent d'atteindre ces besoins grâce à leur bonne conductivité ionique, leur non-inflammabilité et surtout leur état solide. La formulation de ces ionogels peut être modifiée, notamment par l'ajout de cations alcalins dans le liquide ionique, pour atteindre de plus grandes densité d'énergie. L'utilisation simultanée de ionogel, d'électrode 3D et de MnO<sub>2</sub> permet d'obtenir des MSC présentant des performances très encourageantes.

**Mots-Clés:** microsupercondensateur, ionogel, MnO<sub>2</sub>, électrode 3D, IoT

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\*Intervenant

# Mineralomimetism for home, from natural stones to every-day applications.

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Biomimeticism has been very popular for the last two decades. With the biomimeticism approach, science found new inspiration in natural living forms. Either their properties, materials, process or interactions are reproduced providing a potential anthropic application. This approach leads, for example, to the construction of a building using a termite mound as model to keep fresh air inside. We can also cite self-cleaning glasses (for windows or showers) based on the "lotus effect". However, if the living world has plenty of models to offer to science, the non-living, mineral world is also very promising. To emphasize the parallel with biomimeticism, the approach using mineral as models has been called mineralomimetism. Even if less known, mineralomimetism has already several examples in every-day life applications at home. Let us mention synthetic gems precisely synthesized for their beauty in jewellery. Synthetic quartz in watches is the basis of the clock thanks to its piezoelectric property. "Luxury" nail file covered with synthetic nanodiamonds are used for their well-known hardness. Among all possibilities, we study an interesting property discovered two centuries ago in natural gems called hackmanites. Hackmanite is a variety of sodalite and presents an exceptional photochromism. It shows an impressive, reversible, change of colour from white or colourless to deep purple once exposed to ultraviolet irradiation for few seconds. Applications of such a material could reach UV sensors, adaptable sun glasses all the way to a new generation of optical memory. This presentation develops the mineralomimetism process used to get from the observation of natural stones to potential applications through various spectroscopic analyses.

**Mots-Clés:** Hackmanite, photochromism, synthesis, XPS

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\*Intervenant

# Na<sub>7</sub>[SbW<sub>6</sub>O<sub>24</sub>]: A NEW SENSITIVE AND REUSABLE LUMINESCENT SOLID SENSOR FOR WATER DETECTION

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The detection of water either as trace in organic solvents, or as relative humidity (RH) in air have attracted wide interest over the past years, because of their great significance in industrial process controls, batteries life extension and indoor air quality improvement[1]. In the last five years, photoluminescent (PL) solid sensors for water molecules[2] have been considered as an attractive potential alternative to traditional analytical technics due to their faster response, higher sensitivity and ability of *in situ* detection. However, new sustainable and reusable sensors are still highly desirable. Polyoxometalates (POMs) are photoactive molecular oxides of transition metals (W, Mo, V) which are widely investigated as PL sensors of a wide range of analytes,[3] but their ability to detect water have been very scarcely explored. We have recently designed a new anhydrous sodium salt of the lanthanide-free POMs [SbW<sub>6</sub>O<sub>24</sub>]<sup>7-</sup> whom the highly intense luminescence at room temperature is reversibly tunable with its degree of hydration. Indeed, combined powder X-ray diffraction (PXRD), thermogravimetric (TGA) and PL analyses revealed that upon exposure to moisture-laden air (100% RH), Na<sub>7</sub>[SbW<sub>6</sub>O<sub>24</sub>] is progressively converted to the known hydrated phase Na<sub>7</sub>[SbW<sub>6</sub>O<sub>24</sub>].16H<sub>2</sub>O[4], and the rehydration process is accompanied by a drastic luminescence quenching. Moreover, Na<sub>7</sub>[SbW<sub>6</sub>O<sub>24</sub>] particles dispersed into acetonitrile can also detect trace amounts of water (0.008 v%) by rapidly reforming the PL-inactive hydrated salt. Noticeably, the luminescence quenching can be then easily reset by simple thermal dehydration, making Na<sub>7</sub>[SbW<sub>6</sub>O<sub>24</sub>] a promising robust and reusable PL solid sensors for water detection.

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**Mots-Cl es:** Polyoxometalates, photoluminescence solid sensors, water detection, humidity detection

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# Nanofluorures inorganiques pour le stockage chimique de fluor moléculaire F2

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Les agents fluorants à l'état gazeux tels que le fluor moléculaire F2 et HF sont incontournables dans de multiples procédés industriels. Actuellement, ces agents sont commercialisés dans des bouteilles métalliques et à haute pression. Outre les faibles quantités de gaz stockées par rapport au poids de la bouteille, des problèmes tant pour le transport, la manipulation et la sécurité, conduisent à développer de nouvelles solutions de stockage. L'objectif de mes travaux est d'explorer de nouvelles voies de stockage de ces agents fluorants afin d'accroître la capacité de stockage et d'améliorer la sécurité. Concernant le stockage de F2, la chimisorption via des nanoparticules de fluorures inorganiques est privilégiée, mettant en avant la capacité de certains fluorures de haut degré d'oxydation à se décomposer thermiquement avec la libération de F2 ( $MF_3 \rightarrow MF_2 + \frac{1}{2} F_2$ ). Deux systèmes, MF3/MF2 (M = Mn, Co), préparés via deux méthodes de synthèse (précipitation/décomposition et solvothermale assistée par chauffage micro-ondes) seront présentés ainsi que les premiers résultats de cyclages sous F2. L'élaboration de matériaux poreux via une nanostructuration de ces composés est également envisagée afin d'aider à la conservation de la surface spécifique lors des cyclages à des températures relativement élevées ( $T < 600^\circ C$ ) et d'influencer de façon bénéfique la température de restitution de l'agent fluorant. Leur préparation est basée sur l'assemblage de nanofluorures inorganiques en présence de sphères polymériques utilisées comme template suivi d'un traitement thermique afin d'éliminer le polymère et libérer la porosité (Figure 1).<sup>2</sup>

**Mots-Clés:** stockage de gaz fluoré, nanoparticules, fluorures, nanostructuration

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\*Intervenant

# Novel Binder to Obtain High Performance Si based Electrodes for Li-ion Batteries (LIB), for Home Electrical Energy Storage Application

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Electric energy storage through battery has emerged as a way to palliate for the intermittent renewable energy production sources (REPS), like photovoltaics. Applied to housing, the battery usage can be envisioned with a REPS system, but also without it. For the latter, the battery is charged from the grid during off-peak electricity demand and discharged when the demand on the grid is higher. However, despite its usefulness and the fact that it fits well the energy need for a house, these systems might not always be economically profitable. Indeed, researchers argued that it mostly suffered high investment cost[1], in the location where it was found to be not economically viable.

In order to reduce the price of such battery, silicon is a very promising material. Indeed, its  $\sim$  x3 higher volumetric capacity over commercially available graphite would result in  $\sim$  25 % higher volumetric energy in realistic full cell configuration[2]. Moreover, silicon price[3] is around 2.40 USD/kg, whereas graphite[4] is between 8 and 13 USD/kg and graphite accounts for  $\sim$  20 % of the total price of a LIB at the electrode stack level[4]. Combined, these 2 factors will enable cheaper battery for housing application.

Unfortunately, the full lithiation of silicon induces a severe volume expansion ( $\sim$  280%)[2] causing the fragmentation and delamination of the electrode. In this context, binder used for the electrode processing is of prime significance to mitigate mechanical degradations. We present a metal-carboxylate cross-linked binder whose characteristics and influence on electrochemical performances will be discussed.

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**Mots-Clés:** Battery, Energy, Silicon, Binder

# ORGANIC REDOX MEDIATORS FOR Li-O<sub>2</sub> BATTERIES

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As the world moves toward electromobility and a concomitant decarbonization of its electrical supply, modern society is also entering a so-called fourth industrial revolution marked by a boom of electronic devices and digital technologies. Consequently, battery demand has exploded. Introduced on the market in 1991, lithium-ion batteries (LIBs) is becoming a flagship technology possibly able to power an increasingly diverse range of applications from microchips to the emerging large-scale application markets of electric vehicles. However, their energy density is still too low for long range applications especially per unit of volume, as compared to internal combustion engines.

In order to surpass the performances offered by current LIBs, the chemistries based on the Li-O<sub>2</sub> couple in aprotic electrolyte seem promising to really provide ultrahigh-energy density values. The main targeted application is the powering of electrified vehicles with the hope of achieving a reasonable driving range (typically more than 550 km before charging, ca. 340 miles). A typical design for aprotic Li-O<sub>2</sub> batteries is composed of a negative electrode made of metallic lithium, an electrolyte comprising a dissolved lithium salt in an aprotic solvent, a separator, and a porous O<sub>2</sub>-breathing positive electrode composed of black carbon particles.

Li-O<sub>2</sub> batteries could, in principle, double the gravimetric energy density over the current Li-ion technology, but serious side-reaction issues have plagued their development for practical applications. For example, during the discharge process, some undesired insulating products are formed instead of lithium peroxide. Moreover, the blocking/clogging effect on the air electrode due to a selected deposition process leads to an overpotential during both the discharge and charge processes, which results in electrode degradation, electrolyte decomposition, ...

The aim of this work is to use commercial hydrocarbons as additives, synthesized insoluble organic salts and soluble catalysts to improve the electrochemical performance of Li-O<sub>2</sub> batteries.

**Mots-Clés:** Hydrocarbon, Redox mediator, porosity, Li, O<sub>2</sub>, Batteries

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\*Intervenant

# Recycling of components of wasted solid oxide cells and electrolyzers and regeneration of YSZ electrolyte materials

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Decarbonizing hydrogen production is expected to play a pivotal role in the transition toward a sustainable fossil free economy[1]. However, high demand for carbon free hydrogen requires large size Solid Oxide Electrolyzers (SOEs) which in turn have economic, environmental and legislative problems of end of life products[2]. To tackle this problem, we are trying for the first time a strategy of recycling and recovering Solid Oxide Cells (SOCs) components and the regeneration the electrolyte. The separation of electrode-electrolyte assembly was performed through mechanical scratching and grinding followed by thermal and chemical treatments. Recycled materials of SOFCs components; air electrodes ( $\text{La}_x\text{Sr}_{1-x}\text{CoO}_3$ ), nickel oxide (NiO) which constitutes about 50% in weight of the cell and Yttria Stabilized Zirconia (YSZ) were successfully obtained. Detailed crystallographic studies, thermal profiles of recovered hydrated nickel nitrates, microstructure and compositions of the recovered materials were studied respectively by X-Ray Diffraction, Thermogravimetric Analysis / Differential Scanning Calorimetry and Scanning Electron Microscope/Energy Dispersive X-Ray Spectroscopy. The conductivity of the electrolyte made from recycled materials of SOCs wastes was compared with different composition of commercial YSZ materials[3-5] (Fig.1). The lower level of conductivity of the regenerated electrolyte material is discussed and improvements to increase it are suggested.

Fig. 1 Comparison of conductivities of recycled YSZ electrolytes with commercial YSZ from literatures.

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**Mots-Clés:** Hydrogen economy, Recycling wastes, SOFCs, SOECs, YSZ, Ionic conductivity

# Synthèse et caractérisations de complexe de coordination à base de croconate violet pour batterie Li-ion

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Aujourd'hui, les batteries Li-ion sont indispensables pour notre vie quotidienne : elles sont petites et efficaces, et sont utilisées dans de nombreux objets de nos domiciles (tablette, portable, appareils ménagers...). Dans le domaine des matériaux d'électrode positive de batterie, les matériaux inorganiques dominent depuis trente ans. Les matériaux hybrides (organique-inorganique), en particulier les composés de coordination (notamment les polymères), émergent lentement et pourraient concurrencer les matériaux inorganiques. Les premiers exemples se sont concentrés sur l'activité redox du cation métallique uniquement [1] : Ces matériaux peuvent être réduits de manière réversible à l'état solide, et cette réduction est associée à l'insertion d'ions Li<sup>+</sup> au sein de la structure. Des études plus récentes ont montré que l'activité redox du ligand organique et du cation inorganique peuvent être combinées pour atteindre des capacités de stockage d'énergie plus élevées [2]

Dans cette perspective, nous avons porté notre attention sur le croconate violet (CV) : En solution, celui-ci peut s'oxyder deux fois et se réduire une seule fois, d'une manière réversible. [3]. De plus, avec ces fonctions complexantes, il constitue un ligand approprié pour les cations 3d et 4f [4]. Nous avons donc exploré sa réactivité avec divers cations redox actifs (V, Mn, Fe) en solution. Malgré son instabilité intrinsèque dans certaines conditions de synthèse (milieux acides), deux complexes de Fe(II) ont été obtenus. Nous présentons ici leurs structures cristallines et leur comportement thermique qui a été étudié par thermodiffraction et par spectroscopies infrarouge et Mössbauer. L'activité redox de ces complexes sera présentée, et la nature du processus redox en jeu (organique ou inorganique) sera discutée.

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**Mots-Clés:** Complexe de coordination, ligand redox actif, caractérisations

# Toward organic materials for Li-ion Batteries

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Currently, inorganic active materials such as metal oxides or phosphates dominate the field of Li-ion battery electrode materials. However, they stem from mining and their synthesis process around 900°C require an important amount of energy (e.g. 286 kWh for the production of 1 kWh of NMC-based storage capacity). Thus, the environmental footprint of such batteries is not neutral: Global Warming Potential of the aforementioned NMC-based kWh releases in average 160 kgCO<sub>2</sub>eq. Meeting the needs for electrical storage devices while reducing the environmental impact and the demand for unsustainable raw materials call for greener battery technologies. Among the various lines of research, organic redox materials could offer the possibility of rising to those challenges. To date, no Life-Cycle Assessment study proves their environmental footprint is lower than current inorganic materials, but different arguments can be put forward in their favor. As they are composed of naturally abundant chemical elements, they avoid mining and can lead to low-cost chemistry. More, their syntheses are performed below 100°C and can involve raw materials potentially obtained from renewable resources. Finally, their wide choice of chemical structures for organic molecules offers opportunities to tune their redox potential and promote reversible multielectron reactions demonstrating n-type and/or p-type reactivity. For the past 50 years, several kinds of organic redox active moieties have been identified. Our group strives notably for developing air-stable lithiated materials in order to reach high output voltage as recently demonstrated with magnesium (2,5-dilithium-oxy)-terephthalate. It allows reversible delithiation/lithiation electrochemical reaction at an average potential of 3.4 V vs Li<sup>+</sup>/Li coupled with 92% capacity retention over 80 cycles at 20°C, and a specific capacity reaching ~100 mAh/g. Within this background, this contribution aims at reporting the design, the synthesis as well as the electrochemical behavior of other lithiated compounds based on the terephthalate backbone.

**Mots-Clés:** organic materials, battery, cathode

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\*Intervenant

## Posters (tous thèmes)

# A multi-analytical approach for the characterisation of Ni-rich positive material for Li-ion batteries

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The electrification of vehicles presently relies on lithium ion batteries using layered oxides of nickel, manganese and cobalt (NMC) as positive electrode materials. In order to obtain higher energy densities, the market is now heading towards high-nickel content NMCs. Nevertheless, it has been largely demonstrated that these materials suffer from severe gassing issues decreasing the cycle life and causing safety problems. In addition to gases such as H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and CH<sub>4</sub> resulting from the SEI formation at the negative electrode material, the production of O<sub>2</sub>, CO and CO<sub>2</sub> was also demonstrated by different research groups. While it is agreed that the O<sub>2</sub> evolution is from irreversible charge compensation from lattice oxygen due to overcharge, the source of CO and CO<sub>2</sub> is still under debate and different hypotheses have been proposed. In this context, we report here a systematic study of the pristine material surface using a multi-analytical approach in order to elucidate the origin of this gas generation; different characterisation techniques such as Magic Angle Spinning Solid State NMR, XPS, STEM-EELS and FIB-SEM are combined to give a complete description of the material before cycling.

**Mots-Clés:** NMC, Li, ion batteries, Electron Microscopy, MAS NMR, Characterisation

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\*Intervenant

# Adaptive coordination-driven supramolecular chemistry based on pre-assembled luminescent Cu(I) precursors : Straightforward preparation of luminescent 1D Coordination Polymers

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An increasing interest is targeted toward Cu(I) metal complexes as potential new multifunctional molecular materials for several applications as lighting or sensor devices. Those Cu(I) complexes displays a number of interesting luminescent properties and are thus very promising. Using a general supramolecular chemistry synthetic approach developed in our group along with a pre-assembled bimetallic clip, it was possible to overcome the coordination sphere lability issues of Cu(I) ions in order to obtain a blue luminescent tetrametallic luminophore revealing unprecedented conformational flexibility. By utilizing this luminophore as a starting block and combining it with polydentate pyridine ligand, it was possible to achieve the formation of a series of new monodimensional coordination polymers, displaying a large variety in their photophysical properties. This new series of coordination polymers opens the door to the possibility of a multitude of supramolecular architectures, based on different Cu(I) precursors and all displaying a large array of photophysical properties.

**Mots-Clés:** Supramolecular chemistry, Polymetallic complexes, Cu(I) ion, Luminescent materials, Coordination polymers

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\*Intervenant

# Boron and iodine behaviour during nuclear glass vapor hydration

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Highly radioactive and long-lived waste arising from the reprocessing of spent nuclear fuel is vitrified in the form of borosilicate nuclear glass in France. It is planned to dispose of the nuclear glass permanently in the underground geological disposal facilities to ensure the isolation of radionuclides from human beings and the environment. Under the context of disposal cell re-saturation due to the groundwater penetration, the durability of nuclear waste glass in saturated media (or in aqueous solution) has been largely assessed. Before the disposal cell re-saturation, studies show that the geological disposal cell may keep unsaturated for tens of thousands of years due to the presence of hydrogen gas generated via the corrosion of iron canister. Thus, it is probable that nuclear glass will contact water vapor prior to the aqueous solution. As a result, understanding the durability of nuclear glass in the vapor phase becomes essential for evaluating the long-term safety of nuclear glass. The current work studies the vapor hydration of borosilicate and iodine-bearing glass at 90°C and relative humidity at 99%. Hydration kinetics was monitored by analyzing the boron and iodine released during the vapor hydration process. It is found that boron becomes more easily released after iodine being added to the glass matrix. The results related to boron release and retention indicate the possible transformation of tetrahedral [4]B to trigonal [3]B on the hydrated glass surface, which may enhance the release of boron in the form of boric acid afterwards. Release of iodine occurred but at a far lesser extent than boron with 90% of iodine retained in the alteration layer, thus opening good perspectives with regard to the disposal of high-level waste containing iodine.

**Mots-Clés:** nuclear glass, boron, iodine, vapor hydration

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\*Intervenant



# Complexe Ru-oxocyclohexadienyl dans des réactions d'hydrogénation sans base

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Nous sommes actuellement dans "l'âge d'or" [1] de l'hydrogénation par transfert. Toutefois, le nombre de publication varie en fonction de la source d'hydrogène employée. Jusqu'à présent les réactions de réduction par transfert ont été conduites essentiellement en milieu basique et l'acide formique n'a été que très peu utilisé comme source d'hydrogène. Les procédés sans base utilisant l'acide formique comme donneur d'hydrogène sont donc les plus rares. C'est à ce type de défi que nous nous sommes intéressés dans une collaboration avec l'équipe d'Alain Igau du LCC de Toulouse.

Depuis quelques années, cette équipe prépare des complexes originaux Ru-oxocyclohexadienyl [2,3] de type "tabouret-de-piano" qui n'ont, pour le moment, été que très peu étudiés en catalyse. Or, ces complexes présentent beaucoup de caractéristiques théoriques apte à les rendre actifs en catalyse. En effet, un caractère bifonctionnel est envisageable puisque ces complexes présentent un ligand basique et un site vacant acide sur le site métallique. Cette caractéristique pourrait être mise à profit dans des réactions sans base.

J'ai pu, lors de mes travaux de thèse, utiliser ces complexes dans des réactions de catalyse et mettre en évidence leur caractère bifonctionnel. En effet, je les ai mis en oeuvre dans des réactions d'hydrogénation et d'hydrogénation par transfert (iso-propanol et acide formique) sans base en optimisant les conditions sur un substrat test. Ainsi, nous avons pu valider les hypothèses émises en premier lieu: ces complexes de type "tabouret-de-piano" sont actifs en réaction d'hydrogénation et d'hydrogénation par transfert sans base.

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**Mots-Clés:** Catalyse, hydrogénation, sans base, Catalysis, Hydrogenation, base free

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# Cu(I)-phosphine pre-assembled precursors for selective adaptive coordination-driven supramolecular syntheses of new polymetallic Cu(I) luminescent assemblies

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An increasing interest is devoted to Cu(I) metal complexes as new multifunctional molecular materials for lighting and sensors applications.<sup>1</sup> Using a synthetic approach inspired by the general coordination-driven supramolecular (CDS) chemistry strategy,<sup>2</sup> we present herein the straightforward syntheses and solid state characterizations of a novel series of polymetallic Cu(I) supramolecular assemblies.<sup>3</sup> Their specific solid-state luminescent are also reported. These results highlight that, the typical labile, flexible and low-directional coordination sphere of the Cu(I) ion, initially regarded as strongly restrictive in conventional CDS chemistry, turned out to be very valuable to conduct the adaptive and selective preparation of original polymetallic derivatives.

**Mots-Clés:** supramolecular chemistry, Cu(I) ion, Polymetallic complexes

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# Dissipation in rapid gravitational granular flows

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<sup>1</sup> ZHU YAJUAN – Chine

We investigate numerically high speed granular flows down an incline and focus our attention on the influence of the restitution coefficient  $e$  of binary collisions on the nature of the flow regimes. We show in particular that  $e$  plays a major role in rapid flows. Decreasing  $e$  leads in general to denser flows but also quicker flows which was not expected. The increase of the mean flow velocity with decreasing  $e$  is explained as the result of the clustering instability which produces a dense and cold core moving very fast as a plug.

**Mots-Clés:** Granular flow

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\*Intervenant

# Développement d'une plateforme analytique intégrée basée sur la RMN mobile pour la caractérisation des drogues

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Les nouvelles substances psychoactives (NSPs) sont des drogues non-réglémentées qui constituent une menace croissante en termes de santé publique. Les NSPs sont des drogues couramment consommées lors d'évènement festifs et peuvent entraîner la mort par overdose. Pour les réglementer en temps réel, il est essentiel de les caractériser à l'aide d'une approche rapide et accessible. Dans ce cadre, la spectroscopie RMN est un atout de choix puisqu'elle peut fournir la structure moléculaire de ces composés. Cependant, la RMN nécessite des équipements lourds, des coûts d'achat et de maintenance élevés. Au cours des dernières années, de nouveaux instruments compacts, bon marché, et ne nécessitant pas de fluides cryogéniques ont vu le jour. Cependant, la "RMN de paillasse" est limitée par sa faible résolution spectrale et sa sensibilité réduite. Pour améliorer les performances de ces instruments compacts, nous avons récemment mis en œuvre des techniques avancées sur un spectromètre à 1T équipé d'une bobine de gradients, telles que la suppression du signal du solvant, les expériences *pure-shift* et les méthodes 2D ultrarapides. Dans ce contexte, une investigation préliminaire avec deux NSPs modèles nous a permis de déterminer les techniques de RMN les plus adéquates pour leur caractérisation. Différentes séquences hétéronucléaires 2D 1H-13C ont été comparées en termes de sensibilité et de dispersion du signal pour identifier les NSPs à 60MHz. Des outils supplémentaires sont nécessaires pour faire face à la fois à la complexité des structures moléculaires et au fait que les composés saisis sont souvent en mélange. Dans cette optique, nous explorons la combinaison de la RMN 1D et 2D avec des outils de reconnaissance spectrale comme les bases de données expérimentales ou la détermination des déplacements chimiques par la DFT. A terme, ces approches contribueront à la création d'une plateforme intégrée pour identifier, élucider et profiler les NSPs.

**Mots-Clés:** NPS, RMN, DFT

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\*Intervenant

# Electrochemical study of tungsten bronzes $A_xWO_3$ ( $A = Li, Na, \text{ and } K$ ) as electrode materials for fast energy storage devices

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Tungsten oxide  $WO_3$  is a well-studied material due to its electrochromic, photochromic, and catalytic properties and presents a wide diversity of polymorphs. Among them, is the metastable phase of hexagonal bronze (h- $WO_3$ ) which cannot be obtained by purely structural transformation upon temperature [1]. This structure possesses a rigid tungsten-oxygen framework built up of layers containing corner-shared  $WO_6$  octahedra that are arranged in six-membered rings. The layers are stacked along the [001] axis, giving rise to one-dimensional tunnels being able to host different alkali cations such as  $Li^+$ ,  $Na^+$ , and  $K^+$  [2]. This arrangement can result in interesting electrochemical properties when the hexagonal bronze is used as an electrode material for energy storage devices [3].

Hexagonal tungsten oxides were successfully synthesized by hydrothermal synthesis. The materials were characterized by X-ray Diffraction, Scanning and Transmission Electron Microscopy, Energy dispersive X-ray spectroscopy, and BET specific surface area.  $LixWO_3$  shows a nanorod-like morphology where the growth of the stacked hexagonal rings along the  $c$  direction is observed. In this work, we report the synthesis of different hexagonal bronzes of tungsten oxide with the general formula  $A_xWO_3$  ( $A = Li, Na, \text{ or } K$  and  $0 < x < 0.33$ ). We studied the electrochemical behavior in different aqueous electrolytes such as  $LiNO_3$  (5M and 1M),  $Li_2SO_4$ ,  $Na_2SO_4$ , and  $K_2SO_4$  (0.5 M) obtaining specific capacities of  $\sim 70$  C g<sup>-1</sup>,  $\sim 49$  C g<sup>-1</sup>,  $\sim 41$  C g<sup>-1</sup>,  $\sim 24$  C g<sup>-1</sup> and  $\sim 13$  C g<sup>-1</sup>, respectively at 2 mV s<sup>-1</sup> for  $LixWO_3$ . Additional characterization techniques like *operando* X-ray Absorption Spectroscopy were used to unveil the charge storage mechanisms of these tungsten bronze.

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\*Intervenant

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**Mots-Clés:** Tungsten oxide, tungsten bronze, electrode materials, electrochemical devices, fast energy

# Eu<sup>3+</sup>/Tb<sup>3+</sup> mixed Metal-Organic Frameworks (MOFs) for ratiometric luminescent thermometry

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In the past few decades, **Metal-Organic Frameworks (MOFs)** have drawn tremendous attention due to their fascinating topologies coupled with their large domain of application such as catalysis, gas storage/separation or chemical sensing. More recently, these materials have aroused interest in the field of luminescence thermometry. Indeed, luminescent MOFs, and particularly Lanthanide-based MOFs (**Ln-MOFs**), have shown their potential in non-contact luminescence thermometry at the nanoscale due to their large temperature sensing range (from cryogenic to high temperatures up to 400 K) and their unique optical performances. In 2012, Cui *et al.* have shown that lanthanide mixed-MOFs containing two Ln<sup>3+</sup> emitters (*i.e.* Tb<sup>3+</sup> and Eu<sup>3+</sup>) present a great potential for application as **ratiometric luminescent thermometers**. However, no study focuses on the rationalization of the key parameters that control the thermometer's performances such as the **temperature sensing range** or the **relative thermal sensitivity**. In this study, the impact of the lanthanides composition in the mixed-MOFs has been investigated. Thus, two series of mixed-MOFs built on the ligand 1,2,4,5-benzenetetracarboxylic acid (H4Btec) have been studied, with general formula [Tb<sub>1-x</sub>Eu<sub>x</sub>(HBtec)]<sub>n</sub> and [Gd<sub>0.5</sub>Tb<sub>0.5-x</sub>Eu<sub>x</sub>(HBtec)]<sub>n</sub>. These materials are chain compounds where both Tb<sup>3+</sup> and Eu<sup>3+</sup> cations are efficiently sensitized by the ligand due to antenna effect, making them suitable for luminescence-thermometry. More precisely, we proved that a modulation of the relative thermal sensitivity along with the corresponding temperature sensing range is possible by finely tuning the chemical composition.

**Mots-Cl es:** Metal Organic Frameworks, lanthanides, luminescence, thermometry

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# Fast Electron Transfer Kinetics in Deep Eutectic Solvents: Effect of Water Addition

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Deep eutectic solvents (DESs) are an emerging class of solvents, which are considered sustainable and cheap alternatives to ionic liquids.(1) DESs generally consist of mixtures of salts and hydrogen bond donors producing eutectics at the optimized ratio that are liquid at ambient temperature and have unusual solvent properties. Water amount in DESs strongly affects its physicochemical properties from density, viscosity, melting point, surface tension to conductivity,(2) while being part of DESs composition. Recent results from the literature have shown that DESs' nanostructure is varied according to the amount of water present in DES. (3) It is known that DESs spontaneously absorb water when exposing to the air, to a certain extent depending on the hygroscopicity of its components. It is therefore interesting to analyze the effects of water concentration on electron transfer kinetic rate constants. This point is not only a concern for fundamental molecular electrochemistry but is also meaningful for practical utility. In a recent publication, we demonstrate that electron transfer kinetics rate constants involved in two classical oxidation reactions of ferrocene and ferrocyanide in ethaline were remarkably larger than those in ionic liquids while being comparable to values obtained in molecular solvents.(4) In this work, we will study the kinetics of oxidation of ferrocene and ferrocyanide in five DESs, including Ethaline, Reline, Glyceline, choline chloride (ChCl)-lactic acid, and ChCl-malonic acid by varying the water amounts from 0.5 wt% to 10 wt% with particular consideration of ohmic drop compensation. The extracted data in DESs shows that kinetic rate constants value considerably increases with the addition of water in DESs. Electron transfer kinetics increases much faster for the ferrocene/ferrocenium redox couple than for ferrocyanide/ferricyanide redox couple with the addition of water amount in all the five DESs.

**Mots-Clés:** electron transfer, deep eutectic solvents, water addition

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\*Intervenant



# Fast and global authenticity screening of spices using $^1\text{H-NMR}$ profiling: example of black pepper

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According to a recent study from French customs, about half of the commercialized spices are considered as being adulterated, and even more among ground spices. Black pepper samples, representative of the whole world production (Vietnam, India, Brazil, Indonesia ...), were collected over one year and analyzed according to an analytical pathway including organic solvent extraction and untargeted  $^1\text{H NMR}$  spectroscopy. An interpretation tool was developed in order to determine the authenticity of black pepper from our database, whose spectra are displayed on figure 1. Common adulterants such as maltodextrine or starch were detected from 10% addition experiments. Principal Component Analysis (PCA) was used to analyse spectral data in an untargeted unsupervised way, and a geographical discrimination was found between Asia and America (fig. 2). That same fast and untargeted approach can be applied to many other spices.

**Mots-Clés:** Black pepper, authenticity,  $^1\text{H NMR}$

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\*Intervenant

# Formation of molecular alloys and core-shell shaped lanthanide coordination polymers and comparison of their luminescent properties

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Since few decades, lanthanide-based coordination polymers have been studied for their interesting optical properties that make them suitable for anti-counterfeiting application for instance [1]. Coordination polymers are composed with metallic ions that are linked by organic ligands to form infinite one-, two- or tri-dimensional molecular networks [2]. Because of the similar chemical behavior of the lanthanide, ions iso-structural homo- and hetero-lanthanide compounds can be prepared as microcrystalline powders. Hetero-lanthanide compounds may present a random repartition of the metallic ions over the metallic sites and they are called "molecular alloys" [3]. They can also be organized and present a core-shell structure [4].

Herein, we report the synthesis of molecular alloys with terbium and europium as metallic ions and trimesic acid (1,3,5-benzene-tricarboxylic acid or H3tma) as ligand. These coordination polymers with general chemical formula  $TbxEu_{1-x}(tma)(H_2O)_6$ , with  $0 \leq x \leq 1$ , are made as reference for this type of syntheses and will be compared with core-shell microcrystalline powders, with the same composition and crystal structure. The luminescence study of these compounds reveals an efficient Tb-to-Eu energy transfer.

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**Mots-Clés:** Terre rare, luminescence, polymère de coordination

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# Functionalized phenalenones as singlet oxygen photosensitizers for antibacterial applications

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Over the past decades, antibacterial photodynamic therapy (aPDT) has received a great deal of attention for the destruction of bacteria, fungi or viruses. This treatment is based on the light-driven production of reactive oxygen species such as singlet oxygen ( $^1O_2$ ), which is an efficient biocide.[*Crit. Rev. Microbiol.* **2018**, p571] The production of highly reactive  $^1O_2$  is based on the activation of a photosensitizer (PS) through visible light absorption to initially generate its excited singlet state which would then evolve to the excited triple state by intersystem crossing. The PS in its triplet state can interact with ground-state oxygen ( $^3O_2$ ) to form  $^1O_2$  by triplet-triplet energy transfer. These processes are oxygen-dependent which can lead to local hypoxia due to molecular oxygen consumption, lowering the therapeutic effects of aPDT. To circumvent this issue, the delivered light dose could be fractionated into a series of pulse during the treatment (intermittent aPDT).[*Photodiagnosis Photodyn. Ther.* **2015**, p393] Nevertheless, the production of  $^1O_2$  is stopped when light is off. Therefore, our strategy is based on the design of photosensitizers containing a unit able to trap, store and release  $^1O_2$ . A common approach for preparing efficient photosensitizers focuses on the introduction of heavy atoms (i.e., Ir, Ru, Pd, Br, I). Nevertheless, the dark toxicity and cost of heavy-atom-containing PSs are drawbacks for aPDT applications. To overcome these issues, we turned our attention on phenalenone structures as organic photosensitizers owing their propensity to produce  $^1O_2$  in high yield and their photostability. However, the drawbacks of phenalenones such as their absorption in UVA regions and limited synthetic strategies to obtain functionalized structures still constitute important barriers to their widespread adoption. The synthesis of new phenalenone containing a  $^1O_2$  reservoir will be presented in this communication.[*ChemPhotoChem* **2021**, accepted article, doi:10.1002/cptc.202100047]

**Mots-Clés:** Singlet oxygen, Phenalenone, Photosensitizer, Antibacterial photodynamic therapy

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\*Intervenant

# Imagerie TEP in vivo des cancers, vectorisée par un antagoniste des récepteurs CXCR4 radiomarqué au cuivre 64

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Un récepteur cellulaire transmembranaire, CXCR4 attire l'attention des chercheurs depuis quelques années de par son implication dans différentes pathologies comme le VIH ou encore les cancers. CXCR4 ainsi que son unique ligand naturel CXCL12 (également nommé SDF-1) jouent notamment un rôle dans la production de métastases.[1] Plusieurs antagonistes de CXCR4 ont pu être identifiés que ce soit des anticorps, des dérivés de peptides ou encore des petites molécules organiques ouvrant ainsi des perspectives d'imagerie vectorisée des cancers.[2] Parmi ces molécules organiques, certaines sont composées d'un motif tétrahydroquinoline-benzimidazole, fonctionnalisées par différents groupements permettant ainsi de les conjuguer sur un chélateur développé récemment au laboratoire, le *p*-SCN-Bn-TE1PA. Ce dernier a fait ses preuves en tant que chélateur du cuivre-64 en imagerie immuno-TEP sur modèle murin.[3,4] L'objectif est de conjuguer une des petites molécules organiques (PM1) sur le *p*-SCN-Bn-TE1PA permettant ainsi une imagerie ciblée des cancers surexprimant CXCR4, comme le glioblastome. De plus, le cuivre-64 forme avec le cuivre-67 une paire théranostique rendant possible tant le diagnostic que la thérapie des cancers par la même plateforme radiopharmaceutique, pour un meilleur suivi des patients.

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**Mots-Clés:** CXCR4, cancer, imagerie TEP, cyclam

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\*Intervenant

# Implantation de défauts et l'étude de leurs influences sur les propriétés électrochimiques du Nitrure de Vanadium pour l'internet des objets.

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To power the Internet of things, micro-supercapacitors appear to be an efficient and cheap way. In order to have a better understanding of some micro-supercapacitors electrode, we study the influence of defects in VN thin film. The influence of microstructural or structural defects is seldom investigated in pseudocapacitive electrodes. Indeed, most of the synthesized materials do present defects at every scale which contribute to the improvement of the charge storage. In this study, VN thin films were deposited by reactive magnetron sputtering. The as-deposited VN films were compared with similar films implanted with arsenide cations (As<sup>+</sup>) with energies ranging from 20 keV up to 150 keV. The influence of the ionic implantation on the structure and microstructure of the pristine films was characterized by several techniques. The initial curing of the internal stress of as-deposited VN films observed for low implantation energies was lost with increasing implantation energy. Concomitantly, the electrochemical behaviors of the VN films were investigated. All the VN films show a pseudocapacitive behavior at 2 mV.s.

**Mots-Clés:** VN, pseudocapacitive materials, Internet of thing, microsupercapacitors, house

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\*Intervenant

# Insights into Pickering water-in-water emulsions

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Water-in-water (W/W) emulsions are formed by mixing aqueous solutions of incompatible polymers and can in some cases be stabilized by the addition of particles, so-called Pickering emulsions. The understanding of the foundations of the stabilization of W/W emulsions is of major importance for the development of new possibilities in the food industry. Thus, this presentation will provide insights into the features that influence the adsorption of solid particles at the interface of W/W emulsions. This interfacial adsorption is dictated by the interfacial tension between the two aqueous phases and between the particles and each phase. It should therefore be possible to induce and fine-tune adsorption by adding small amounts of a third polysaccharide that is compatible and soluble with one or both phases. To investigate this statement, W/W emulsions formed by mixing pullulan (PUL) and amylopectin (AMP) and adding protein microgels (MG) were studied. The microstructure and positioning of the MG were monitored using confocal laser scanning microscopy. The effect of adding small amounts of different types of polysaccharides on the adsorption of the MG at the interface was studied as well as their partitioning between the phases. The addition of all types of polysaccharides led to a progressive shift of the MG from the PUL phase to the AMP phase and to adsorption of the MG at the interface when the partition was not extreme. Finally, the partition could be fine-tuned to be equal in both phases, and in that case, the particles adsorbed at the interface remained there even very close to the binodal.

**Mots-Clés:** water in water emulsions, Pickering emulsions, protein microgels.

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# Insights into the Chemistry of astrophysical environments

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Gas-phase ion-molecule reactions may play some role in the synthesis of large interstellar molecules. However, the nature of the products and the kinetics of ion-molecule reactions relevant for cold environments are not well known, in particular at low temperature. We have recently developed a unique approach to investigate the reactivity of ions. Our method relies on the implementation of a mass-selective source of ions on the uniform supersonic flow chamber (better known as the CRESU – Cinétique de Réaction en Ecoulements Supersoniques Uniformes). Our efforts first focused on the reactivity of  $N_2^+$  with propyne ( $HC\equiv C-CH_3$ ) and allene ( $CH_2CCH_2$ ) at 24, 36, 49 and 72 K. We also explored the reaction of the molecular ion  $CH_2CN^+$  with four hydrocarbons: methane ( $CH_4$ ), acetylene ( $HC\equiv CH$ ), ethylene ( $H_2C=CH_2$ ), and ethane ( $H_3C-CH_3$ ) over the 36-300 K range. Branching ratios into the various exit channels were measured. In addition, we have studied recently the reactivity of  $O_2^+$  ion with propyne, allene, ethene and propylene at very low temperature. Our results will be discussed and preliminary conclusions drawn. Beyond the interstellar medium, our work may also have some implications for the chemistry of Titan's atmosphere

**Mots-Clés:** Titan, planetary atmospheres, Interstellar medium, CRESU technique, ion, mol reactions

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# Isotopomics analysis of small quantities of cholesterol using an optimized 2D NMR experiment: Application to cheese authentication

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Cholesterol is involved in the synthesis of many steroid molecules and is related to many health problems. Determination of the <sup>13</sup>C position-specific contents of this compound allows to trace foodstuffs from animal origin and can afford powerful biomarkers for metabolic and cardiometabolic disorders as well as for nutritional epidemiologic studies. The existing <sup>13</sup>C IN-EPT (Insensitive Nuclei Enhanced by Polarization Transfer) adiabatic method permits such an isotopic analysis but requires 80 mg of cholesterol in order to be carried out in a reasonable time. This NMR method is therefore restricted to products high in cholesterol. Thus, we aimed to develop a new NMR sequence allowing to extend the analysis to matrices of low cholesterol contents, such as dairy products. A symmetric and adiabatic Heteronuclear Single Quantum Coherence (HSQC) 2D NMR sequence was used to reach this goal. Adiabatic pulses were used for winning in precision and sensitivity, while keeping experiment time short. Moreover, Variable Recycling Times (VRT), Non-Uniform Sampling (NUS), and Linear Prediction (LP) were evaluated and optimized in order to reduce the NMR experiment duration. Additionally, number of *t*<sub>1</sub> increments and spectral range were also adjusted. Using this newly developed HSQC sequence, 5 mg of cholesterol can be analyzed while maintaining a precision as high as 2 permil on the 24 non-quaternary carbon atoms of the molecule in 31 min instead of 16.2 hours with the previous method. In order to evaluate the applicability of the method on biological matrices and the potential of cholesterol as an authenticity biomarker, cheese samples from different origin were collected and cholesterol was quantitatively extracted and analyzed. Molar fractions of cholesterol isotopomers obtained from HSQC spectra were used as inputs in the construction of classification models for cheese authentication. Cheese samples were successfully classified according to their producing species, geographical origin and type.

**Mots-Clés:** Cholesterol, Quantitative NMR, 2D HSQC, <sup>13</sup>C isotope analysis, Isotopomics, Cheese authentication

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# Ligand-driven light switching of Single Molecule Magnets

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Single Molecule Magnets (SMM) are molecules comprising one or more metal centers and showing slow relaxation of the magnetization at low temperature. The importance of SMM lies in their magnetic bistability, which has a molecular origin. SMMs offer unique features that may allow information to be stored with much higher densities. They are considered as the smallest chemically tunable components for spin-based devices and hold promises for applications in information storage. [1] For such applications, it would be a great advantage to control the magnetic properties by applying external stimuli. Light is fascinating in this purpose due to its easy and contactless application. [2]

The goal of our project is to create an efficient strategy to switch reversibly the molecular magnetic behavior with light, relying on the photochromic abilities of a ligand, and on the influence of the coordination environment on the SMM property.

Scheme 1 (a) photo-isomerization of photoactive ligand, (b) complex design

In our target complexes, dysprosium (III) was selected to promote magnetic anisotropy, and the photochromic ligand was designed to produce large light-induced changes in the coordination environment hence affecting the electronic structure and magnetic behavior. [3] In this presentation, we will present the synthesis of several macrocyclic photochromic complexes, and discuss the influence of different parameters on the equilibrium. [4]

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**Mots-Clés:** Single molecule magnets, photochrome, spiropyran, macrocycle, Dysprosium(III)

# MoO<sub>x</sub>:MoS<sub>y</sub> hybrid thin film as anode buffer layer for organic solar cells application

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Anodic Buffer Layer (ABL) plays a crucial role in improving the performance of organic solar cells (OSC) by adjusting the electrode work function, transporting the holes from the organic semiconductor to the electrode, and avoiding the charges recombination by blocking the electrons at ITO/photoactive layer interface. The MoO<sub>3</sub> thin film is well known as an efficient ABL, which has good hole transporter property, but on the other hand, lacks the ability to block electrons. Therefore, the aim of this work is the synthesis of a new buffer layer to reduce the free charge losses at the interface electrode/active layer.

In this work, we opted for a hybrid buffer layer synthesized by a wet process based on molybdenum trioxide and molybdenum disulfide (MoO<sub>3</sub>/MoS<sub>2</sub>) according to partial oxidation of MoS<sub>2</sub> using hydrogen peroxide as oxidant. The chemical reaction was carried out at room temperature while other reaction parameters are controlled to adjust the atomic percentages of each component. Promising results are obtained by X-ray photoelectron spectroscopy analysis, which confirms that there is a growth of the two materials (MoO<sub>x</sub> and MoS<sub>y</sub>).

The synthesis of the thin films was followed by morphological, optical characterization to fulfill the conditions for a good ABL.

**Mots-Clés:** Thin film, wet chemical synthesis, hybrid buffer layer, interface electrode/organic material

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# Modélisation In Silico du Marquage avec le Radioisotope 211 de l'Astate

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L'isotope radioactif 211 de l'astate (At), émetteur de particules alpha produit sur la région nantaise grâce au cyclotron ARRONAX, est particulièrement intéressant en tant qu'agent thérapeutique potentiel en médecine nucléaire en raison de sa période (7,2 h) et de l'énergie des particules alpha émises lors de la désintégration du noyau.[1] L'astate peut ainsi être vectorisé vers les cellules tumorales afin de détruire celles-ci via les particules émises lors de la désintégration du noyau radioactif.[1] Jusqu'à présent, les protocoles de marquage de l'astate principalement développés reposent sur la formation d'une liaison avec un carbone d'aryle comme dans le N-succinimidylastatobenzoate (SAB). Cependant, ce type de liaison At–C présente *in vivo* une stabilité insuffisante pour une injection systémique du radiopharmaceutique.

Mon travail vise à étudier, exclusivement par des approches de chimie quantique (DFT) relativiste, (i) l'interaction de PhAt avec des modèles d'acides aminés, et (ii) la stabilité de la liaison C–At dans PhAt et des modulations chimiques permettant de la stabiliser.

Nos résultats permettent d'établir un ordre énergétique préférentiel d'interaction de PhAt avec les différents fragments d'acides aminés. Par ailleurs, les descripteurs théoriques sélectionnés montrent de façon concordante une moins grande stabilité de la liaison C–At par rapport à son homologue C–I.[3]

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**Mots-Clés:** astate, radiomarquage, médecine nucléaire, SAB, chimie quantique, DFT, relativité, acides aminés

# Modélisation de l'auto-affinement spectral laser assisté par effet Brillouin

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Les lasers sont omniprésents dans notre vie quotidienne. Si dans la plupart des applications il est possible de se contenter de simples diodes laser certaines au contraire nécessitent des sources optiques aux propriétés bien particulières. Par exemple, le développement de lasers très fins spectralement est un enjeu majeur dans de nombreux domaines de la physique fondamentale et appliquée. Cependant l'obtention de sources laser présentant une largeur de raie optique de l'ordre du Hertz demande des développements lourds et coûteux. L'objet de la présentation est de décrire un nouveau principe d'affinement spectral développé à l'institut Foton et ne faisant pas appel aux techniques habituelles de la métrologie temps-fréquence. Le contenu de la présentation permettra de comprendre comment il est possible d'auto-affiner spectralement un laser solide en s'aidant de l'effet Brillouin. Nous verrons notamment qu'il est possible d'obtenir de manière simple des raies laser sub-Hz en combinant les actions d'un résonateur actif kilométrique et d'une boucle à verrouillage de phase. Ensuite nous présenterons la modélisation du système d'affinement sous la forme de fonctions de transfert permettant de comprendre comment ce dernier permet de corriger les variations de phase non désirées d'une source optique bruitée. Cette modélisation nous offre notamment la possibilité d'évaluer les limites du système et de trouver les meilleurs compromis en terme de réalisation expérimentale.

**Mots-Clés:** Affinement laser, Diffusion Brillouin stimulée, Résonateur fibré, Modélisation

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# Modélisation structurale de fluorures inorganiques désordonnés.

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De nombreux matériaux cristallisés présentent un désordre de nature chimique (sites cristallographiques occupés à la fois par des atomes de natures différentes ou des lacunes) ou topologique (occupation des sites interstitiels) et des propriétés physiques intéressantes (absorption, conductivité ionique, propriétés diélectriques). Pour mieux comprendre et améliorer ces propriétés, une description structurale de ces matériaux est nécessaire. Leur caractérisation structurale est difficile par des techniques de diffraction classiques qui ne permettent d'obtenir qu'une description moyenne. En revanche, la sensibilité de la Résonance Magnétique Nucléaire (RMN) à l'environnement local du noyau sondé en fait une sonde idéale pour les solides désordonnés. Même si leurs spectres sont peu résolus, des informations structurales précises peuvent en être extraites en confrontant résultats expérimentaux et calculs DFT (Théorie de la Fonctionnelle de la Densité) issus de modèles structuraux, des supermailles reflétant à la fois les caractères périodiques et désordonnés du matériau.

Dans ce contexte, ma thèse vise à décrire aussi précisément que possible la structure de (halogéno)-(hydroxy)-(oxy)-fluorures inorganiques désordonnés d'intérêt en appliquant aux composés sélectionnés la démarche suivante:

- Synthèse et caractérisation par diffraction et par RMN du solide (<sup>19</sup>F, noyaux quadripolaires);
- Construction et sélection de supermailles à l'aide du programme " Supercell "(**1**), optimisation des positions atomiques et calculs ab-initio des paramètres RMN en appliquant l'approche GI-PAW(**2,3**) implémentée dans le code CASTEP (**4**);
- Comparaison des résultats RMN expérimentaux et calculés.

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**Mots-Clés:** DFT, DRX, RMN, Synthèse

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# Multiscale modelling of polonium chemistry in solution

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Polonium is one of the rarest and most toxic elements found in nature. Despite being discovered in 1898, it is still scarcely studied due to its dangerous properties. Nowadays, scientists face the problem of detecting this perilous element in the environment using *in situ* sensors. This progress is complicated by the narrow knowledge of polonium chemistry. Conducting experiments is quite complex with this element, especially given its extreme toxicity. Instead, the goal of this study is to predict the theoretical chemical behavior of polonium in solution without performing any experimental work, thus saving the experimenter's health, time, and money. This is achieved by doing theoretical chemical calculations based on methods of quantum mechanics as well as by coupling them with classical physics. Our project is divided into several steps, which include carrying out a systematic study of small systems ("benchmark"), developing a force field (defining parameters used in classical equations to calculate properties of the systems), and performing molecular dynamics studies (studies of bigger systems). After computing a benchmark on complexes of polonium with water ligands and finding the most satisfying methodology for calculations, we have first confirmed that Po can create hydrated complexes with up to 9 water molecules in the 1st hydration shell (further addition of ligands results in starting to fill the 2nd hydration shell). Currently, we plan to compute the properties of these complexes with different methodologies and also carry out the same type of calculations but this time with complexing ligands (Cl<sup>-</sup>).

**Mots-Clés:** Polonium, modelling, quantum mechanics, quantum chemistry, theoretical chemistry

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# New developments for studying in-situ radium behavior for environmental impacts and monitoring

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Natural radiogenic Radium has been drawn high attention because of its radio-toxicity and chemical similarity to Calcium, an element indispensable in bones and other organs. A reliable, efficient and rapid method is expected to be developed aiming at quantifying the "labile" part of Radium in natural water. A project has been started since 2015 in collaboration with TrisKem International, aiming at developing a specific Radium resin for environmental applications. The innovative resin (entitled Resin SK below) consists of a metal-selective ligand, which has shown a potentially high affinity and selectivity to Radium in environmental conditions.

The objectives of this research mainly include 3 aspects, firstly, selecting resins which are not only capable of capturing Radium but also suitable for further geological research; secondly, introducing the potentially applicable resins into the DGT (Diffusive Gradients in Thin films) sensors, then conducting a series of laboratory tests in order for DGT characterization; finally, acquiring the in-situ data for improving the knowledge of Ra geochemistry. Several sites in France will be involved, i.e. the Loire estuary and two former uranium mines

The Radium adsorption capacities of the SK resin showed a high affinity of Radium when environmental pH was higher than 5. It could be an appropriate binding matrix in DGT sensors, but only in freshwater system.

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Apart from SK resin, several resins could also be promising, i.e., TK-100, TK-101 Strontium-specific resins, Chelex-100 chelating resin and AnaLig Ra-01 Radium-specific resin. The performances of these resins have been tested under 5 commercial mineral water: Cristaline, Evian, Hépar, Rozana and Volvic. AnaLig Ra-01 has the best performance among all. Salinity is an important factor influencing Radium adsorption capacity.

Fabrication of DGT gels and DGT characterization have been completed, and the DGT kinetics experiments in lab and in-situ are on the go.

**Mots-Clés:** Radium, Diffusive gradient in thin films (DGT), environmental monitoring

# New host materials for high performance single layer phosphorescent light emitting diodes

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Nowadays, OLEDs (Organic Light-Emitting Diodes) technology is present in everyday life. It is mainly found in smartphone and television screens, but also, more recently, for lighting. Organic electrophosphorescent diodes (PhOLEDs) are the second and most mature generation of OLEDs. In this technology, all the high-efficiency PhOLEDs are multi-layer devices constituted, in addition to the emissive layer (EML), of a stack of functional organic layers. These layers play a crucial role in the device performance as they improve the injection, transport, and recombination of charges within the EML. However, in order to fit with the energetic and ecological transition, PhOLED technology should still be improved. Single-layer PhOLEDs (SL-PhOLEDs) represent ideal OLEDs, consisting only of the electrodes and the EML. Simplifying the multilayers structure is then crucial to reduce the amount of commodities, the manufacture complexity, the production and recycling costs for real-life applications. However, reaching high-performance SL-PhOLED is far from easy, as removing the functional layers of an OLED stack dramatically decreases the performance. To achieve high SL-PhOLED efficiency, the efficient injection, transport, and recombination of charges should be insured by the EML, and particularly, by the host material. Herein, two host materials have been investigated. They are constructed on the association of an electron-rich unit (indoloacridine or dihydroquinolinoacridine) connected by a shared spiro carbon atom to an electron-deficient 2,7-bis(diphenylphosphineoxide)-fluorene. In addition to a high ET value, adequate highest occupied molecular orbital/lowest unoccupied molecular orbital energy levels and important thermal stability, the key point in this molecular design is the suitable balance between hole and electron mobilities, which leads to good performance in a SL-PhOLED. In this work, the synthesis and the study of photophysical, electrochemical and charges transfer properties are reported and rationalized by theoretical calculations. Then, the performances of the SL-PhOLEDs using these semi-conductors as host materials are presented.

**Mots-Clés:** Host material, organic electronics, single, layer phosphorescent organic light, emitting diode, triplet energy, ambipolar charge transport

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# On twisted $\pi$ -conjugation: theoretical outlooks on intersystem crossing efficiency on fused BODIPY derivatives

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Triplet photosensitizers (PSs) have been widely studied for various applications from photocatalysis to photodynamic therapy (PDT). Obtaining an efficient intersystem crossing (ISC) within chromophores usually requires to follow the El-Sayed rule or to use the heavy atom effect. However, it has been reported that the non-coplanarity in helicenes significantly increases the spin-orbit coupling (SOC) to the point where such twisted  $\pi$ -conjugated compounds become competitive. In this context, strongly deformed Boron dipyrromethene (BODIPY) derivatives have shown up to 63% of singlet oxygen generation. A better understanding of the interplay between of the degree of twisting and the ISC efficiency is presented in this contribution for two BODIPY derivatives of different sizes: Benzo[b]-fused BODIPY (BDP-B) and [a]Phenanthrene-fused BODIPY (BDP-P). For the two systems, we calculated the photophysical properties using post-HF methods as the cyanine-like BODIPY undergo strong differential electronic correlation effects. Counter-intuitively (with respect to the previous works related to the relationships between twisting in  $\pi$ -conjugated derivatives and ISC efficiency) we report here that the least twisted molecule shows both higher ISC efficiency and the weakest fluorescence. This behavior is well rationalized by theoretical calculations that also demonstrate the first non-Kasha behavior in a BODIPY derivative.

**Mots-Clés:** ISC, BODIPY, Fluorescence, theoretical

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# PLANAR ORGANIC SOLAR CELLS BASED ALUMINIUM PHTHALOCYANINE CHLORIDE AS ACCEPTOR

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Phthalocyanines (Pcs) and their hybrid derivatives are thermally and chemically stable. They present an intense absorption in the red/near-infrared (NIR) region of the solar spectrum, which make them excellent candidates in many fields of applications; in catalysis, photodynamic therapy (PDT) and especially in the different generations of photovoltaic solar cells; in dye sensitized solar cells, in perovskite cells as hole transporting material (HTM), and in planar and bulk heterojunction solar cells as donor material [1].

Herein, we investigate for the first time the use of Aluminum Phthalocyanine Chloride (AlPcCl) as acceptor material in a planar heterojunction:  $\alpha$ -sexithiophene ( $\alpha$ -6T) /AlPcCl instead of fullerene and we have demonstrated that the use of AlPcCl as acceptor increases the PCE by about 16% in comparison with the heterojunction-based Fullerene as acceptor  $\alpha$ -6T/C60. The figure on the right represents the J-V characteristics of the both heterojunctions.

**Mots-Clés:** Planar organic solar cells, Alpha, sexithiophene, AlPcCl, Fullerene

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\*Intervenant

# Proximity effect in parallelized microfabrication using two-photon polymerization

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Two-photon polymerization (2PP) is a photochemical process usually initiated by tightly focusing an ultrafast laser pulse into a volume of photosensitive photoresists with a high-numerical-aperture objective. Scanning a write "voxel" in 3D enables near free-form fabrication, but at a limited speed for industrial purposes. Several strategies have been implemented to improve the fabrication speed, one such strategy is massive parallelization which is the approach used in our PHENomenon H2020 European project. Massive parallelization can be realized by beam-splitting diffractive optical elements.

In our project, we report on a major unexpected obstacle encountered in massively parallelized fabrication. Using several spots simultaneously to polymerize, local changes in the 2PP threshold have been observed. We linked this to the presence of other light spots in the neighborhood of a studied light spot (spatial proximity effects) and/or to any previous exposure of the resist (whether producing polymerization or not) by spots scanned across the same plot area previously (temporal proximity effects).

Several experiments are performed to understand and quantify the effect: 1) calibration DOEs with the same number of spots but differing separation 2) comparison of the proximity effects obtained with commercial and project-developed resins 3) Influence of the Objective Numerical Aperture.

Through computational modeling, we show that these effects can be fully modeled and interpreted by simply taking into account PSF overlap and radical diffusion processes, partially quantifying the range of the effect under specific conditions.

This study aims to use simulation to predict the behavior of parallel fabrication to avoid the proximity effect. Promising experimental solutions are adding quencher molecules to the resists, using thinner photoresist layers to increase oxygen penetration, or use a minimum inter-spot distance.

**Mots-Clés:** Two, photon polymerization, diffractive optical element, massively parallel fabrication,

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\*Intervenant

photoresist, proximity effect, simulation.

# Pump-probe experiments and solid-state materials : validation of a high field THz-TDS set-up

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TeraHertz (THz) radiations ( $10^{12}$  Hz) were first obtained using large scale facilities but the breakthrough came from the ability to develop table-top setups generating intense THz pulses. In the middle of the 1980's, the emergence of the THz-Time Domain Spectroscopy [1] has filled a spectral gap and permitted the measurement of spectra in a region complementary to the far-IR classical spectra. Contrary to the common transmission measurements, this technique can directly measure the electric field as a function of time, allowing time-resolved and phase-sensitive experiments. It is already widely used for detection of drugs and explosive devices. In solid-state physics, intense THz pulses are of particular interest for several reasons. First, their energies correspond to the typical energies of optical phonon modes or other structural motions. Also, their important amplitudes might be crucial for inducing phase transitions and control some physical properties. We can therefore use intense THz pulses to trigger phenomena and monitor optical properties as a function of time.

In the Institute of Physics of Rennes, we are developing a pump-probe THz-optical set-up with femtosecond resolution and temperature control. In this poster, I present the high field THz-TDS part of the set-up, that uses optical rectification in LiNbO<sub>3</sub> [2] to generate intense THz pulses, and electro-optical detection. The set-up capabilities are highlighted through the discussion of test experiments [3]. In particular, I will show how the study of birefringent systems induces peculiar time (and frequency) domain profiles as a function of polarization. The ability of performing THz-TDS in the non-linear regime is also discussed [4].

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**Mots-Clés:** TeraHertz, Time Domain Spectroscopy

# Single-crystal to single-crystal transition of Single-Chain Magnet

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The Digital Revolution is a part of our daily life for a few decades now, with the democratisation of the computers, Internet, cell phones and other connected devices. Adding to this, the upcoming rise of cloud computing, streaming and artificial intelligence will lead to an exponential growth of data consumption (and *de facto* its storage). To tackle this issue, a net increase of the areal density of hard drive disks will be needed, by miniaturizing the size of its elementary storage units.

With this aim in mind, physicists and coordination chemists have designed jointly promising molecular magnets, able to store information by addressing its spin orientation ( $\uparrow = 1$  and  $\downarrow = 0$  for example) at the nanoscale level, and working up to the liquid nitrogen temperature. However, these 0D molecular magnets, called Single-Molecule Magnets (SMMs), are subject to parasitic demagnetization effects (such as quantum tunnelling, Raman, *etc*), which is not the case for infinite Single-Chain Magnets (SCMs) because of their inherent infinite 1D topology. Taking this into consideration, we have synthesised two new SCMs based on a strongly anisotropic magnetic centre, the Tb(hfac)<sub>3</sub>, and a bridging nitronyl nitroxide (NIT) radical, the NITPhO-Hexyl. By monitoring the crystallization conditions, we have shown that we can selectively obtain either a chiral helical chain or a finite hexanuclear complex depending on the presence of atmospheric water or not. Surprisingly, if a magnetic SCM behavior was expected for the chain, the finite hexanuclear complex share similar properties, usually observed only for infinite molecules.

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\*Intervenant

**Mots-Clés:** Coordination chemistry, Molecular magnetism, chirality, magnets, lanthanides, radicals

# Spatial organization of magnetic nanoparticles induced by optical stimuli

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The search for high-density storage materials prompted a considerable number of studies involving nanoparticles and nanostructured materials. Remote and reversible optical activation opens new perspectives in terms of speed and easiness of implementation. Furthermore, many parameters of light such as intensity, polarization and energy can be controlled. [1] In this work, the possibility to organize magnetic nanoparticles is reported, thanks to the photoinduced displacement of photochromic matrices and the application of a magnetic field.

The first step involves the synthesis of photochromic azo molecules with bulky groups to facilitate solid-state photochromism. [2] Superparamagnetic magnetite nanoparticles with a diameter of 20 nm are synthesized. Superparamagnetism shows advantages thanks to the absence of magnetization at ambient temperature, thus limiting aggregation.

The organization of nanoparticles is based on a method of holographic inscription on thin molecular films made exclusively of azo molecules. Under structured light irradiation, the photochromic molecules undergo an intensive matter transport caused by continuous E-Z photoisomerization reaction. Surface relief gratings are then formed in a reversible manner and with controlled height.

The superparamagnetic nanoparticles, embedded in the azo matrix, are dragged by the bulk migration of the photochromic thin films and accumulate in the azo patterns. Exposure to a magnetic field during photoillumination brings an additional driving force to the nanoparticles and helps to maintain them in place during optical erasure. Magnetic patterning can be promoted from such an organization. References:

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\*Intervenant

**Mots-Clés:** Photochromisme, magnétisme, azo, nanoparticules, inscription holographique

# Stereoselectivity control in intramolecular carbolithiation of alkynes.

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The carbolithiation reaction consists of the addition of an organolithium reagent to a carbon-carbon double or triple bond. Its synthetic power lies in its ability to simultaneously create a new carbon-carbon and carbon-lithium bond. The newly generated organolithium species can then be reacted with various electrophiles to yield highly functionalized compounds. This reaction has proved particularly useful for the synthesis of five-membered carbo- and heterocyclic ring systems. Herein is reported our investigation towards the stereoselective intramolecular 5-exo-dig carbolithiation of alkynes. It is shown that the substituent at the propargylic position exerts a profound effect on the configuration of the double bond in the final product. In addition, our preliminary results on enantioselective desymmetrizing carbolithiation of bis-alkynylated compounds are presented.

**Mots-Clés:** alkynes, carbolithiation, organolithium, stereoselectivity

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\*Intervenant

# Synthesis and characterization of chiral and chromophores based DTEs for the optical control of luminescence properties

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Luminescent molecules are present in a variety of domains, such as biology (bio-imaging), optoelectronics (data processing, molecular storage) or electroluminescent devices that are now part of our daily lives (OLED screens). In this highly competitive field, our approach aims to bring two additional dimensions. The first one is to control the luminescence by an external stimulus, here, light. Indeed, our research group has an expertise in the synthesis and study of the optical properties of photochromic luminescent molecules. [1] The second dimension is to introduce chirality in these photochromic units in order to access light-switchable circularly polarized luminescence. [2] This will pave the way for particularly promising multifunctional optical systems.

The introduction of chirality in dithienylethenes via atropoisomerism strategy was reached by blocking the interconversion between the two antiparallel forms and opens an opportunity for studying their chiroptical properties after separation of enantiomers. [3] The introduction of a chromophore allowed the photocontrol of the circularly polarized luminescence property.

**Figure 1:** Design of the chiral DTEs

**Figure 2:** blocked interconversion by atropoisomerism

The design strategy and the synthetic pathways, along with the optical properties of the synthesized molecules will be presented. The results of the following of the photochromism by <sup>1</sup>H and <sup>19</sup>F NMR and UV-Visible absorption will be discussed. The dynamic of the system was also studied via variable temperature experiments.

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\*Intervenant

**Mots-Clés:** dithienylethenes, chirality, atropisomerism, photochromism, luminescence



# Synthesis of new chromophoric ligands for the elaboration of photo/redox active Metal-Organic Frameworks

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Over the past three decades, Metal Organic Frameworks (MOFs) have triggered increasing attention and extensive researches **(1)**. This interest is justified by the immense variability of structures and properties, coming from the combination of both organic and inorganic chemistries, as well as by the inherent potential porosity of this type of material. More recently, the possibility to incorporate chromophores and/or molecular catalysts in the structure, as ligands or guests, appeared as a way to access appealing applications like photo(electro)catalysis, artificial photosynthesis, organic solar cells, photoswitches, electrochromism **(2)**... Moreover, accessing such applications is eased by the fact that MOFs can be immobilized on surface, either as polycrystalline thin films, or as SURMOFs **(3)** (SURface-anchored MOFs).

Currently, the elaboration of MOFs is more and more understood and controlled, therefore the incorporation of complex dye-derived ligands become more accessible. In this context, it is necessary to push out the limits of the efficiency of MOFs by introducing new ligands in this research field.

In this poster, we are reporting the synthesis of new sophisticated arylene diimide ligands, as well as their use for the elaboration of various photo/redox active MOFs. The focus will be on the n-type electrochromic properties of such porous hybrid material.

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**Mots-Clés:** MOF, electrochromism, photo, activity, redox, activity, functionalized electrode, chromaticity

# TAPIOCA STARCH GELATINIZATION PROPERTIES MONITORED BY TD-NMR AND COMPLEMENTARY CLASSICAL TECHNIQUES

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Low amylose starches or starches from roots like cassava show dramatically different gelatinization behaviour when compared to wheat starch. The investigation of these starches’ hydrothermal properties and their characteristics is crucial due to their broad application in food industry and, more specifically cereal industry.

TD-NMR is the unique technique allowing investigation in a quantitative way and in real time of the gelatinization sub mechanisms of starch, such as amylose leaching, starch water absorption, and crystal melting. To our knowledge, this is the first NMR report on tapioca starch upon heating which elucidates these subtle gelatinization sub mechanisms. The evolution of solid-phase components, which are attributed to non-exchangeable protons rising from amylopectin and amylose put evidence on the loss of crystallinity and organization of starch as a result of solubilizing (before 60°C) and releasing the solid material and starch granule disintegration due to gelatinization (after 60°C). The evolution of the liquid phase components, which are attributed to intra and extra granular water, respectively, put evidence on the granule water absorption and amylose leaching to the extra granular phase before 60°C and the gelatinization phenomenon after 60°C by adjunction of the extra granular and intra granular proton pools.

In contrary to the solid phase results, which were entirely consistent with results obtained on wheat starch, the evolution of the liquid phase components of tapioca starch did not follow the same trend as for wheat starch, which is consistent with different gelatinization properties of tapioca starch measured in parallel (RVA, DSC). Hence, new assumptions and attributions are proposed for tapioca regarding its higher swelling capacity and cohesiveness.

**Mots-Clés:** Tapioca, starch, NMR, RVA

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# The Cis $\rightarrow$ Trans Photoisomerisation of Azobenzene: a Fresh Theoretical Look

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The *cis*  $\rightarrow$  *trans* photo-isomerisation mechanism of azobenzene, after excitation to the  $n\pi^*$  and  $\pi\pi^*$  states, is revisited using high-level *ab initio* surface hopping mixed quantum-classical dynamics in combination with multi-reference CASSCF electronic structure calculations. A reduction of photoisomerisation quantum yield of 0.10 on exciting to the higher energy  $\pi\pi^*$  state compared to the lower energy  $n\pi^*$  state is obtained, in close agreement with the most recent experimental values(1) which re-examined previous literature values which showed larger changes in quantum yield. By direct comparison of both excitations, we have found that the explanation for the decrease in quantum yield is not the same as for the reduction observed in the *trans*  $\rightarrow$  *cis* photoisomerisation. In contrast to the *trans*  $\rightarrow$  *cis* scenario,  $S1 \rightarrow S0$  decay does not occur at ‘earlier’ C–N=N–C angles along the central torsional coordinate after  $\pi\pi^*$  excitation, as in the *cis*  $\rightarrow$  *trans* case the rotation about this coordinate occurs too rapidly. The wavelength dependency of the quantum yield is instead found to be due to a potential well on the  $S2$  surface, from which either *cis* or *trans*-azobenzene can be formed. While this well is accessible after both excitations, it is more easily accessed after  $\pi\pi^*$  excitation - an additional 15-17% of photochromes, which under  $n\pi^*$  excitation would have exclusively formed *trans*-azobenzene, are trapped in this well after  $\pi\pi^*$  excitation. The probability of forming *cis*-azobenzene when leaving this well is also higher after  $\pi\pi^*$  excitation, increasing from 9% to 35%. The combination of these two factors results in the reduction of 0.10 of the quantum yield of photoisomerisation on  $\pi\pi^*$  excitation of *cis*-azobenzene, compared to  $n\pi^*$  excitation.

## References:

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**Mots-Clés:** Photochemistry, Azobenzene, Photochromes, Ab initio, Surface Hopping Dynamics

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\*Intervenant

# Émulsions de bitume stabilisées par des composés biosourcés

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L’industrie de la construction et de l’entretien des routes doit prendre en compte la nécessité de réduire l’impact environnemental tout en préservant les propriétés des matériaux de construction. Dans ce contexte, le procédé de fabrication d’enrobés à basse température, qui consiste à utiliser des émulsions de bitume pour enrober les granulats, est une solution alternative pertinente aux procédés traditionnels lors desquels le bitume et les granulats sont chauffés à haute température. En effet, ce procédé réduit la consommation d’énergie, la production de gaz et les effets sur la santé des travailleurs.

L’émulsion de bitume est constituée de gouttelettes de bitume dispersées dans une phase aqueuse contenant un tensioactif pétrochimique amphiphile. Le tensioactif permet de stabiliser la dispersion des gouttelettes et d’améliorer l’enrobage des granulats par le bitume après rupture de l’émulsion. Afin de diminuer la dépendance de l’industrie routière aux émulsifiants pétrochimiques et de limiter leur impact environnemental, le projet vise à développer des émulsions de bitume stabilisées par des matériaux biosourcés, plus respectueux de l’environnement, comme alternative à ces tensioactifs, pour répondre aux futures exigences techniques/sanitaires.

Pour ce faire, les ressources biosourcées appropriées et les procédés adéquats capables d’émulsifier le bitume et de stabiliser la dispersion huile-dans-eau doivent être identifiés. Des composés aux propriétés chimiques différentes ont été testés et l’influence de la ressource sur les caractéristiques et la stabilité des émulsions a été étudiée. En outre, une étude de faisabilité a été réalisée sur les mélanges incorporant l’émulsion et les granulats afin de mesurer leurs performances de base.

**Mots-Clés:** Emulsion, bitume, matériaux bio, sourcés, performances des mélanges

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# **JED 3M – LE MANS 2021 – EDITION VIRTUELLE**

**Merci à toutes et tous pour votre participation !**

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