

# Welcome to the Scientific Days of the Doctoral School “Sciences Fondamentales”

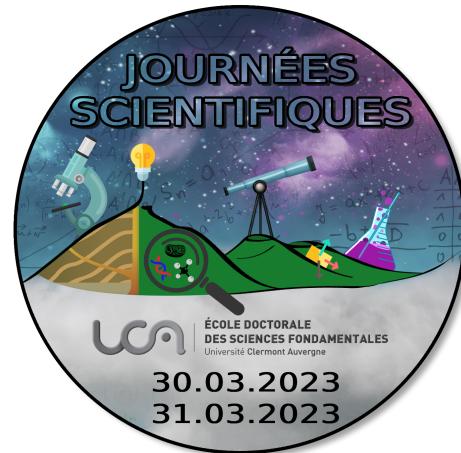
Thursday 30<sup>th</sup> and Friday 31<sup>th</sup> of Mars 2023  
Amphithéâtre de recherche, pôle Physique (Bat. EUPI)



Organization team:

- Adrien Gautier (*LMV*)
- Victoria Rafflin (*LMV*)
- Clément Bazantay (*LaMP*)
- Gaëtan Raymond (*LPC*)
- Océane Perrin (*LPC*)

Thanks to Maxime Pypiec for the logo...



With the contribution of :



## Thursday, 30<sup>th</sup> of Mars 2023

9h00 - 9h30	<b>Reception and opening speech</b>
9h30 - 9h50	<b>Design of nanostructured layered double hydroxides using sacrificial metal-organic framework materials to form efficient catalytic degradation of Bisphenol A</b> Mengwei LI- ICCF - page 3
9h55 - 10h15	<b>Use of radioactive isotopes as a tracer and timer of pre-eruptive processes beneath Hekla volcano, Iceland</b> Garance HERVE - LMV - page 4
10h20 - 10h40	<b>Classifier les plus grands relevés astronomiques avec Fink</b> Etienne RUSSEIL - LPC - page 5
10h40 - 11h00	<b>Session Posters 1:</b> Eléonore POUGET (IMoST - page 21) - Tara BUZDON (ICCF - page 22) Pavel KOKHANCHIK (IP - page 23) - Giuseppe ARBIA (ICCF - page 24)
11h00 - 11h30	<b>Coffee break</b>
11h30 - 11h50	<b>Large impacts and their contribution on the volatile budget of the early Moon</b> Tristan ENGELS - LMV - page 6
11h55 - 12h15	<b>Topological synthetic Andreev bands in a polaritonic analog of multi-terminal Josephson junctions</b> Ismaël SEPTEMBRE - IP - page 7
12h20 - 12h40	<b>Incorporation de luminophores dans des pièces d'acier inoxydable 316L par fabrication additive</b> Christina BASLARI - ICCF - page 8
12h40 - 14h00	<b>Lunch break</b>
14h00 - 14h20	<b>Assess real time interaction of disease causing protein with DNA by Total Internal Reflection Fluorescence microscopy (TIRF)</b> Martial MARTUCCI - LPC - page 9
14h25 - 14h45	<b>La réversibilité des graphites fluorés en batterie au lithium</b> Marie COLIN - ICCF - page 10
14h45 - 15h15	<b>Intervention 1 : Clermont Auvergne Innovation, PEPITE and Doct'Auvergne</b>
15h15 - 15h40	<b>Session Posters 2:</b> Mariana FARHAT (LaMP - page 25) - Leslie NUNEZ (ICCF - page 26) - Freddy VASCONEZ (LMV - page 27) Marion LEROUX (ICCF - page 28) - Yagizalp OKUR (LMBP - page 29)
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16h20 - 16h40	<b>Toward a better understanding of peroxymonosulfate and peroxydisulfate activation using a nano zero-valent iron catalyst supported on graphitized carbon</b> Minjuan CAI - ICCF - page 11
16h45 - 17h05	<b>Disséquer un volcan : le système magmatique de l'île de Petite Terre (Mayotte, Océan Indien occidental)</b> Tristan LACOMBE - LMV - page 12
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## Friday, 31<sup>th</sup> of Mars 2023

9h00 - 9h20	<b>Nanofils III-Arséniures épitaxiés par procédé HVPE et appliqués aux dispositifs pour l'infrarouge et le bêtavoltaïque</b> Emmanuel CHEREAU - IP - page 13
9h25 - 9h45	<b>Thermochemical Heterogeneities at the top of the lower mantle</b> Siddarth KHAN - LMV - page 14
9h50 - 10h10	<b>Matériaux lamellaires hybrides organique-inorganique pour dispositifs avancés de l'énergie</b> Julien SARMET - ICCF - page 15
10h10 - 10h40	<b>Session Posters 1:</b> Lucie ARNAUD (IMoST - page 31) - Laurence NIQUET (LaMP - page 32) Clara THORAL (ICCF - page 33) - Nafise ELAHOOUR (LPC - page 34) Nicolas SUCHET (ICCF - page 35) - Léo HAHN (LMBP - page 36)
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11h20 - 11h40	<b>Etude de la violation CP dans les désintégrations B- en D0h- avec D0 en K0spi+pi-pi0 à LHCb</b> Jessy DANIEL - LPC - page 16
11h45 - 12h05	<b>Soil CO<sub>2</sub> degassing, thermal flux and self potential at la Soufrière de Guadeloupe: evidence for changing patterns of fluid motion within the dome</b> Amélie KLEIN - LMV - page 17
12h10 - 12h30	<b>Study of new fructose-6-phosphate aldolases from extremophilic organisms</b> Léo PAULAT - ICCF - page 18
12h30 - 14h00	<b>Lunch break</b>
14h00 - 14h20	<b>Evaluation of new 68Ga-Complexes in osteoarthritis pet imaging</b> Florent MAGOT - IMoST - page 19
14h25 - 14h45	<b>Viscosity of crystal-free silicate melts from the active submarine volcanic chain of Mayotte</b> Pauline VERDURME - LMV - page 20
14h45 - 15h40	<b>Intervention 2 : Albin association, Jeunes Chercheurs Associés and UCA/CNRS:Management and setting up of scientific projects</b>
15h40 - 16h00	<b>Session Posters 4:</b> Lucas PAILLER (LaMP - page 37) - Giovanni CHERCHI (ICCF - page 38) Hiba BEJI (IP - page 39) - Sébastien DE WINDT (ICCF - page 40)
16h00 - 16h45	<b>Coffee break</b>
16h45 - 17h30	<b>MT 180 - Closing speech and prizes giving</b>

20h00	<b>A Drink in The Still Irish Bar</b> 7 Bd Léon Malfreyt, 63000 Clermont-Ferrand
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# Design of nanostructured layered double hydroxides using sacrificial metal-organic framework materials to form efficient catalytic degradation of Bisphenol A

Mengwei LI

Minjuan Cai<sup>1,2</sup>, M. Brigante<sup>1</sup>, G. Maillhot<sup>1</sup>, Vanessa Prévot<sup>1</sup>, Claude Forano<sup>1</sup>

Institut de Chimie de Clermont-Ferrand

The interest of Layered Double Hydroxides (LDH) for environmental remediation applications has been reported since more than twenty years and is nowadays well established. Adsorption and ion exchange properties of LDH or modified LDH (hybrids, nanocomposites, calcined LDH) allow to efficiently remove a large range of pollutants such as pesticides, phytosanitary molecules, drugs, heavy metals from contaminated waters or wastewaters. In addition to adsorption, transition metal containing LDH may display catalytic and photocatalytic performances for pollutant degradation. Based on both synergistic behaviors, they constitute promising materials for the development of novel advanced oxidation processes. Optimization of degradation performances has been focused not only on chemical composition but also on the tuning of LDH particle size and aggregation morphology. Thanks to the recent advances in synthesis methods, 3D hierarchical and porous LDHs can be prepared. Conversion of 3D sacrificial templates based on organic or hybrid structures into LDHs is a soft strategy that preserves the original architecture and leads the formation of nano-structured mesoporous LDH macrostructures. MOFs are transition metal-based hybrid nano and macrostructures that display various topology and morphology, with enhanced surface properties and reactivates. Conversion of MOFs into LDHs offers a very new and interesting strategy route for the preparation of LDH with novel architectures suitable for simultaneous adsorption/oxidation of organic pollutants.

In this study, we optimized and compared the preparation of a Fe-based MOF (MIL-88A) by hydrothermal-assisted and microwave-assisted precipitation in order to tune the size and shape of particles. In a second step, under a screening of microwave conditions, the MIL-88A was rapidly and efficiently converted into Ni-Fe LDH with the maintain of the original 3D architecture by simultaneous local etching and co-precipitation reactions in mixed solutions. Changes in structure and morphology were monitored by X-ray diffraction, Raman and FTIR spectroscopy, electron microscopy (SEM, TEM), DLS and N<sub>2</sub> physisorption. LDH synthesized using conventional co-precipitation methods was used for comparison. This new LDH was further modified by calcination at 200°C, 300°C and 400°C to increase its specific surface area and reactivity. Finally, the as-prepared and calcined Ni-Fe LDH were used to catalyze persulfate at 20 °C, for the degradation of Bisphenol A and other less conventional pollutants found in wastewaters. The results showed some LDH exhibited superior catalytic ability accomplishing more than 80% degradation efficiency of BPA in 10 min. The recycling experiments showed that the catalysts have recyclable properties, which matches with the green chemistry concept.

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# Use of radioactive isotopes as a tracer and timer of pre-eruptive processes beneath Hekla volcano, Iceland.

Garance HERVE

Laboratoire Magma et Volcans

Time is an important parameter when studying the volcanology field. Volcanic processes (e.g. the injection of magma into a magma chamber or the gas accumulation in a plumbing system) take place on a variable time scales, and these can sometimes lead to eruptions. Therefore, constraining this parameter could be key to understanding these processes and post facto, predicting future eruptive events. Several techniques have been developed to examine their associated time scales; one will be present and apply to a volcano located in Iceland: Hekla.

Hekla is characterised by recent eruptive activity with five new eruptions in the last century, each spaced 10-20 years apart (the last one being in 2000). A new study developed the idea that the recurrence of these eruptions is due to the accumulation of gases at the top of the magma chamber.<sup>[1]</sup>Called the auto-cycle model, it gives a new schematic behind the forces driving an eruption. It is commonly considered that the rise of magma at the surface is forced by the injection of new magma coming into a plumbing system.

The main objective of the study is to refute or confirm this physical model by showing whether there is a real gas accumulation at the top of Hekla's magma chamber, how long does this process take and what are the implications on the eruptive intensity of these events?

To this end, we have used some of the short half-life radioactive isotopes of the <sup>238</sup>U series and exploited their possible radioactive disequilibrium in the first products of the last five Hekla eruptions. Radioactive isotopes are used as a timer to quantify the temporality of some processes. In this case, as we wanted to track the gases' behaviour, we focused on <sup>222</sup>Rn, a member of this radioactive series that has a high affinity for the gas phase. However, during an eruption, the gases present in the plumbing system escape, so <sup>222</sup>Rn cannot be measured directly. We have therefore analysed it indirectly by measuring the activity of <sup>226</sup>Ra (parent isotope) and <sup>210</sup>Pb (daughter isotope) by gamma and alpha spectrometry.

We will discuss all these principles, nuclear techniques, and their limits to finally find out whether the preliminary results are relevant to the auto cyclic model confirming or not, a gas accumulation at the top of the Hekla's magma chamber.

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## Classifier les plus grands relevés astronomiques avec Fink

Etienne RUSSEIL

Laboratoire de Physique de Clermont

L'Observatoire Vera-C.-Rubin est l'un des futurs plus grands télescopes au monde et débutera son activité en 2024. Il fonctionnera automatiquement à la recherche de phénomènes transitoires, et photographiera ainsi l'ensemble du ciel austral tous les trois jours pendant 10 ans. On estime que chaque nuit le LSST devrait détecter 10 millions de ces phénomènes, ce qui représente 20 téraoctets de données brutes. Face à de tels volumes, il est impossible pour les astronomes d'analyser manuellement l'ensemble des observations, et il est nécessaire de recourir à des méthodes d'apprentissage machine.

C'est dans ce contexte que l'infrastructure Fink est créée. Ce broker a pour objectifs de nettoyer, traiter, analyser et classifier les données en temps réel avant de les redistribuer aux communautés scientifiques concernées par les découvertes. Il est composé de modules scientifiques de machine learning, individuellement conçus pour répondre à des questions scientifiques précises.

Dans cette présentation/poster je présenterais le contexte général, le télescope, l'infrastructure Fink ainsi que les modules scientifiques de classification de galaxies actives et de supernova par production de paires que j'ai implémenté depuis le début de ma thèse.

# Large impacts and their contribution on the volatile budget of the early Moon

Tristan ENGELS

Laboratoire Magma et Volcans

The Earth/Moon system likely results from a giant impact between a Mars-size object and the proto-Earth 70 to 100 Myrs after the formation of the first solids of the Solar System. This high-energy context leads to extreme conditions under which volatile elements would not normally be preserved in the protolunar disk. However, recent measurements of lunar samples highlight the presence of a significant amount of water in the Moon's interior (1.2 to 74 ppm). The aim of the present work is to quantify the water contribution of the late accretion on the early Moon. Here, we use a 2D axisymmetric model with the hydrocode iSALE-Dellen to study the fate of a large impactor on a target body similar to the early Moon with a crust, a magma ocean, and a mantle. For this purpose, we compute different models to monitor the depth to which the impacted material is buried at the end of the impact event and the degree of devolatilisation of the impactor. Three parameters are explored: the crustal thickness (ranging from 12 to 100 km), the impactor radius (ranging from 25 to 400 km) and the impactor velocity (ranging from 0.5 to 10 km s<sup>-1</sup>). Our models show that impactors with a radius greater than 50 km impacting a partially molten lunar body with a crust thinner than 40 km could significantly contribute to the water content of the lunar mantle even for impact velocities of less than 5 km s<sup>-1</sup>. For larger impact velocities ( $\geq 10$  km s<sup>-1</sup>) the impactor material is significantly molten and its water content is devolatilised within the lunar atmosphere. Depending on the water content of the impactor material and the ability of the lunar magma ocean to maintain chemical heterogeneities, the late lunar accretion following the Moon-forming giant impact could explain the differences in water content between the lunar samples.

# Topological synthetic Andreev bands in a polaritonic analog of multi-terminal Josephson junctions

Ismaël SEPTEMBRE

Institut Pascal

A driven-dissipative nonlinear photonic system (e.g. exciton-polaritons) can operate in a gapped superfluid regime. In this talk, I will show theoretically that the reflection of a linear wave on this superfluid is an analogue of the Andreev reflection of an electron on a superconductor<sup>[1,2]</sup>. A normal region (empty of superfluid) surrounded by two superfluids is found to host Andreev-like bound states. These bound states form topological synthetic bands versus the phase difference between the two superfluids. When bands of different nature (signal-like and idler-like) are approaching the one to the other, they interact through an anti-hermitian coupling giving rise to exceptional points and Fermi arcs<sup>[1]</sup>. On the other hand, when bands of same nature are approaching, they can cross giving rise to Hermitian topological singularities. In particular, I will show the case of the p-like bands of a 5-terminal junction in the 4D parameter space created by the superfluid phases acting as quasi-momenta<sup>[3]</sup>. We find 4/6 Weyl points in 3D subspaces with preserved/broken time-reversal symmetry. We link the real space topology (vortices) to the parameter space one (Weyl points). We derive an effective Hamiltonian encoding the creation, motion, and annihilation of Weyl nodes in 4D. These effects were predicted in electronic Josephson junctions giving great hopes to implement topological quantum computing without the need to use topological superconductors, but their experimental observation remained elusive. Our work paves the way to the study of exotic topological phases in a platform allowing direct measurement of eigenstates and band topology.

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# Incorporation de luminophores dans des pièces d'acier inoxydable 316L par fabrication additive

Christina BASLARI

Hicham Maskrot<sup>1</sup>, Wilfried Pacquentin<sup>2</sup>, Sonia de Sousa Nobre<sup>3</sup>, Daniel Zambon, Rachid Mahiou

Institut de Chimie de Clermont-Ferrand

Les pièces métalliques exposées en milieux corrosifs nécessitent beaucoup de maintenance préventive ce qui est chronophage et coûteux. Dans la plupart des cas, les composants sont remplacés avant leur fin de vie pour éviter tout risque de défaillance. Dans une approche d'économie circulaire, il serait pertinent de s'intéresser à l'allongement de la durée d'usage des composants métalliques et de proposer de nouvelles solutions pour l'écoconception des pièces et la gestion intelligente des maintenances. Pour cela une méthode de diagnostic est proposée afin d'assurer le suivi de la perte de matière liée à la corrosion et à l'usure. Cette solution consiste à incorporer dans les pièces métalliques par fabrication additive des poudres luminescentes aux propriétés optiques. Ainsi le suivi du signal luminescent déterminera l'avancement de la dégradation du matériau<sup>[1]</sup>. La fabrication additive est adaptée pour ce type d'applications car elle permet de combiner des matériaux de natures différentes sans interrompre le cycle de construction de la pièce. Dans cette étude, la technologie Laser Powder Bed Fusion (L-PBF) a été utilisée pour incorporer des luminophores dopés aux terres rares dans l'acier inoxydable 316L<sup>[2]</sup>. Les pigments luminescents ont été insérés avec succès et un signal luminescent a été détecté après fabrication par spectroscopie laser. Les interactions de la matrice métallique avec les particules luminescentes ainsi que les modifications structurales et physico-chimiques induites par le procédé L-PBF ont été étudiées. Par ailleurs l'analyse microstructurale et les propriétés du 316L aux inclusions luminescentes ont également été investiguées par microscopie optique, microscopie électronique à balayage, analyse EBSD et microdureté.

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- [2] Chowdhury, S.; Yadaiah, N.; Prakash, C.; Ramakrishna, S.; Dixit, S.; Gupta, L. R.; Buddhi, D. *Laser Powder Bed Fusion: A State-of-the-Art Review of the Technology, Materials, Properties & Defects, and Numerical Modelling*. *Journal of Materials Research and Technology* 2022, 20, 2109–2172

Presentation

## **Assess real time interaction of disease causing protein with DNA by Total Internal Reflection Fluorescence microscopy (TIRF)**

Martial MARTUCCI

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Mitochondria are the powerhouse of the cell. They contain their own DNA (called mitochondrial DNA or mtDNA). This DNA is copied (replicated) by a set of a few factors (proteins), including the mitochondrial single stranded binding protein (mtSSB). Since 2018, several clinical reports have described that alterations (mutations) of mtSSB are associated with human disease. However, these reports lack mechanistic explanations. My project focus on understanding the molecular basis for the pathogenicity of one of these mutations (R107Q).

For this, I have studied real-time interactions of mtSSB with DNA using a single molecule approach involving Total Internal Reflection Fluorescence microscopy (TIRFm). I measured compaction efficiency and rate, dissociation rate, and I performed competition binding assay between wild-type and mutant SSB. All together the results suggest that the mutation could affect the binding pattern and the compaction rate of the protein. These changes could affect the proper functioning of the protein and its ability to ensure mtDNA replication.

# La réversibilité des graphites fluorés en batterie au lithium

Marie COLIN

Katia GUERIN<sup>1</sup>, Killian HENRY<sup>2</sup>, Elodie PETIT<sup>1</sup>, Marc DUBOIS<sup>1</sup>

Institut de Chimie de Clermont-Ferrand

Après la récente interdiction de vente de véhicules thermiques neufs à partir de 2035 en Europe et les rapports du GIEC sur l'urgence de diminuer l'utilisation d'énergie fossile, le développement de systèmes de stockage de l'énergie électrique plus performants est alors nécessaire. Les batteries primaires (piles) au lithium à électrode positive de carbone fluoré ( $\text{Li}/\text{CF}_x$ ) délivrent une densité d'énergie deux fois supérieure aux batteries  $\text{Li}/\text{SOCl}_2$  ou  $\text{Li}/\text{MnO}_2$ <sup>1</sup>; 2180 Wh/kg sont attendus. Ces piles délivrent une capacité de 865 mAh/g pour une composition CF1, nettement supérieure aux capacités délivrées par les meilleures cathodes du marché. Par exemple, les oxydes de Nickel-Manganèse-Cobalt ont une capacité d'environ 200 mAh/g. De plus, les ressources en carbone sont illimitées contrairement au Cobalt et au Nickel. Tout problème environnemental ou éthique lié à l'extraction, comme pour le Cobalt, est aussi évité. Les piles  $\text{Li}/\text{CF}_x$  ont également une large gamme de température d'utilisation et une longue durée de vie. Ces systèmes sont utilisés dans le domaine médical pour des appareils implantables, ou bien dans les domaines militaire et spatial et ont été commercialisés pour la première fois en 1975 par Matsushita Electronic Co. (renommé Panasonic Corporation) au Japon.<sup>2</sup>

Lors de l'utilisation de la batterie, les liaisons C-F se rompent pour former du carbone et du fluorure de lithium LiF selon la réaction suivante :  $\text{CF}_x + \text{xLi} \rightarrow \text{C} + \text{xLiF}$ . Le composé LiF étant très stable ( $\Delta H_f^\circ = -616 \text{ kJ/mol}$ ), il empêche la réversibilité de la réaction, c'est-à-dire la reformation du  $\text{CF}_x$  nécessaire à une autre réduction électrochimique. Pour limiter la formation de LiF très stable et donc favoriser la réversibilité, les paramètres électrochimiques (électrolyte) et/ou le matériau  $\text{CF}_x$  peuvent être modulés. La réaction de fluoration est l'étape clé durant laquelle des liaisons se forment entre les atomes de fluor et de carbone (liaisons C-F). Selon les conditions opératoires (température, durée, quantité de fluor...) et le précurseur carboné, les liaisons établies sont plus ou moins fortes. La versatilité des liaisons C-F permet de moduler la tension de fonctionnement de la batterie selon l'application souhaitée. Plus les liaisons C-F sont fortes, plus la tension de la pile sera faible ; cette valeur peut ainsi varier entre 3,5 et 2,0 V vs  $\text{Li}^+/\text{Li}$ . Les conditions de fluoration permettent également de moduler la quantité de fluor présente dans le matériau. D'autres composants de la batterie peuvent aussi être ajustés, comme l'électrolyte, qui assure le passage des ions entre les deux électrodes.

Dans ces travaux, un graphite fluoré composé de liaisons C-F faibles est utilisé comme électrode positive avec un électrolyte polymère commercial et a démontré de la réversibilité sur de nombreux cycles. La réversibilité est expliquée par une analyse fine du LiF formé selon les étapes de réduction ou d'oxydation.

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# Toward a better understanding of peroxymonosulfate and peroxydisulfate activation using a nano zero-valent iron catalyst supported on graphitized carbon

Minjuan CAI

Peng Cheng<sup>2</sup>, Jinjun Li<sup>1\*</sup>, Feng Wu<sup>1</sup>, Mohamed Sarakha<sup>2</sup>, Gilles Mailhot<sup>2</sup>, Marcello Brigante<sup>2\*</sup>

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Degradation of estrogenic compounds has been achieved through heterogeneous activation of peroxymonosulfate (PMS) and peroxydisulfate (PS), a promising approach for environmental remediation. However, these processes usually require the use of an expensive or toxic catalyst. Here, nano zero-valent iron (nZVI) catalysts supported on graphitized carbon (GC) have been prepared characterized by appropriate techniques. A GC-nZVI catalyst with an Fe:C ratio of 0.07 was finally selected for the activation PMS/PS and tests on bisphenol A (BPA) degradation at circumneutral pH. Under optimal conditions (0.25 mM PMS/PS and 0.05 g L<sup>-1</sup> catalyst), 25 µM BPA was completely removed in 30 min, and around 80% was mineralized after 2 h. Chemical quenching experiments using selective probes and kinetic modelling have been used to determine the involvement of reactive species and quantify their steady-state concentrations in dark and under irradiation. Activation of PMS/PS by GC-nZVI is shown to produce sulfate radicals ( $\text{SO}_4^{\bullet-}$ ), hydroxyl radicals ( $\cdot\text{OH}$ ) and ferryl ions ( $\text{Fe}^{\text{IV}}\text{O}^{2+}$ ). GC-nZVI shows good stability in the recycling experiments and can be used over a wide pH range of 3.0–7.0 with almost no loss of degradation efficiency. This study has shown that highly efficient GC-nZVI /PS/UVA or GC-nZVI/PMS/UVA system has great potential for application in different water matrix, and our findings provide

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# Disséquer un volcan : le système magmatique de l'île de Petite Terre (Mayotte, Océan Indien occidental)

Tristan LACOMBE

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J.C. Komorowski<sup>3</sup>, P. Besson<sup>3</sup>, P. Verdurme<sup>1</sup>

Laboratoire Magma et Volcan

La découverte du nouveau volcan au large de Mayotte en 2019 a montré que le volcanisme sur cette zone, que l'on croyait éteint, était bien actif. L'île de Petite Terre, située dans le lagon de Mayotte, présente un exemple parfait de quatre volcans explosifs supposés être très jeunes (10 Ka) et recouvrant des volcans effusifs plus anciens. La position de Petite Terre, à cheval à la fois sur l'ancien bouclier, éteint, du volcan de Mayotte et sur la chaîne volcanique sous-marine se terminant par le volcan récemment actif pose la question de son affiliation à l'un ou l'autre système.

Nous présentons ici les caractéristiques pétrologique et géochimiques de ce système magmatique, en intégrant des données provenant d'échantillons de lave et pyroclastiques issus du volcanisme de Petite-Terre, afin d'étudier le lien entre les phonolites (explosives) de Petite Terre et les cônes de scories (effusifs). Les éléments majeurs et traces montrent que les cônes de scories et les phonolites de Petite Terre représentent deux séries magmatiques différentes, les cônes de scories appartenant au bouclier tandis que les phonolites peuvent être rattachées à la chaîne sous-marine.

La présence de morceaux de manteau dans les phonolites, ne montrant aucun signe de réaction, suggère que ces phonolites ont évolué dans le manteau (17 km/ 1015 °C). La présence de xénocristaux de biotite et d'amphibole riches en Fe montre que ces phonolites chaudes (954 °C) ont croisé le chemin d'une lentille de magma de composition similaire plus ou moins solidifiée (8 – 14 km, 785 °C). Ces phonolites ont également évolué dans des conditions très réductrices ( $\Delta\text{NNO} = -2,35$  unités log) ce qui expliquerait leur forte teneur en fer (jusqu'à 6 % en poids).

Ces résultats montrent que le volcanisme de l'île de Petite Terre, et probablement de la chaîne volcanique à l'est de Mayotte, se superpose à l'activité de l'ancien bouclier et se déroule dans un système très dynamique où les magmas évoluent à des profondeurs lithosphériques (> 20 km). Ils montrent également que les magmas dans la zone peuvent interagir avec des lentilles partiellement fondues stockées à un niveau plus faible près de la base de la croûte, les remobilisant potentiellement avec des implications pour les scénarios éruptifs.

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# Nanofils III-Arséniures épitaxiés par procédé HVPE et appliqués aux dispositifs pour l'infrarouge et le bêtavoltaïque

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Les téléphones, les ordinateurs ou tout autre objet électronique partagent le même point commun, ils sont constitués principalement d'un seul et même type de matériau : les semi-conducteurs. Ces semi-conducteurs ont en effet une propriété particulière qui est de conduire l'électricité dans certains cas mais pas dans d'autres, ce qui est essentiel pour contrôler un courant électrique. C'est dans ce contexte que s'inscrit mes recherches.

Le but de ma thèse est de synthétiser à l'échelle nanométrique, c'est-à-dire 1000 fois plus fin qu'un cheveu, des structures appelées nanofils semi-conducteurs. Pour fabriquer ces nanofils, il est nécessaire de se placer dans des conditions particulières de pression et de température. Dans notre laboratoire, nous disposons d'une méthode spécifique qui est l'épitaxie en phase vapeur par la méthode aux hydrures (HVPE).

Mes recherches portent sur deux matériaux semi-conducteurs : l'arséniure de gallium (GaAs) et l'arséniure d'indium (InAs), qui se destinent tous deux à des applications différentes. Le GaAs est un candidat idéal pour les générateurs bêtavoltaïques ou « batteries nucléaires », leur principe de fonctionnement est le même qu'un panneau solaire, mais au lieu d'utiliser l'énergie du soleil pour produire de l'électricité, on utilise l'énergie des déchets nucléaires. L'utilisation de nanofils de GaAs vise à fortement améliorer l'efficacité des générateurs conventionnels<sup>[1]</sup>.

L'InAs est un matériau à fort potentiel pour la future génération de détecteurs infrarouges. Il représente une alternative aux capteurs actuels à base de mercure-cadmium-tellure (MCT) qui sont toxiques et non recyclables. Ces détecteurs sont indispensables pour un très grand nombre d'applications telles que l'industrie, l'instrumentation scientifique, l'astronomie, la surveillance ou encore la télécommunication. De plus, les nanofils d'InAs ont le potentiel d'améliorer la résolution et la vitesse de l'imagerie infrarouge<sup>[2]</sup>.

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# Thermochemical Heterogeneities at the top of the lower mantle

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The high water storage capacity of minerals in Earth's mantle transition zone (410 – 660 km) implies the possibility of a water reservoir in deep Earth. This enables the possibility of melting, as water is carried to the lower mantle by the subducting-slabs. Water in a dry geologic system acts as an impurity, which reduces the solidus temperature below the geotherm, such that melting is initiated in natural conditions *vis à vis* dehydration melting.

Seismic discontinuities at the top of lower mantle (660 km) concurrent with perovskite phase transformation, has been attributed to partial melting in association with overlying H<sub>2</sub>O reservoir. More precisely, the contrasting 1-3 wt. % H<sub>2</sub>O storage capacity of major mineral phases, Wadsleyite- Ringwoodite and dry Bridgmanite gives us an impetus to analyze the activity of water and its effects on partial melting at a global scale in deep mantle. The high wetting character of hydrous silicate melt at such high pressure implies that small degree of melting can dramatically affect the propagation of seismic waves at high depth.

Our study aims to synthesize and quantify the equilibrium melt relations and effects of water in perovskite stability field in order to reconcile geochemical and geophysical observations of such low seismic velocity zones. We perform high-pressure laboratory experiments using the multi-anvil press with starting material of model pyrolite composition and pre-defined amounts of H<sub>2</sub>O in a closed system at conditions relevant to top of the lower mantle, in order to synthesize melt co-existing with the major phases in the lower mantle. The melt chemical composition is buffered iteratively in order to converge and quantify the eventual incipient equilibrium melt with the rest of the mantle to best replicate the natural process. The synthesized samples are mapped chemically in terms of major elements using Focused Ion Beam Scanning Electron Microscope (FIB-SEM) and quantified using Electron Probe Micro-Analyzer (EPMA).The coexisting solid phases are identified using Raman spectroscopy.

The chemical quantification of the primary melt in deep Earth, its chemical evolution and effects of variations in H<sub>2</sub>O content in the system will enable us to model these geochemical reservoirs and extrapolate physical parameters of melts like density, viscosity on theoretical fronts using established Equations of State to finally comment on the geodynamics and better understand the evolution of Earth as a whole.

# Matériaux lamellaires hybrides organique-inorganique pour dispositifs avancés de l'énergie

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Après des années de recherche consacrées à la préparation de la technologie post-lithium, il existe un besoin grandissant de trouver de nouveaux systèmes de stockage électrochimique, polyvalents, robustes et, plus particulièrement, de réguler les fluctuations de production et de consommation des équipements électriques. De tels systèmes doivent s'appuyer sur des matériaux à transfert de charge rapide, dont tous les composants doivent être optimisés. Pour cela les matériaux lamellaires de type hydroxydes sont une alternative intéressante déjà étudiée par le passé de par leur versatilité de composition. Cependant, un changement de paradigme par rapport à ce qui est étudié aujourd'hui dans les hydroxydes lamellaires est de se concentrer ici sur leur capacité à accueillir des espèces organiques électroactives comme cela a été fait pour la première fois avec l'anthraquinone-sulfonate (AQS), les dérivés de ferrocènes, pour une utilisation en tant que capteur mais jamais comme une source de stockage de l'énergie possible. Dans ce travail, publié récemment, nous nous concentrons sur l'électroactivité des dérivés de la flavine, notamment le phosphate de riboflavine dérivé de la vitamine B, catalysant un grand nombre de réactions redox.

Par conséquent, en sélectionnant deux espèces électroactives, l'une comme électrode positive et l'autre négative, il est possible de concevoir de nouveaux dispositifs de stockage d'énergie. Chaque matériau d'électrode est basé sur des espèces électroactives, le phosphate de riboflavine d'un côté et le carboxylate de ferrocène de l'autre, intercalées dans une structure hôte d'hydroxyde double lamellaire (HDL). Une fois les molécules intercalées avec succès, le comportement électrochimique de chaque assemblage hybride est examiné séparément dans un électrolyte aqueux pour caractériser les réactions d'oxydoréduction au cours du cyclage. Puis les deux matériaux d'électrodes sont placés dans un dispositif à trois électrodes pour former un nouveau supercondensateur asymétrique original.

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# Etude de la violation CP dans les désintégrations B- en D0h- avec D0 en K0spi+pi-pi0 à LHCb

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The observable Universe is mainly made up of matter, while almost all the antimatter disappeared in the very early times. One explanation is that the Universe obeys the Sakharov conditions, which mean the existence of a C (charge) and CP (charge - parity) symmetry violation. An area of Particle Physics deals with the comprehension and measurement of this symmetry breaking and the potential discovery of a Physics beyond the Standard Model (SM).

In particular, the  $\gamma$  angle of the Cabibbo-Kobayashi-Maskawa (CKM) matrix sets a benchmark for CP violation, to be compared with the SM predictions. The accumulated statistics by the LHCb detector allows expecting an even more precise measurement of the  $\gamma$  angle. Its accuracy is currently around  $4^\circ$ , nevertheless, a precision around  $1^\circ$  is desirable to test SM up to dozens of TeV.

The purpose of this study is to make a measure of this angle through the  $B^- \rightarrow D^0(\rightarrow KS\pi^+\pi^-\pi^0)$   $K^-$  decay, using LHCb data from Runs 1 and 2 (2011-2018), thanks to a generalized GGSZ method. This measurement, with a tree-diagram decay, can typically be used for the direct gamma measurement, setting a “standard candle” for the SM.

I will firstly quickly describe the SM of Particle Physics, insisting on C and CP symmetries. I will then rapidly describe LHCb Detector (and LHC accelerator complex). Then after introducing the CKM matrix and its  $\gamma$  angle, I will focus on the interest of such a measurement and its principle. If I have time, I will then present the analysis, in particular events selection, background study and nominal fit.

# **Soil CO<sub>2</sub> degassing, thermal flux and self potential at la Soufrière de Guadeloupe: evidence for changing patterns of fluid motion within the dome**

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Active arc volcanoes often hold a hydrothermal system that typically manifests itself as fumaroles, hot springs or boiling pools at the surface. Hydrothermal fluid motion within a volcanic edifice is sustained by a constant supply of heat and gas from a magma reservoir at depth interacting with shallow ground water. Circulation of acid hydrothermal fluids causes micro-seismicity and alteration of the host rock, potentially leading to mechanical weakening and/or gradual self-sealing of the edifice. This increases the likelihood of flank/edifice collapse or shallow overpressurisation that can result in violent eruptions. As recently demonstrated by the deadly events at Ontake volcano (Japan, 2014) or White Island (New Zealand, 2019), even purely steam-driven eruptions (without magma emission) can be very hazardous given their sudden onset. Therefore, monitoring the spatial distribution and temporal evolution of hydrothermal signals at volcanoes with long-lived hydrothermal activity is crucial to detect and interpret precursory signs of explosive activity.

Our study focuses on La Soufrière de Guadeloupe, one of the most active and dangerous volcanoes of the Lesser Antilles, that since its last phreatic eruption in 1976-77 is closely monitored. In recent years, it has been in a phase of accelerating unrest characterized by the formation of new fumaroles on the summit, increased seismicity, deformation, ground heating and soil degassing.

In May 2022 we performed mapping of soil CO<sub>2</sub> flux, ground temperature and self-potential (SP), a method measuring the natural electric ground potential used to constrain subsurface fluid flow. By comparing these maps to each other and to previously obtained data, we aim to trace the temporal changes in fluid motion within the dome. Time-series from a permanent SP array installed on the summit of La Soufrière in April 2022 will allow us to study how external factors like rainfall and internal forcing like seismicity affect the hydrothermal system.

So far, our data show a clear spatial shift in hydrothermal fluid circulation towards the NE sector of the summit, presumably as a result of increased ground permeability in that area. This is in line with observed progressive fracture opening, increasing fumarole temperature, progressing vegetation die-off and shallow condensation level as inferred from our temperature data. Higher permeability allows fluids to rise more easily to the surface (increased measured CO<sub>2</sub> flux, maximum SP anomaly) and promotes vapor condensation close to the surface. Due to the high latent heat of water vapor, this may cause the observed extensive ground heating.



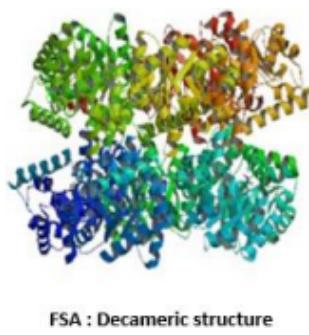
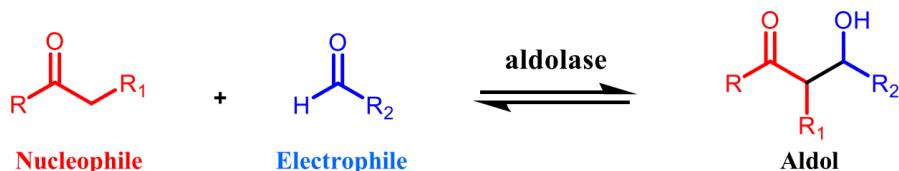
# Study of new fructose-6-phosphate aldolases from extremophilic organisms

Léo PAULAT

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Biocatalysis is a tool to access new products of interest in a greener and more eco-friendly way. It allows us to respond to many current issues related to the 12 principles of green chemistry. In this context, Aldolases are C-C bond forming enzymes of particular interest for synthetic applications. Indeed, the aldol reaction allows to generate up to 2 asymmetric centers, providing chiral adducts. Depending on the aldolases used, the stereochemistry of these asymmetric centers can be controlled<sup>[1]</sup>.



Fructose-6-phosphate aldolase (FSA) belonging to class I aldolases, was discovered in *E. coli* by Schürmann and Sprenger<sup>[2]</sup> in the 2000s. It was demonstrated as the first aldolase able to use hydroxyacetone<sup>[3]</sup>, as nucleophile substrate, and furthermore particularly robust, efficient and versatile towards other nucleophiles such as dihydroxyacetone, hydroxybutanone<sup>[4]</sup> and glycolaldehyde<sup>[5]</sup>. These discoveries were the basis for mutagenesis<sup>[1]</sup> work or for the search from biodiversity for new aldolases presenting for example different stereochemistries.

In the framework of our collaboration with the Génoscope (Evry), two FSA from acidophilic organisms are studied, one from, Acidobacteria Bacterium (A0A399XV01) and one from Acidiplasma Aeolicum (A0A0Q0RVA3). These catalysts have revealed atypical properties. Molecular modeling and their kinetic constants determination helped their characterization. These results will be presented here, as well as some synthetic applications.

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## Evaluation of new $^{68}\text{Ga}$ -Complexes in osteoarthritis pet imaging

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Osteoarthritis (OA) is a degenerative disease leading to progressive destruction of articular cartilage. It is the most common joint disease in France with approximately 10 million people affected. It is widely accepted that the impact of OA will continue to increase in developed countries due to the aging population and obesity epidemic, setting serious public health issues associated with an extremely high economic burden[1]. Today, there are only symptomatic treatments for the pain and stiffness caused by OA. Through better understanding of mechanisms of action, new therapeutic strategies have emerged. Among them, disease-modifying osteoarthritis drugs (DMOADs) have been developed with the aim of preventing, halting or reversing the progressive joint destruction in OA. Despite promising results, the emergence of an effective DMOAD in humans remains a failure. The reasons are partly due to the lack of a sufficiently accurate monitoring method to assess changes within the cartilage matrix. Developing molecular imaging by targeting a cartilage biomarker is considered to be the most sensitive and functional approach for assessing OA at earlier stages, and demonstrating DMOAD efficacy. To address this issue, UMR 1240 UCA-INSERM IMoST has already validated a promising radiotracer for single-photon emission computerized tomography (SPECT) functional imaging of joints in nuclear medicine<sup>[2]</sup>. This radiotracer designed as [ $^{99\text{m}}\text{Tc}$ ]Tc-NTP 15-5, is a bi-functional agent containing a polyazamacrocyclic for  $^{99\text{m}}\text{Tc}$  labelling and a quaternary ammonium function for its ability to bind to negative charges of cartilage proteoglycans. This molecule is currently in a "first into human" CARSPECT clinical trial<sup>[3]</sup>. In parallel our team have synthesized and evaluated new copper-64 ( $\beta^+$ emitter) labelled complexes allowing positron emission tomography (PET) imaging as cartilage radiomarkers<sup>[4]</sup>. In the continuity of these works and due to improved  $^{68}\text{Ga}$  radioisotope availability, we are currently working on new gallium complexes for cartilage PET imaging applications. A dozen complexes have so far been synthesized from two polyazamacrocycles (cyclen and pycyclen). We report their synthesis, radiolabelling methods and first in vivo evaluations.

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# Viscosity of crystal-free silicate melts from the active submarine volcanic chain of Mayotte

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Laboratoire Magma et Volcans

Following an unprecedented seismic activity that started in May 2018, a new volcanic edifice, Fani Maoré, was constructed on the ocean floor 50 km east of the island of Mayotte (Indian Ocean). This volcano is the latest addition to a submarine volcanic chain characterized by an alkaline basanite- to-phonolite magmatic differentiation trend. Here, we performed viscosity measurements on five silicate melts representative of the East-Mayotte Volcanic Chain compositional trend: two basanites from Fani Maoré, one tephri-phonolite and two phonolites from different parts of the volcanic chain. A concentric cylinder viscometer was employed at super-liquidus conditions between 1500 K and 1855 K, and a creep apparatus was used for measuring the viscosity of the undercooled melts close to the glass transition temperature in the air. At super-liquidus temperatures, basanites have the lowest viscosity (0.11 to 0.99 log10 Pa·s), phonolites the highest (1.75 to 3.10 log10 Pa·s), while the viscosity of the tephri-phonolite falls in between (0.89 - 1.97 log10 Pa·s). Viscosity measurements at undercooled temperatures have only been performed for one phonolite melt because Raman spectroscopy showed nanolites within the basanite and tephri-phonolite glass samples. The phonolite has a viscosity of 10.19 to 12.30 log10 Pa·s at 1058 to 986 K. Comparison with existing empirical models revealed discrepancies up to 2.0 log units with our experimental measurements. This emphasizes (i) the lack of data falling along the alkaline basanite-to-phonolite magmatic differentiation trend to calibrate empirical models, and (ii) the complexity of modeling the variations in viscosity as a function of temperature and chemical composition for alkaline magmas. The presented new measurements indicate that, at eruptive temperatures between 1050 °C and 1150 °C, the anhydrous, crystal- and bubble-free basanite melt is very fluid with a viscosity around 2.6 log10 Pa·s whereas the anhydrous phonolite crystal- and bubble- free melt at eruptive temperatures ranging from 800 to 1000 °C has a viscosity around 6 - 10 log10 Pa·s. These new viscosity measurements are essential to define eruptive models and to better understand the storage, transport and ascent dynamics of Comoros Archipelago magmas, and of alkaline magmas in general, from the source to the surface.

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# Comparaison de deux approches d'apprentissage supervisé dans la conception d'un observateur canalisé pour l'évaluation de la qualité image en scanographie

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Imagerie Moléculaire et Stratégies Théranostiques

Objectifs : L'évaluation de la qualité image selon une approche spécifique s'est inscrite comme approche consensuelle en scanographie, en particulier depuis l'avènement d'outils logiciels autorisant l'amélioration du compromis entre qualité de l'image et exposition du patient. Parmi ces outils, les plus populaires sont les algorithmes de reconstruction itératifs dont l'apport clinique n'est plus à démontrer. Chacun d'eux opère selon une implémentation spécifique, complexifiant l'optimisation et l'homogénéisation des protocoles entre différents systèmes. Dans ce contexte, la littérature priviliege le recours à l'observateur idéal, lequel est capable d'extraire la totalité de l'information diagnostique disponible dans l'image. Il n'a toutefois pas d'issue analytique en pratique supposant d'envisager des techniques alternatives, parmi lesquelles les techniques de réduction dimensionnelle ont été largement investiguées dans le but d'extraire les caractéristiques informatives de l'image. Cette approche a permis d'introduire la notion d'observateur canalisé, lequel n'agit plus sur la totalité de l'image mais sur un nombre restreint de variables, les données canalisées. Les canaux sont dits efficents dès lors qu'ils autorisent l'observateur canalisé à approximer les performances de son homologue non contraint. Pour ce faire, des travaux antérieurs ont démontré le bénéfice d'introduire un algorithme d'apprentissage supervisé dans la conception d'un observateur canalisé. L'objet du travail présenté ici est d'évaluer la façon dont ce paradigme est le plus efficacement introduit au sein d'un observateur: une première approche envisage son introduction dans l'étape de réduction dimensionnelle tandis qu'une seconde approche consiste à substituer la fonction de décision de l'observateur linéaire idéal par un algorithme d'apprentissage supervisé.

Matériel et méthode : Une machine à vecteurs de support (SVM) a été employée et comparée à l'observateur linéaire idéal canalisé (CHO) en termes de capacité à prédire les performances de l'observateur linéaire idéal non contraint. La SVM et le CHO ont tous deux été estimés sur des données canalisées, dérivées de la décomposition linéaire de matrices. Cette approche, empruntée à la théorie classique des matrices, utilise ici la décomposition en valeurs singulières (SVD) de la matrice système, l'analyse en composantes principales (PCA) et la méthode des moindres carrés partiels (PLS). Les propriétés de généralisation de ces observateurs numériques ont été évaluées suivant un processus en deux étapes : 1) en utilisant des images d'entraînement et de test reconstruites avec la même stratégie de régularisation et 2) en considérant des images reconstruites différemment. En effet, l'hétérogénéité des stratégies de régularisation, et plus largement de reconstruction, adoptées par les principaux constructeurs positionne les propriétés de généralisation d'un observateur numérique comme un point clé à considérer en vue de son implantation en routine clinique. Pour cela, plusieurs tâches de détection ont été simulées, dans lesquelles différentes structures de bruit ont été générées en faisant varier les stratégies de régularisation.

Résultats : Les performances de l'algorithme SVM se sont avérées supérieures à celles du CHO quel que soit le type de canaux ou de régularisation envisagés. De plus, même si tous deux ont montré de bonnes capacités de généralisation lorsque les images de test étaient reconstruites de la même façon que celles utilisées lors de la phase d'entraînement, les performances du CHO ont fortement diminué lorsqu'elles étaient reconstruites de façon distincte. A l'inverse, l'algorithme SVM a réussi à atteindre de bonnes performances quel que soit le schéma de généralisation envisagé. Enfin, en considérant une base d'apprentissage de dimension limitée, en cohérence avec le nombre d'images réalisable en clinique, l'observateur numérique faisant l'usage conjoint des canaux PCA et de l'algorithme SVM a permis d'atteindre de meilleures performances que le CHO associé aux canaux PLS.

Conclusion : Les résultats obtenus dans ce travail argumentent en faveur de l'introduction d'un algorithme d'apprentissage supervisé dans la fonction de décision plutôt que dans le processus d'extraction des données lors de la conception d'un observateur canalisé. En particulier, l'algorithme SVM en association avec les canaux PCA s'est inscrit comme une bonne alternative à l'observateur linéaire idéal dans l'évaluation de la qualité image.

# HIGHLY FLUORINATED G-C<sub>3</sub>N<sub>4</sub> OBTAIN BY GAS-SOLID FLUORINATION AND ITS APPLICATION IN PHOTODEGRADATION

Tara BUZDON

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Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) is a widely studied semiconductor with a tunable band gap that makes it useable in different application fields. It can be used as a photodegrader material in photocatalysis thanks to its good opto-electronic properties.<sup>[1]</sup> Moreover, the weak Van der Walls bonds between sheets makes it easy to exfoliate and works as a solid lubricant.<sup>[2]</sup> It's also a material that can promote H<sub>2</sub> production through water splitting, another property we will work on.

In order to improve its catalytic activity, mostly electronic conduction and light sensitivity to visible light spectrum, g-C<sub>3</sub>N<sub>4</sub> has already been doped by different process such as with Br<sup>[3]</sup>, B<sup>[4]</sup> or even codoped with B/F<sup>[5]</sup>. g-C<sub>3</sub>N<sub>4</sub> has also been fluorinated by HF<sup>[6]</sup> or mainly with NH<sub>4</sub>F<sup>[7,8]</sup> by hydrothermal methods. However, all these methods provide only few fluorine atoms into the material (less than 1at.% and maximum 7.05at.%)<sup>[9]</sup> without to know exactly how and where F atoms are bond onto the structure.

Here, we present for the first time fluorination of g-C<sub>3</sub>N<sub>4</sub> with pure F<sub>2</sub> followed by some diluted fluorination. To understand the fluorination process and adjust it, two parameters, time and dilution, were adjusted during the different fluorination, and optimized parameters were determined. The obtained materials are analyzed and characterized through XRD, MET, IR-ATR, RMN, XPS, DRS and UV-vis to quantify and qualify fluorination but also to see how the morphologies of the materials were changed. Transmission Electron Microscopy (TEM) reveled the nanostructure and exfoliated structure of the material induced after fluorination. XPS spectra show that high fluorination rates, as high as 26%, were obtained, without dilution. Another effect of fluorination was highlight with DRS showing that fluorination induced a decrease of energy band and so on the bad gap of the material. Then, photodegradation measures are made on methyl orange (MO, a common dye) and the mechanism reactions are studied in particular the role of F- ion. Our studies show that photodegradation of MO was improved in the presence of fluorine in the solution. Finally, the reversible fluorination of g-C<sub>3</sub>N<sub>4</sub> was successfully demonstrated through the use of hydrazine.

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# Modulated Rashba-Dresselhaus Spin-Orbit Coupling for Topology Control and Analog Simulations

Pavel KOKHANCHIK

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We show theoretically that Rashba-Dresselhaus spin-orbit coupling (RDSOC) in lattices acts as a synthetic gauge field. This allows us to control both the phase and the magnitude of tunneling coefficients between sites, which is the key ingredient to implement topological Hamiltonians and spin lattices useful for simulation perspectives. We use liquid crystal based microcavities in which RDSOC can be switched on and off as a model platform. We propose a realistic scheme for implementation of a Su-Schrieffer-Heeger chain in which the edge states existence can be tuned, and a Harper-Hofstadter model with a tunable contrasted flux for each (pseudo)spin component. We further show that a transverse-field Ising model and classical XY Hamiltonian with tunable parameters can be implemented, opening up prospects for analog physics, simulations, and optimization.

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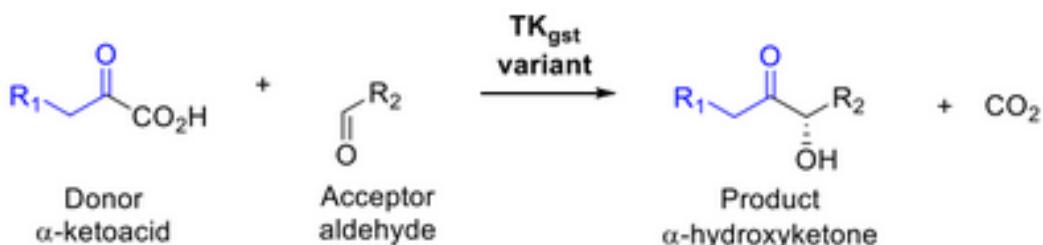
# Evolved transketolase from *Geobacillus stearothermophilus* for new -hydroxyketones synthesis

Giuseppe ARBIA

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*Geobacillus stearothermophilus* thermostable transketolase enzyme (TKgst) catalyzes, in one step a stereoselective and irreversible carboligation reaction using  $\alpha$ -ketoacid, hydroxypyruvate (Li-HPA) as donor substrate and an aldehyde as acceptor to generate various  $\alpha$ -hydroxyketones valuable in food and pharmaceutical areas<sup>[1-4]</sup>. Our current goal consists in TKgst engineering by mutagenesis to broaden the substrate specificity towards pyruvate analogs and polyhydroxylated aldehydes with different configurations and carbon chain length. We will present some recent results showing the high synthetic potential of TKgst variants for obtaining new  $\alpha$ -hydroxyketones.



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# Highlighting the industrial origin of terpenoids in a coastal city in northern France: a source-apportionment approach of non-methane hydrocarbons (NMHC)

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Volatile organic compounds (VOCs) including terpenoids (isoprene and monoterpenes) play a key role within the atmospheric system acting as precursors of ground-level ozone, new particles and secondary organic aerosols; hence the growing interest of better characterizing them and identifying and quantifying their emission sources. While terpenoids have long been recognized to originate from natural sources, there is a growing body of evidence of an origin from human-made activities in cities, in particular from household solvents. Here we explore for the first time the potential role of industrial activities on the terpenoid burden in the urban atmosphere as part of the DATAbASE (Do Anthropogenic Terpenoids mAtter in AtmoSpheric chemistry?) project.

This study is based on the analysis of continuous VOC observations from an intensive field campaign conducted during summer 2014 at an urban-industrial background site located in Dunkirk (northern France) and impacted by metallurgy, chemicals, petrochemicals, pharmaceuticals and food processing plant emissions. More than 40 compounds were measured by on-line Thermal Desorption Gas Chromatography with a Flame Ionization Detector, and Proton Transfer Mass Spectrometry. Isoprene,  $\alpha$ -pinene, and limonene were the most abundant detected terpenoids at average mixing ratios of  $0.038 \pm 0.031$  ppbv,  $0.023 \pm 0.016$  ppbv and  $0.021 \pm 0.012$  ppbv, respectively. Toluene ( $0.22 \pm 0.40$  ppbv), benzene ( $0.09 \pm 0.16$  ppbv), xylenes, C2-C5 alkanes, C2-C3 alkenes, and acetylene were the most abundant hydrocarbons, accounting for 85% (mol/mol) of the concentration of total VOCs. Surprisingly, the VOC average composition is consistent with the one found in non-industrial urban atmosphere of temperate latitudes (AIRPARIF 2013). However, several peak concentrations are depicted in some VOC time series like anthropogenic aromatics and, even terpenoids, corresponding to periods under the influence of the industrial and urban-industrial wind sectors.

A careful crossed analysis of those events has been performed and the urban and industrial emission ratios of terpenoids have been estimated. Finally, Positive Matrix Factorization (PMF) has been performed to identify emission sources of VOCs: first results show the presence of terpenoids in industry-like factors.

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# The role of bacterial biodegradation for atmospheric budgets of formic and acetic acids

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Formic and acetic acids are ubiquitous components in the atmosphere, representing the main organic acids in the gas and condensed phases (clouds, particles, fogs). Their sources comprise various anthropogenic activities and biogenic processes, like direct emissions from biomass burning, fossil fuel combustion, vegetation, and soil, besides secondary production from gas and aqueous phase photochemistry. Meanwhile, their sinks are usually considered limited to wet and dry deposition, and oxidation by radicals ( $\text{OH}$ ,  $\text{NO}_3^-$ ). Lab and model studies suggest that atmospheric budgets of acetic and formic acids can be affected by the presence of metabolically active bacteria. Even is suggested that the highest metabolic activity of bacteria is favored by their residence time in warm clouds, the presence of liquid water, and substrate availability.

As opposed to current atmospheric models neglecting the activity of bacteria in clouds, we explore the potential role of biodegradation as an additional sink of formic and acetic acids. We implemented the biodegradation of acetic and formic acids in cloud droplets in a detailed atmospheric multiphase chemistry model. In contrast with chemical reactions occurring in all droplets, biodegradation occurs in a small fraction of cloud droplets (0.1%), based on the small number concentration of bacteria cells in the atmosphere. Furthermore, the model includes detailed chemical processes in the gas phase and cloud droplets and biodegradation rates that were measured by the BioMeta group.

We perform model sensitivity studies to identify atmospheric conditions (e.g., pH, cloud droplet size) under which biodegradation represents a significant sink of the two acids, taking into account the possible amount of acids degraded by bacteria, and the rate at which each acid could be potentially metabolized by bacteria. We show that the loss of formic and acetic acids may be overestimated by up to 5% (~20 ppt) and 3% (~8 ppt), respectively if biodegradation is not included. The net formation or loss rates are predicted to be reduced by up to 20%. We will broadly discuss the reasons for these trends, influenced by different physicochemical parameters, and their impact on biodegradation as an important acid sink.

We conclude that current atmospheric chemistry models may be incomplete to assess the loss of organics in the atmospheric multiphase system as biodegradation might be a significant loss of formic and acetic acids and possibly similar organics.

# OROVOLC: USING ROBOTIC METHODS TO WATCH VOLCANOES

Freddy VASCONEZ

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Laboratoire Magma et Volcans

Volcanic explosions are widely recognized as the most dangerous of all volcanic processes, since they represent large amounts of energy released in short periods of time. The consequences of past volcanic explosions include destroyed infrastructure, damaged means of production, displaced people and even fatalities, including among scientists. In order to understand the dynamics behind the explosive activity in a safe way, we studied the Reventador volcano with two objectives in mind. The first is to observe the explosions produced in the volcano. The second is to measure the composition of the gas. We are using robotic methods in both objectives to reduce the associated risk to personnel.

Our observation of the explosions is based in visible and infrared imaging. We have developed an instrument called VIGIA that uses computer vision and other computational routines to: distinguish whether the volcano is clear; detect explosions and trigger a recording sequence; save thermal and visible-range videos and pictures; add a GPS-based timestamp to the recorded data; obtain periodic statistics and send reports directly to the volcanologist's cellphone. With VIGIA we have recorded more than 500 explosions from the Reventador volcano, from which we analyze the duration of the explosion, the exit velocity of pyroclastic material, the height and volume of the plume generated, and the mass of gas and pyroclasts emitted.

Aiming at measuring the composition of the gas we use a remote-controlled hexacopter to directly sample the plume. The hexacopter is equipped with a GasSampler instrument, designed to indicate to the pilot when the vehicle traverses the plume and automatically fill up a sample bag with the gas. The hexacopter returns to the pilot with the sample that is immediately analyzed using a MultiGAS instrument. By using this method, we can obtain the gas composition ( $H_2O$ ,  $CO_2$ ,  $SO_2$ ,  $H_2$  and  $H_2S$ ) without subjecting the volcanologist to any high-risk area.

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# Conception et synthèse de sondes fluorescentes originales pour une utilisation en microscopie sur un organisme modèle : *Caenorhabditis elegans*.

**Marion LEROUX**

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Institut de Chimie de Clermont-Ferrand

Le suivi d'une substance active au sein d'un organisme est un enjeu complexe majeur, permettant notamment de faciliter la découverte de nouvelles cibles d'intérêt. Pour ce faire, la microscopie de fluorescence est un outil particulièrement bien adapté.

L'objectif de mes travaux de recherche est de mettre au point une technique de marquage fluorescent permettant de suivre le devenir d'une molécule ou d'un microorganisme *in vivo*, dans l'intestin du nématode *Caenorhabditis elegans*. Pour cela, une sonde fluorescente sera synthétisée et couplée à une molécule ou un microorganisme d'intérêt via un lien potentiellement clivable.



Schéma 1 : Représentation schématique d'un composé d'intérêt

Après ingestion, nous pourrons suivre le parcours du vecteur d'intérêt grâce à la transparence du nématode, et en étudier le devenir et l'impact *in vivo*.

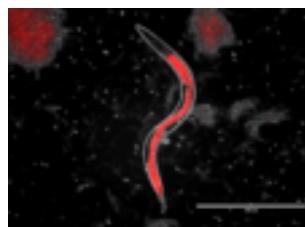


Figure 1 : Exemple d'image obtenue par microscopie sur *C. elegans*

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# Creep Characteristics Along the Central Part of the Philippines Fault on Leyte Island from ALOS-2 Time-Series Analysis

Yagizalp OKUR

Laboratoire de mathématiques Blaise Pascal

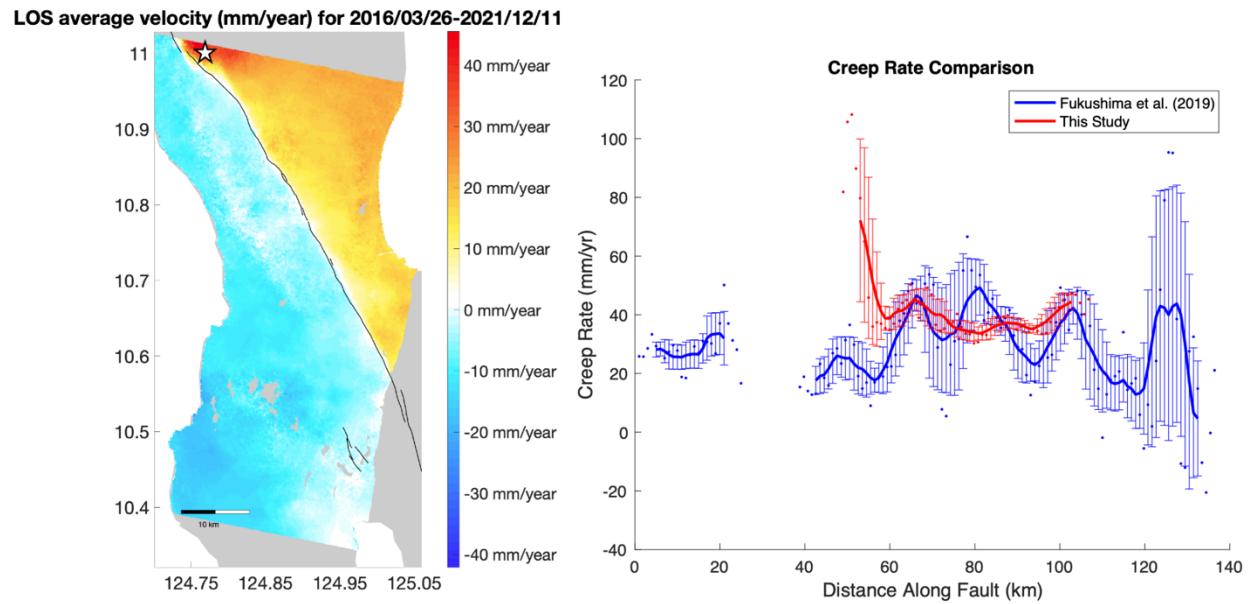
Observations reveal that slip characteristic varies on sections of active faults. Some sections of the fault may be seismically locked, whereas other sections may exhibit creep. Thus, it is usually difficult to characterize these faults with a single slip rate. Analyzing slip distributions along active faults allows the creation of elaborate fault models for the region and developing earthquake hazard scenarios.

Detection and detailed analysis of creeping faults on land have been progressing thanks to the increased number of observations from synthetic aperture radar interferometry (InSAR). Here, we present results of surface creep rates along the central part of the Philippines Fault on Leyte Island using ALOS-2/PALSAR-2 descending data sets acquired between March 2016 and December 2021. A total of 31 interferograms created by the RINC software were analyzed using the small baseline subset algorithm for InSAR time series analysis (DeNTiS). Radar observation geometry of the descending path was favorable for the northwest-southeast oriented left-lateral strike-slip fault. To overcome the decorrelation in the InSAR signal, we multi-looked the interferograms, resulting in a pixel size of 203 m and 198 m in range and azimuth directions, respectively. We used the split spectrum analysis for ionospheric noise correction and GACOS for mitigating noises caused by the troposphere.

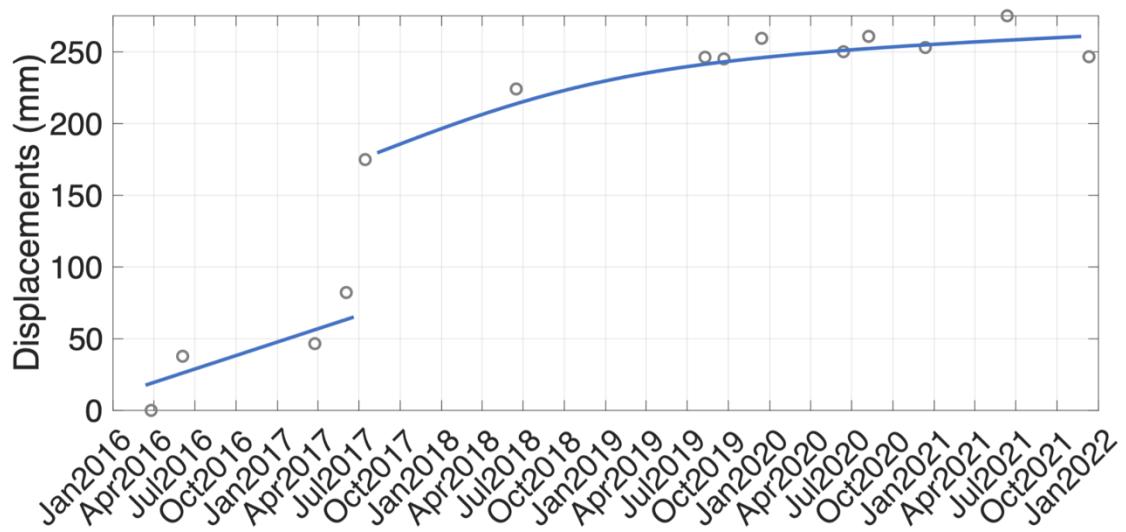
We estimated the fault creep rates by using the velocity offsets between the sides of the fault, assuming pure left-lateral motion. Our result indicates creep rates between 30-50 mm/year with a mean of  $39 \pm 4$  mm/year along the fault, which is comparable to Fukushima et al. (2019), who inferred a creep rate of  $33 \pm 11$  mm/year by using the ALOS/PALSAR data obtained between October 2006 and January 2011. A comparison of creep rates along the fault between this study and Fukushima et al. (2019) shows that the mean creep rates are consistent. More prominent spatial fluctuation in the creep rates was observed from the result of Fukushima et al. (2019), likely due to un-corrected tropospheric noise on the ALOS/PALSAR data analysis.

The anomalously high creep rate (up to ~100 mm/year) in the northwest part of the study region was a manifestation of the effect of the Ormoc earthquake that occurred on 6 July 2017 (Figure). The time series indicates the signature of the coseismic slip as an offset and afterslip as logarithmic decay in the time series.





Time-series plot for the location (white star) in the LOS mean velocity map



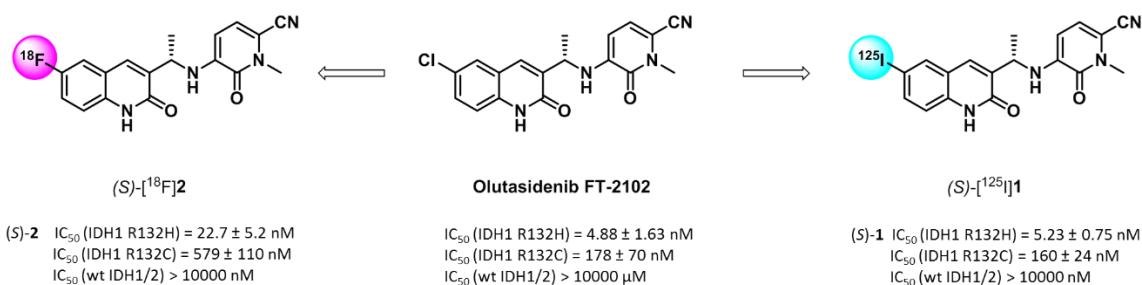
# SPECT or PET Imaging of IDH1 Mutant Cancers with Novel Radiohalogenated Analogues of Olutasidenib

Lucie ARNAUD

V. Weber, S. Dukic-Stefanovic,<sup>1</sup> B. Wenzel,<sup>1</sup> V. Roux, J.M.Chezal, T.H. Lai,<sup>1,2</sup> R.Teodoro,<sup>1</sup> K. Kopka,<sup>1,3</sup> E. Miot-Noirault, W. Deuther-Conrad,<sup>1</sup> A. Maisonnial-Besst

# Imagerie Moléculaire et Stratégies Théranostiques

Isocitrate dehydrogenases (IDHs) are metabolic enzymes frequently mutated in a wide spectrum of human cancers including glioma, acute myeloid leukaemia (AML), chondrosarcoma (CHS), and intrahepatic cholangiocarcinoma<sup>[1]</sup>. Mutated IDHs (mIDHs) confer neomorphic activity resulting in the conversion of  $\alpha$ -ketoglutarate to an oncometabolite D-2-hydroxyglutarate involved in tumourigenesis. These mutant enzymes have become promising targets for new therapies, and several mIDH specific inhibitors have been developed, leading to the approval of two of them by the food and drug administration (FDA) for AML treatment. The FDA is also emphasising the importance of developing companion diagnostics that could become a predictive marker of response to novel anti-mIDH therapies and could be of valuable help to select patients who could benefit from these therapeutic alternatives. To this end, the present study reports the development of radioiodinated and radiofluorinated analogues of an inhibitor in clinical trials, olutasidenib (FT-2102), as tools for non-invasive single photon emission computed tomography (SPECT) or positron emission tomography (PET) imaging<sup>[2]</sup>. Olutasidenib was chosen for its nanomolar binding affinity for mIDH1 combined with its selectivity compared to wtIDH1 and mIDH2, favourable blood-brain barrier penetration, and its low efflux rate<sup>[3]</sup>. Non-radiolabelled derivatives 1 and 2, halogenated at position 6 of the quinolinone scaffold, were synthesised and tested in vitro. They showed a good retention of inhibitory potency and selectivity in comparison with the lead olutasidenib. Therefore, both compounds were selected for further radiolabelling and stability studies. Using a common organotin precursor, (S)-[<sup>125</sup>I]1 and (S)-[<sup>18</sup>F]2 were efficiently synthesised by radio-iododemettallation and copper-mediated radiofluorination, respectively. Both radiotracers were stable at room temperature in saline or DPBS solution and at 37 °C in mouse serum, allowing future planning of their in vitro and in vivo evaluations in glioma and CHS models.



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# Evaluation of the representation of raindrops breakup in bulk models using multifrequency radar retrievals

Laurence NIQUET

Frédéric Tridon<sup>1,2</sup>, Antoine Causse<sup>1</sup>, Baptiste Bordet<sup>3</sup>, Pierre Grzegorczyk<sup>1</sup>, Wolfram Wobrock<sup>(1)</sup>, Céline Planche<sup>(1)</sup>

Laboratoire de Météorologie Physique

Over the last decade, floods were the type of disaster causing the most material damages and fatalities. A better knowledge of the atmospheric processes leading to precipitation is mandatory to better predict severe floods and mitigate their impact on human societies, in particular in the context of a changing climate.

This study focuses on a squall line system which occurred over the ARM (South Great Plain Central Facility) site in Oklahoma on June 2011 and was observed by multifrequency radars. In particular, we analyze the temporal and vertical evolution of the drop size distribution (DSD) provided by a recently developed retrieval technique combining the Doppler spectra observed by two co-located vertically pointing cloud radars.

One of the most uncertain rain microphysics process is the breakup of drops. It is represented in bulk models via vastly different versions of a parameterization combining the collection and breakup processes. By exploiting the variations of the bulk properties of the DSD, we evaluate the ability of the different parameterizations to reproduce the observations. These results suggest that such radar observations have the potential for reducing the uncertainty associated with the representation of the breakup process in models.

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# The influence of photo and thermooxidative ageing on NBR/PVC blends cracks

Clara THORAL

Gérald Soulagne<sup>1</sup>, Pierre-Olivier Bussière, Sandrine Therias

Institut de Chimie de Clermont-Ferrand

Blends of Nitrile butadiene Rubber/Poly(vinyl chloride) are commonly used for the fabrication of hoses conveying fluids, such as fuel for the automobile sector. This particular application calls for NBR due to its good resistance to oils and solvents. To improve the mechanical properties, NBR is blended with PVC, this will bring both higher thermal resistance and stiffness<sup>[1]</sup>. However, as the majority of unsaturated polymers, the presence of double bonds in the backbone of the NBR (found in butadiene units) makes it particularly sensitive to thermo- and photoageing<sup>[2,3]</sup>. This study has been conducted in collaboration between Trelleborg Industrie SAS and the Institute of Chemistry of Clermont-Ferrand.

Indeed, NBR/PVC hoses have shown a loss of their usual properties during its lifespan, leading sometimes to cracks occurrence on the surface during lifetime. The aim of this work is to perform a multiscale study of the materials under thermo- and photoageing conditions in order to determine the main contributor involving cracks formation. The results obtained show significant differences between the effect of photooxidation exposure, occurring only at the extreme surface of NBR/PVC blends and leading to micro-cracking under stress, and thermooxidation which tends to make the whole material brittle.

To reach this objective, different characterisation techniques have been investigated at molecular scale, exhibiting modifications corresponding to the formation of oxidation products monitored by infrared spectroscopy. At macromolecular scale where crosslinking was followed by Differential Scanning Calorimetry (DSC) and Dynamic Mechanical Thermal (DMTA) analyses. As we can see in Figure 1, Atomic Force Microscopy (AFM) was used to follow not only the polymer modulus but also cracks formation at the surface during ageing. This approach allows us to explain how the

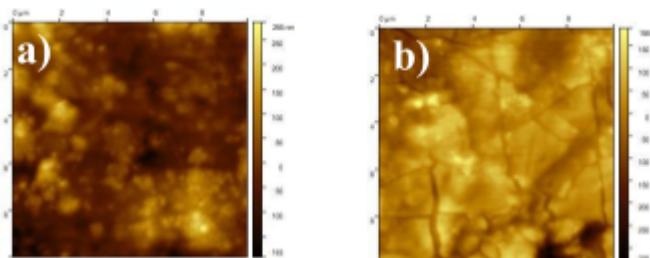


Figure SEQ Figure \\* ARABIC 1. AFM images of a NBR/PVC (66/33 %wt) blend a) at 0h and b) after 100h of irradiation

crosslinking mechanism, taking place in both photo- and thermoageing, can initiate cracking effects in one case and of a material breaking in the second.

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# Zinc-doped Bioactive glass/ Polycaprolactone hybrid scaffolds manufactured by direct and indirect 3D Printing methods

Nafise ELAHPOUR

Laboratoire de Physique de Clermont

This work aims at studying a novel organic-inorganic hybrid material, based on SiO<sub>2</sub>-CaO-ZnO (75/15/10 Si/Ca/Zn relative atomic percent) bioactive glass (BG) and polycaprolactone (PCL) for its organic part. Hybrids consisting of 30 wt. % BG – 70 wt. % PCL were produced by conducting the acid-based catalyzed silica sol-gel process inside a solution of PCL, mixing a solution of PCL with the BG sol right before its gelation. The hybrid sol was then additively manufactured into scaffolds in two manners: one based on the direct printing of dried hybrid xerogel, the other one based on a templating method involving 3D printed paraffin templates infilled with the hybrid sol. In vitro apatite-forming ability tests in Simulated Body Fluid (SBF) confirm the ion release along with the hybrid's bone-like apatite forming ability. However, the kinetics differ significantly between directly and indirectly 3D-printed scaffolds, the former requiring longer soaking periods to degrade, while the latter demonstrate faster calcium phosphate formation. These distinct behaviours can be attributed to the denser structure obtained with 3D direct printing using FDM (Fused Deposition Modelling), which results from the coarse (several hundred  $\mu\text{m}$ ) printing resolution and hot extrusion, while the 3D indirect templated method leads to finer pore sizes, thinner struts with internal porosity therefore enhancing apatite nucleation. Remarkably, diffusion and accumulation of zinc are observed at the surface of both kind of hybrids, within the newly-formed active calcium phosphate layer. Zn release was found to be dependent on the scaffold printing method but also on the medium, with Zn<sup>2+</sup> concentrations released being 2 orders of magnitude higher in Muller-Hinton Broth bacterial culture medium compared to a simple saline solution such as SBF, reinforcing observations from previous studies about the ability of proteins to enhance the dissolution of ZnO by creating highly soluble complexes. Direct and indirect cellular assays involving bone marrow human mesenchymal stem cells (hMSCs) were conducted. Indirect cell viability assay evidences no cytotoxic effects of the Zn-hybrid under normal experimental conditions, a major concern to be addressed given the relative sensitivity of eukaryote cells exposed to Zn and possible Zn<sup>2+</sup> homeostasis deregulation. LIVE/DEAD staining of hMSCs 3D cultured in the scaffolds for prolonged periods of times<sup>3</sup> demonstrate excellent biocompatibility with cell attachment, growth and proliferation for at least 7 weeks.

# Ajustement de l'hydrophobicité et de l'oléophobicité du polypropylène par fluoration directe sous différentes conditions

Nicolas SUCHET

Nicolas BATISSE, Marc DUBOIS

Institut de Chimie de Clermont-Ferrand

La fluoration est un procédé efficace pour modifier la surface des polymères. Il s'agit d'une réaction gaz solide avantageusement utilisée de manière industrielle pour le traitement de géométries complexes telles que des réservoirs de véhicules.

La réaction de fluoration sur une polyoléfine se traduit par une substitution partielle ou totale des atomes d'hydrogène en surface par des atomes de fluor sans affecter les propriétés macroscopiques du cœur du polymère. Elle s'établit de manière spontanée et est extrêmement exothermique d'où la nécessité d'étudier les paramètres permettant de la contrôler.

Cette étude vise à montrer qu'il est possible de moduler l'énergie de surface du polypropylène en faisant varier les paramètres de fluoration tels que la composition du mélange réactif et la température de la réaction.

De manière générale, la fluoration à température ambiante par du fluor moléculaire pur donne un caractère hydrophile au polypropylène qui se traduit par une diminution de l'angle de contact à l'eau. Ceci s'explique par l'incorporation de groupements oxygénés polaires à la surface des échantillons fluorés. En présence d'oxygène dilué dans le mélange réactionnel et par post-réactivité à l'air, davantage de groupements oxifluorés sont générés tandis que la réaction de substitution des atomes d'hydrogène par le fluor est perturbée. Il en résulte une surface plus voire extrêmement polaire après hydrolyse des groupements oxifluorés. Les mesures d'angles de reculé à l'eau sur les échantillons traités deviennent impossibles car l'eau s'étale à la surface de l'échantillon lorsqu'elle est rendue totalement hydrophile.

Des fluorations sous atmosphère de fluor élémentaire pur ( $F_2$ ) ont été réalisées entre 2°C et 110°C. Une augmentation de la température induit une substitution plus importante et plus en profondeur des atomes d'hydrogène par ceux de fluor. La spectroscopie infrarouge permet d'affirmer qu'à partir de 70°C la totalité de l'épaisseur sondée dans le mode employé (ATR), environ 2 $\mu$ m, est totalement fluorée. La mesure des énergies de surface par la formule d'Owens Wendt montre une diminution globale de la composante dispersive pour une température de fluoration entre 2°C et 110°C et une composante polaire minimale à 90°C. La fluoration à haute température a donc permis d'obtenir un polypropylène plus hydrophobe et plus oléophobe, contrairement à ce qui est généralement reporté dans la littérature.

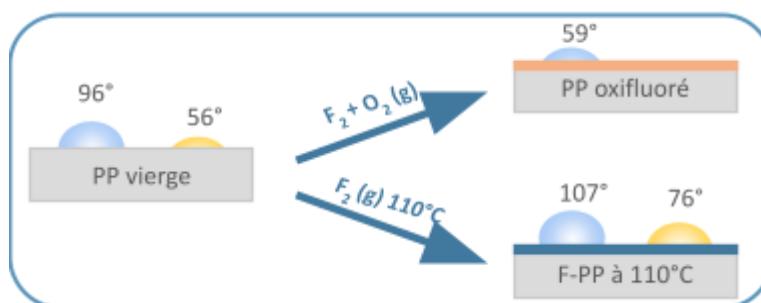


Figure SEQ Figure 1\*  
ARABIC 1: Angles de contact statiques à l'eau (bleu) et au diiodométhane (jaune) du polypropylène avant et après traitements de fluoration

# Modelling run-and-tumble particles using piecewise-deterministic markov processes

Leo HAHN

Arnaud GUILLIN, Manon MICHEL

Laboratoire de mathématiques Blaise Pascal

Run-and-tumble particles change direction at random times between which they move in straight lines. This class of active particles can be used as a particle-level model for bacteria such as *E. coli*. Our goal will be to deduce mesoscopic properties from this particle-level description. In particular, we want to better understand motility-induced phase separation (coexistence of high-density and low-density areas). Using a piecewise-deterministic Markov process allows us to obtain a continuous-space model for two mutually blocking persistent random walkers. We focus on two models : one where the tumbles are assumed to be instantaneous and another where the tumbles are assumed to have a finite duration. Using the generator of the process, we are able to exactly determine the non-equilibrium steady state of our system. Furthermore, we are able to determine scaling of the mixing time of our processes in terms of our model parameters. Both the non-equilibrium steady state and the mixing time highlight two regimes : a persistent regime and a diffusive regime.

## Assessing the efficiency of water-soluble organic compounds biodegradation in clouds under various environmental conditions

Lucas PAILLER

Pascal Renard<sup>1</sup>, Angelica Bianco<sup>1</sup>, Camille Mouchel-Vallon<sup>1,a</sup>, Maud Leriche<sup>1</sup>, Luc Patryl<sup>2</sup>, Patrick Armand<sup>2</sup> and Laurent Deguillaume<sup>1,3,\*</sup>.

Laboratoire de Météorologie Physique

Atmospheric chemistry and transport modelling is crucial to better apprehend air quality and climate. However cloud processes in chemistry/transport models are still roughly represented. Indeed, many complex and uncertain bio-physico-chemical processes take place in clouds controlling their formation, their lifetime and the transformation occurring within them. Strong uncertainties still exist for example on the phase partitioning of chemical compounds among the gas, liquid and particulate compartments and the chemical and biological transformations in cloud droplets.

In order to address that issue, we use and develop a multiphasic atmospheric chemistry box model that considers detailed chemical and microphysical processes. It aims at reproducing simultaneously the kinetic transfer and reactivity using highly detailed gaseous (MCM) and aqueous (CLEPS) phase chemical mechanisms. The CLEPS aqueous phase mechanism was developed to describe the chemical transformations adapted to simulate biogenically influenced environments. Recently, the mechanism took into account the biological activity highlighting the efficient role of microorganisms in the multiphasic atmospheric transformations of chemical compounds such as small organic compounds and hydrogen peroxide. It appears, for example, that formic acid is largely biodegraded in cloud droplets drastically decreasing both its aqueous and gaseous concentrations. Sensitivity tests (pH and water content) further demonstrated the added value of modulating the biodegradation efficiency according to the concentrations of each compound.

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# Generative Models of Transient Anomalous diffusion in Polymer Melts

Giovanni Michele CHERCHI

Institut de Chimie de Clermont-Ferrand

Molecular Dynamics simulations are often highly computational expensive when simulating physical systems and materials with a lot of degrees of freedom. In particular, in soft-matter systems, polymer melts can be challenging because of complicated non-linear interactions and diverse diffusion regimes.

They often display subdiffusive regimes which relax to normal diffusion after a long simulation time. Reaching these timescales remains expensive and one of the solutions often adopted is coarse-graining. In this work, on the other hand, we try to employ generative Machine learning techniques to model the conditional distribution of single polymers in an homopolymer system. This gives us the chance to use single polymer degrees of freedom to train a Neural Network with a Score-Based regularization able to reproduce faithfully both the stationary distribution and autocorrelation function; We use short-term molecular dynamics simulations but the objective is, therefore, extrapolating the long-term relaxation behaviour.

We then model the Center of Mass dynamics, which displays transient anomalous diffusion, with a Generalized Langevin Equation with an integrable kernel, which gives a solution in the overdamped limit that exploits a set of stochastic processes corresponding to the relaxation modes of the single polymer.

Future research perspectives include evaluating the generalization capabilities of the Model with respect different temperatures or other thermodynamical coordinates.

# Elaboration and characterization of a thin SiN<sub>x</sub> interfacial layer between the silicon and the anti-reflection layer to improve the performance of solar panels

Hiba BEJI

Eric Tomasella, Christine Robert-Goumet

Institut Pascal and Institut de Chimie de Clermont-Ferrand

Thin dielectric films are nowadays widely used in the photovoltaic field (PV). But thermal silicon dioxide (SiO<sub>2</sub>) has become undesirable for industrialization due to high temperatures deposition and relatively long processing times. While silicon nitride turns out to be a good candidate for photovoltaic applications, combining excellent surface passivation quality with excellent anti-reflective properties. These films are very suitable for backside passivation of bifacial solar cells, as evidenced by efficiencies above 20% due to optimization of certain characteristics compared to SiO<sub>2</sub>.

The a-SiN<sub>x</sub> is known for its high band gap (Eg= 4.5 eV) as well as a high refractive index n of the order of 2 and a high density of the order of 3.2 to 3.5 g/cm<sup>3</sup> which give it interesting properties in this field.

In this work, a-SiN<sub>x</sub> films are elaborated by a reactive deposition process using non-toxic gases (N<sub>2</sub>, Ar<sub>2</sub>) involving radio-frequency plasma on Si (100) and (111) substrates. However, the interface between antireflective films and the Si substrate play a key role on the yield of PV cells. Thus, we focused our attention on an original surface passivation method, consisting on a nitriding process using N<sub>2</sub> plasma glow discharge source (GDS) under ultra-high vacuum.

Several experimental parameters as nitridation temperature and time, initial substrate state have been studied to create a very thin SiN<sub>x</sub> film (less than 10 nm). In situ Angle Resolved-X-ray Photoelectron Spectroscopy (XPS) measurements combined with surface models and Density functional theory (DFT), allow controlling the stage of the elaboration and allow the determination of the composition and the thickness of the nitride layer formed.

The aim of the elaboration of SiN<sub>x</sub> thin film is to minimize the dangling bonds and therefore to reduce the interface state density. Metal-Insulator-Semiconductor (MIS) electrical characterizations have been applied in order to extract information from the interface.

## Acknowledgment:

"This work was sponsored by a public grant overseen by the French National Research Agency as part of the "Investissements d'Avenir" through the IMobS<sup>3</sup> Laboratory of Excellence (ANR-10-LABX-0016) and the IDEX-ISITE initiative CAP 20-25 (ANR-16-IDEX-0001).

# Strategies to achieve stable manganese oxyfluorides by tuning the reactivity of pure molecular fluorine

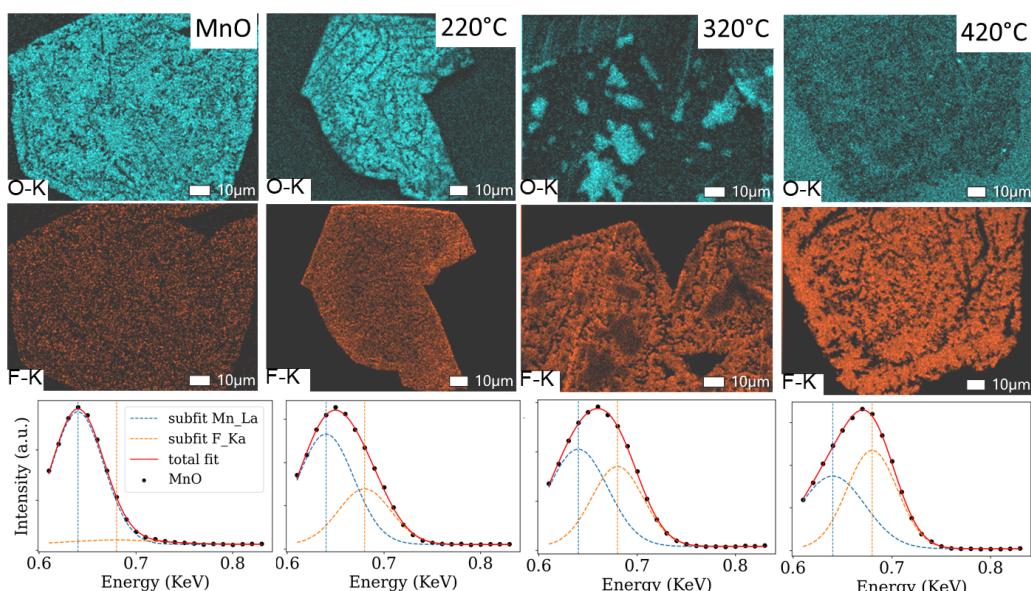
Sébastien DE WINDT

Auvergniot J.<sup>1</sup>, Gschwind F<sup>1</sup>, Kumakura S.<sup>1</sup>, Cabelguen P-E.<sup>1</sup>, Dubois M., Guerin-Araujo Da Silva K.

Institut de Chimie de Clermont-Ferrand

Thanks to their high initial electrochemical properties and broad compositional flexibility, lithium-rich disordered rocksalts cathode active material including high-performance manganese-only materials, appear as potential replacement to the cobalt-based current market leader “NMC” material<sup>[1]</sup>. They however lack stability, but recent works have identified bulk fluorination as a potential solution to stabilize these compounds<sup>[2]</sup>.

There is nonetheless a clear lack of diversity in fluorination agents used to synthesize these disordered rocksalts, as most publications used LiF, a very stable compound<sup>[3]</sup>. To achieve manganese-only materials, manganese oxy-fluorides represent potentially promising precursors, but literature reports only two which are both hazardous<sup>[4,5]</sup>. We developed several strategies for synthesis and a tailored characterization methodology to explore the chemical space of direct fluorination of manganese oxide MnO with molecular fluorine, and showed how to finely tune its reactivity to reach exotic manganese fluoride or novel, safe and air-stable manganese oxyfluorides.



Cross-section scanning electron microscopy EDX mappings, with deconvoluted EDX point spectra

<sup>1</sup> Umicore, 31 rue du Marais, 1000, Brussels, Belgium.

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## **Interventions:**

**Doct'Auvergne** is an association created by PhD students for PhD students and young doctors. This association was created with the aim of developing opportunities for exchanges and meetings between doctoral students. It also organizes numerous events throughout the year, where university research actors share their knowledge with the general public. Doct'Auvergne is an association created by PhD students for PhD students and young doctors. This association was created with the aim of developing opportunities for exchanges and meetings between doctoral students. It also organizes numerous events throughout the year, where university research actors share their knowledge with the general public.

**Albin** is an association composed of students and academics, who wish to contribute to the reintegration of detainees, as well as to the debate on places of detention. Its function is primarily that of transmitting knowledge through lectures given to prisoners in penitentiary centers. The action of the association continues on the benches of the faculties, where they propose to make known what the detention is or could be. Albin is an association composed of students and academics, who wish to contribute to the rehabilitation of prisoners, as well as to the debate on places of deprivation of liberty. Its function is first and foremost transmitting knowledge through lectures given to prisoners in penitentiary centers. The action of the association continues on the benches of faculties, where it is proposed to discuss on what the detention is or could be.

**Clermont Auvergne Innovation** is a company that supports the development and innovation of research work, through public-private partnerships, detection and analysis of projects with development potential. It offers its assistance in the maturation of projects via the creation of companies, start-ups, associations, and communities. Clermont Auvergne Innovation is a company that supports the development and innovation of research work, through public-private partnerships, detection and analysis of projects with development potential. It offers assistance in the maturation of projects through the creation of companies, start-ups, associations and communities.

**Clermont Auvergne PEPITE** (for Pôles Etudiants Pour l'Innovation, le Transfert et l'Entrepreneuriat) is a university service for all students of the EPE UCA. This service makes it possible to weave a link between research and entrepreneurship from the point of view of skills, through awareness-raising, training and support for PhD students. Clermont Auvergne PEPITE (for Pôles Etudiants Pour l'Innovation, le Transfert et l'Entrepreneuriat) is a university service for all students of the EPE UCA. This service ease at weaving a link between research and entrepreneurship under the angle of competences, through devices of sensitization, training and accompaniment for the doctoral students.

**Jeunes Chercheurs Associés** is a cooperative society of collective interest which allows to valorize the competences acquired with the doctorate in order to facilitate the pursuit of career of the young doctors in all the economic sectors. This company offers doctoral students a contractual expertise and consulting service, which can be an alternative to the doctoral teaching service. Jeunes Chercheurs Associés is a cooperative society of collective interest which allows to value the competences acquired with the PhD, in order to facilitate the pursuit of career of the young doctors in all the economic sectors. This company offers PhD students a contractual expertise and consulting service, which can be an alternative to the doctoral teaching service.

### **UCA / CNRS : Management and setting up of scientific projects**

Oraline Wiart (European Projects Engineer at the CNRS "European Grants" Pole) and Claire Soriano (Head of the UCA Project Engineering Pole) will present an overview of the main funding for research through the various units for setting up and monitoring scientific projects. Oraline Wiart (European Projects Engineer at the "European Grants" Pole of the CNRS) and Claire Soriano (Head of the Project Engineering Pole of the UCA) will present a panorama of the main fundings for research through the different cells for setting up and monitoring scientific projects.

# Ma thèse en 180 secondes (MT180)



Three minutes on top of the clock !

On March 6, 2023 at 5:30 pm, **the 10th edition of the Clermont-Ferrand final** of this competition took place. This competition allows PhD students to present their research topic, in French and in simple terms, to a lay and diverse audience. Each student must make a clear, concise, yet convincing presentation of his or her research project in three minutes and not a second more.

Ten PhD students from the University of Clermont Auvergne, representing the different doctoral schools of Clermont-Ferrand, participated. At the end of an emotional evening, the verdict was given for the 1st and 2nd prizes of the Jury, the 1st prize of the Public and the prize of the Internet users.

This year, the 1st prize of the Jury and of the Public was awarded to the same candidate, Héloïse CHAT from M2iSH. This qualification will allow her, as well as the 2nd prize of the Jury, to reach the national semi-final which will take place in April 2023, in Paris.

The **2nd prize of the Jury** was awarded to **Adrien GAUTIER** (from the Magma and Volcanoes Laboratory), part of the **Doctoral School of Fundamental Sciences (Ecole Doctorale des Sciences Fondamentales)**.

We would like **to congratulate him for his performance and give him all our support** for the next step that awaits him in Paris.

**Do not hesitate to follow him in this adventure or to participate in the next editions**, to represent the University, but especially, **to make known your work to all**.



The last word ...

The organizing committee thanks  
the doctoral school of basic sciences for  
giving the opportunity to set up these  
scientific days 2023 .

Thank you all for your participation

Have a nice day and see you next year!  
Océane, Victoria, Adrien, Clément, Götton

PS: Places in the organizing committee  
are available, join us!

