SCIENTIFIC DAYS

Doctoral School of Fundamental Sciences

CAMPUS DES CEZEAUX

Amphithéâtre recherche
Pôle physique

Opening

Soap film physics

Seminar by Thierry Charitat

physicist and professor
at Université de Strasbourg

MAY
26 • 27

Posters and talks on current thesis projects

Full program on : sf.ed.uca.fr

**ÉCOLE DOCTORALE
DES SCIENCES
FONDAMENTALES**

Graphic design by Camille Valadeau

Organising team

- Lou Breton (ICFF)
- Marie Bretonniere (ICCF)
- Pauline Fombelle (LaMP)
- Alexis Guérin (LMBP)
- Romain Jouanneaud (IP)
- Aela Le Brun (LPCA)
- Paul Stos (LMBP)

With the contribution of

+ clermont auvergne métropole

UCA UNIVERSITÉ Clermont Auvergne

UCA ÉCOLE DOCTORALE DES SCIENCES FONDAMENTALES

ICCF Institut de Chimie de Clermont-Ferrand

LaMP

lmv

lmbp

LPC Particules pLasmas Univers applicationS Laboratoire de Physique de Clermont

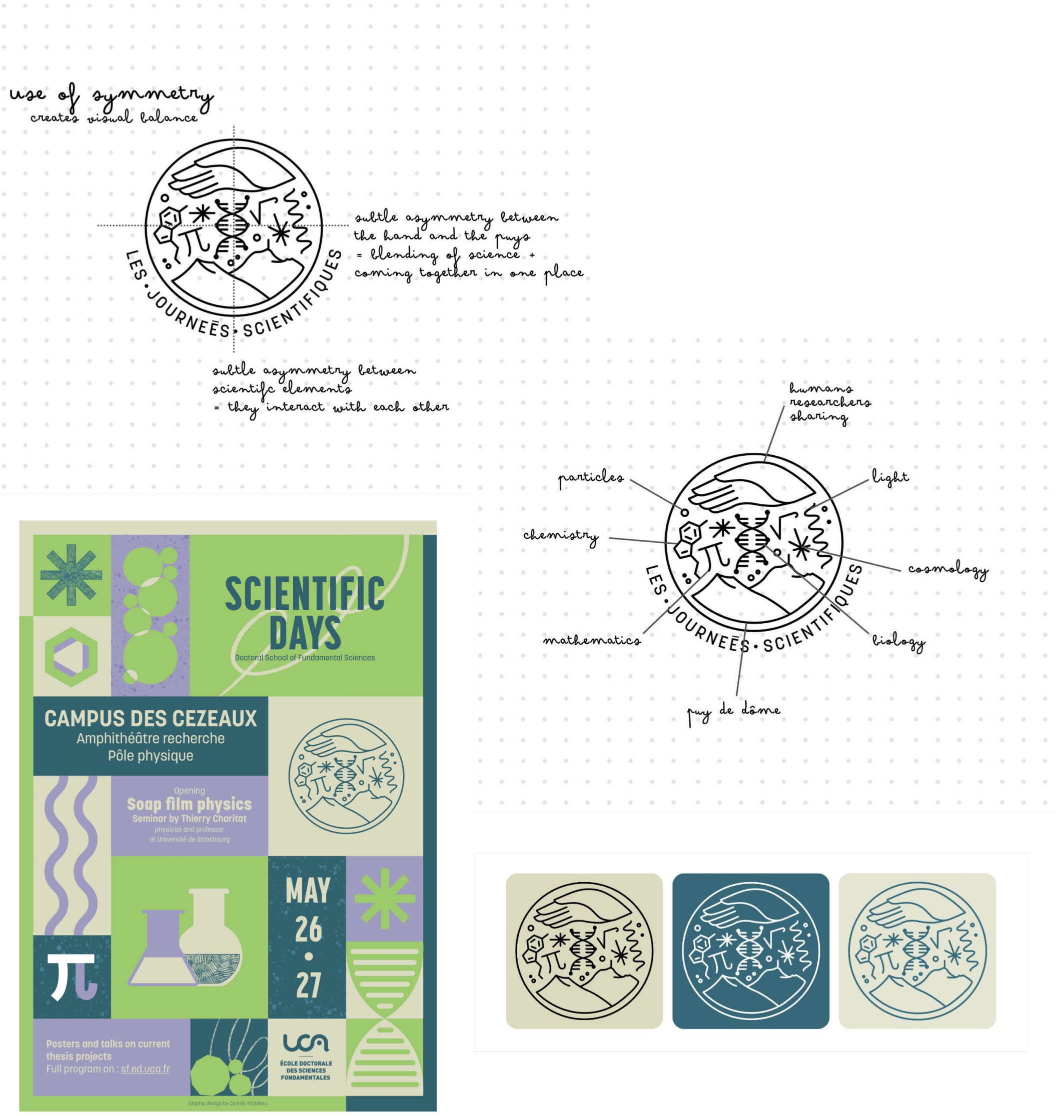
INSTITUT PASCAL sciences de l'ingénierie et des systèmes

IMoST Imagerie Moléculaire et Stratégies Théranostiques

Graphic design

Special thanks to Camille Valadeau for handling the graphic design
for this edition of the Scientific Days!

Camille has always had a strong passion for applied arts. A self-taught graphic designer, she uses her skills to showcase her projects. After earning a science-track high school diploma, she pursued a DNMADE (National Diploma in Art and Design) in Bordeaux. She then completed a Master's in Innovation Engineering at the École des Mines de Nancy, finishing with an internship at Kardham, an independent firm specializing in workplace design. Currently, she is continuing with the same company through a work-study program while completing a specialized Master's in Design-Driven Innovation at ENSCI – Les Ateliers in Paris. This path will soon lead her to a role as an Innovation Director.



Once again, a big *thank you* to Camille for her time and dedication!

Guest speaker

Thierry Charitat

Physicist and professor at the University of Strasbourg, France

We are honoured to welcome Prof. Thierry Charitat, physicist and professor at the University of Strasbourg, as our guest speaker for the opening session of the 2025 edition of the JS EDSF.

His talk, titled

**Soap films and curvature:
minimum surfaces, Delaunay surfaces and beyond**

will open this year's event.

Further information to be announced shortly.

Monday, 26 May 2025

09:00 - 09:30	Reception	
09:30 - 10:00	Opening speech	
10:00 - 12:00	**Invited talk:** Thierry Charitat (ICS), *Soap films and curvature: minimum surfaces, Delaunay surfaces and beyond*	
12:00 - 13:30	Lunch break	
13:30 - 13:50	Arthur Lafarge (LPCA), *Study of the Higgs self-Coupling with the ATLAS detector and characterization of ALTIROC performance*	p. 7
13:50 - 14:10	Thi Hòa Émilie Nguyen (LMBP), *What is dimension?*	p. 8
14:10 - 14:30	Arjun Babu (ICCF), *Sol-Gel derived luminescent coatings incorporating $YVO_4:Eu^{3+}$ nanoparticles*	p. 9
14:30 - 15:00	**Posters:** Zacharie Bordas (ICCF), Jessy Dominique (LMV), Yongrong Zou (ICCF), Sidy Diarra (LaMP), Laeticia Guerry (LPCA), Alexy Duchamp (ICCF), Romain Thévenet (ICCF)	p. 23-29
15:00 - 15:30	Coffee break	
15:30 - 15:50	Martin Metodiev (LMBP), *A structured estimator for large covariance matrices in the presence of pairwise and spatial covariates*	p. 10
15:50 - 16:10	Amr Saleh (ICCF), *Exploring the interaction between plasma proteins and PVC in medical devices: Insights from molecular simulations*	p. 11
16:15 - 16:30	Snack	

Tuesday, 27 May 2025

09:00 - 09:30	Reception	
09:30 - 09:50	Saida Moumen (ICCF), *Fluorination by solid-gas reaction of high-performance compounds for rechargeable batteries*	p. 12
09:50 - 10:10	Clément Legrand (LMBP), *Knot theory and knot invariants*	p. 13
10:10 - 10:30	Chloé Barjou-Delayre (LPCA), *Study of anisotropic cosmic expansion with type Ia supernovae from the Zwicky Transient Facility*	p. 14
10:30 - 11:00	**Posters:** Yunge Bai (ICCF), Nicole Vizuete (LMV), Aho Yapi (LMBP), Ghazal Borhan (ICCF), Loïc Méchin (IP), Hao Wang (ICCF)	p. 30-35
11:00 - 11:30	Coffee break	
11:30 - 11:50	Hugo Clermont (ICCF), *Development of a new method for temporal monitoring of hydroxyl radicals during UV-based AOPs*	p. 15
11:50 - 12:10	Pauline Nibert (LaMP), *Photobiological transformation of organic compounds in clouds*	p. 16
12:15 - 13:30	Lunch break	
13:30 - 13:50	Thomas Rouyer (LMV), *Carbon origin of carbonatites: Constraints given by short-lived radioactive systems* ^{146}*Sm*-^{142}*Nd and* ^{182}*Hf*-^{182}*W*	p. 17
13:50 - 14:10	Yi Wu (ICCF), *Photochemical transformation of triphenyl phosphate with reactive species in cloud water*	p. 18
14:10 - 14:30	Thomas Clouvel (LPCA), *Search for the coherent neutrinoless conversion of a muon bound to a nucleus into an electron at J-Parc*	p. 19
14:30 - 15:00	**Posters:** Hugo Lajoie (ICCF), Jérémie Moukambi Moukambi (LMBP), Killian Malosse (ICCF), Otmane Hammouti (ICCF), Michael Galárraga (LMV), Stephany Bouzid (ICCF)	p. 36-41
15:00 - 15:30	Coffee break	
15:30 - 15:50	Florian Tillet (LMBP), *Spikes traps and geometry of numbers*	p. 20
15:50 - 16:10	Marina Anastasiou (ICCF), *Investigation of sorption and photochemical capacity of sewage sludge derived materials for the removal of emerging contaminants*	p. 21
16:15 - 16:30	Coffee break	
16:30 - 17:00	Closing speech and rewards	
20:00	Closing social event (venue to be determined)	

Talks

Study of the Higgs self-Coupling with the ATLAS detector and characterization of ALTIROC performance

Arthur Lafarge

Supervisors : Djamel Boumediene (LPCA), Louis D'Eramo (LPCA)

Keywords: *di-Higgs; $HH \to b\bar{b}\gamma\gamma$; self-coupling; High Granularity Timing Detector; ALTIROC; HL-LHC.*

The Standard Model (SM) is the most predictive framework describing interactions among the fundamental constituents of matter. It includes 19 free parameters, measured experimentally, notably with the ATLAS detector at the Large Hadron Collider (LHC) at CERN. These parameters encompass particle masses, phases, and coupling values. Among them, the Higgs boson self-coupling is particularly significant: only a scalar can possess a self-coupling, a key parameter in shaping the Higgs potential and explaining the origin of particle masses. Precisely determining this coupling is crucial—either to reinforce the SM's predictive power and constrain the Higgs potential, which directly impacts the stability of our universe, or to open the door to new physics.

This coupling plays a role in the rare simultaneous production of two Higgs bosons via a virtual Higgs boson, with a cross-section 1,000 times smaller than single Higgs production. Detecting this process is challenging, as the Higgs bosons decay into various particles with different probabilities. One of the most sensitive signatures is the decay into two b-quarks and two photons ($HH \to b\bar{b}\gamma\gamma$). Although currently limited by available data, this signature has set the best existing constraint on the self-coupling. The new ongoing study, leveraging the latest developments and increased statistics, promises a significant improvement over the most up-to-date published results [1].

The High Luminosity LHC (HL-LHC) upgrade will increase data collection by a factor of 20, enabling an unprecedented measurement of this coupling. A sensitivity projection study [2], based on ATLAS Run 2 legacy results [1], estimates the expected constraint at the end of the HL-LHC program. However, handling such an increase in data comes with challenges, notably a higher track density in the detector. To address this, a High Granularity Timing Detector [3] is under development, enhancing track reconstruction by adding a temporal dimension. A key challenge is ensuring the robustness of its readout ASIC, ALTIROC, against radiation effects while maintaining high time resolution.

This presentation will explore the challenges of detecting di-Higgs events through the $b\bar{b}\gamma\gamma$ channel in ATLAS and assess the prospects of discovering the di-Higgs signature at the HL-LHC.

References

[1] JHEP 01 (2024) 066

[2] ATL-PHYS-PUB-2025-001

[3] ATLAS-TDR-031

What is dimension?

Thi Hoà Émilie Nguyen
Supervisors : Julien Bichon (LMBP)

Keywords: *dimension; vector spaces; non-commutativity*.

Dimension is a fundamental concept in mathematics, often used to describe the "size" or "complexity" of a space. A vector space is a collection of vectors (which can be thought of as arrows in space), that can be added together or multiplied by numbers called scalars. The dimension of a vector space tells us how many independent vectors are needed to create all the other vectors in the space by combining them in different ways.

For example, in a two-dimensional space (like a flat sheet of paper), two independent vectors are enough to represent all the other vectors in this space. The more dimensions a space has, the more "complex" it becomes, because it contains more possible directions.

In my thesis, I focus on the cohomological dimension (a way to measure the complexity of certain algebraic structures) of certain non-commutative algebras, that are mathematical structures where the order in which we multiply elements matters (i.e. in these algebras, yx is not always equal to xy).This non-commutative behavior is important in modeling certain physical theories like quantum mechanics and quantum field theory. Calculating the dimension of these objects can sometimes be much more complicated. To simplify this process, I introduce a criterion based on a smoothness condition—proven by Serre—that provides a more accessible way of understanding these complex dimensions.

References

[1] J.-P. Serre, *Local Algebra*, Springer Monographs in Mathematics, 2000.

Sol-Gel derived luminescent coatings incorporating YVO_4:Eu^{3+} nanoparticles

Arjun Babu

Supervisors : François Réveret (ICCF), Damien Boyer (ICCF)

Keywords: *YVO_4:Eu^{3+} nanoparticles; sol-gel synthesis; luminescent coating; particle size.*

Recently, the development of luminescent nanoparticles (NPs) exhibiting high quantum yield has emerged as a tremendous goal in the race for miniaturization of optical systems like LED lighting or display devices [1]. Herein, we studied the optical properties of YVO_4:Eu^{3+} NPs synthesized by two distinct hydrothermal protocols (S1 and S2). As shown in Figure 1, the averages size of the synthesized nanoparticles were 340 nm and 10 nm [2,3]. This lanthanide ions doped vanadate is well-known to produce a strong red emission upon UV excitation. Then, structural, morphological and optical characterizations were performed to analyse these nanophosphors in detail. Eu^{3+} concentration was evidenced by elementary analysis and Rietveld refinement. Afterwards, these YVO_4:Eu^{3+} NPs were incorporated in a sol-gel based hybrid material with different loading rates and then luminescent coatings were achieved by spin-coating these suspensions onto glass substrates [4]. Their thickness was determined by profilometry and micro-reflectivity measurements. Furthermore, the effect of mass loading and NPs size on the optical properties of luminescent films was also investigated by conducting photoluminescence and UV-visible spectroscopies. Finally, the angular distribution of the red-emitting light upon UV excitation (Figure 1) was analysed to estimate the photons trapped inside the structure depending on the surface roughness and the NPs size.

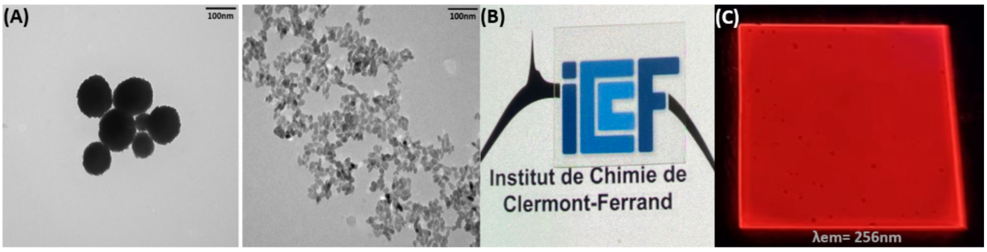


Figure 1. TEM Images of YVO_4:Eu^{3+} NPs synthesized by (A) S1 and (B) S2 hydrothermal protocol, Images of luminescent hybrid coating under (C) daylight and (D) UV excitation.

References

[1] Terraschke et. al., Chem. Rev., 2015, 115, 11352.

[2] Chen. et. al, Phys. Chem. Chem. Phys., 2010, 12, 7775.

[3] K. Riwotzki et. al., J. Phys. Chem. B, 1998, 102, 10129.

[4] Toide et. al., J Sol-Gel Sci Technol, 104, 2022, 478.

A structured estimator for large covariance matrices in the presence of pairwise and spatial covariates

Martin Metodiev

Supervisors : Pierre Latouche (LMBP), Guilhem Fouetillou (Medialab, Sciences Po), Marie Perrot-Dockès (Université Paris Cité, CNRS, MAP5)

Keywords: *large covariance matrix estimation; pairwise covariates; spatial effects*.

We consider the problem of estimating a high-dimensional covariance matrix from a small number of observations when covariates on pairs of variables are available and the variables can have spatial structure [1]. This is motivated by the problem arising in demography of estimating the covariance matrix of the total fertility rate (TFR) of 195 different countries when only 11 observations are available. We construct an estimator for high-dimensional covariance matrices by exploiting information about pairwise covariates, such as whether pairs of variables belong to the same cluster, or spatial structure of the variables, and interactions between the covariates. We reformulate the problem in terms of a mixed effects model. This requires the estimation of only a small number of parameters, which are easy to interpret and which can be selected using standard procedures. The estimator is consistent under general conditions, and asymptotically normal. We assess its performance under our model assumptions, as well as under model misspecification, using simulations. We find that it outperforms several popular alternatives. We apply it to the TFR dataset and draw some conclusions.

References

[1] M. Metodiev et al., *A Structured Estimator for large Covariance Matrices in the Presence of Pairwise and Spatial Covariates*, 2024, <`hal-04777439`>.

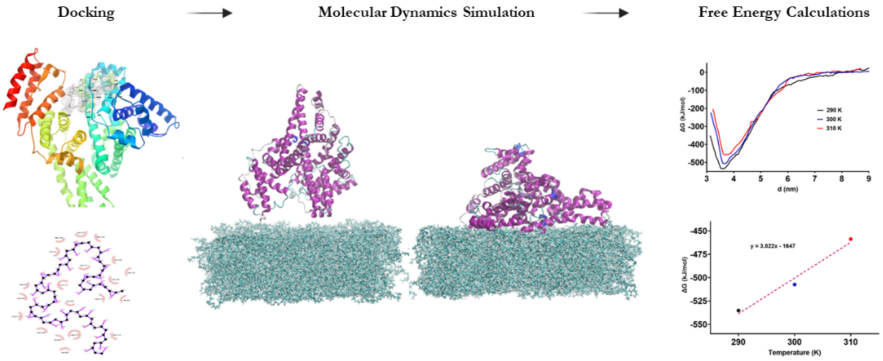
Exploring the interaction between plasma proteins and PVC in medical devices: Insights from molecular simulations

Amr Saleh

Supervisors : Patrice Malfreyt (ICCF), Mehdi Sahihi (ICCF)

Keywords: *plasma proteins; PVC; molecular simulations; biofouling.*

Understanding the physio-chemical factors underlying the process of biofouling is of crucial relevance for enhancing the design of new biomaterials. In this study, we initially evaluated the affinity of plasma proteins towards Polyvinyl chloride (PVC) using molecular docking. Human Serum Albumin was found to be the most relevant plasma protein to study its adsorption on the PVC surface. From 0.5 μs long MD simulations, we quantitatively studied the interactions between HSA and PVC while carefully monitoring potential structural changes of the protein during the adsorption process. HSA was found to spontaneously adsorb on the PVC surface without enduring substantial damage to its secondary structure. Moreover, we evaluated the thermodynamics parameters governing the adsorption process by calculating the Potential of Mean Force (PMF). The Gibbs free energy of adsorption was found to be -507.38 kJ/mol at 300 K, indicating that the process is spontaneous and thermodynamically favored. We also studied the adsorption process at different temperatures (290 K and 310 K) and we have found that the results are consistent and that the process is enthalpy-driven. The findings of this molecular study provide an extensive evaluation of one of the most critical processes determining medical devices compatibility. Future investigations involving other plasma proteins and more complicated biomaterials are recommended to provide more insights to guide the design of new materials in the biomedical industry.



Fluorination by solid-gas reaction of high-performance compounds for rechargeable batteries

Saida Moumen

Supervisors : Laurent Jouffret (ICCF), Kevin Lemoine (ICCF), Enora Lavanant (ICCF), Laura Albero Blanquer (Umicore)

Keywords: *solid electrolytes; chalcogens; stability; gaseous fluorination; rechargeable batteries*.

Lithium-ion (LiB) batteries are pivotal to modern energy storage systems, powering electric vehicles and many everyday electronic devices. The market for rechargeable lithium batteries is booming as new technological applications demand higher energy densities and advances in storage and safety. From a safety perspective, the nucleation and growth of lithium dendrites can cause the battery to short-circuit when the two electrodes are connected. On the other hand, battery overheating can cause fires or system explosions because liquid electrolytes contain flammable solvents. The development of non-flammable solid electrolytes seems to be the solution to this safety problem, forming a barrier that inhibits the growth of lithium dendrites, thus preventing contact between the two electrodes. [1, 2] Solid electrolytes are becoming increasingly popular in research due to their recent interest in the energy field.

In this talk, we will present the state of the art of studies carried out to improve the performance of these materials. In particular, we will focus on one of the approaches being explored: fluorination. Fluorination has emerged as a promising technique to optimize the properties of solid electrolytes, especially in terms of ionic conductivity and electrochemical stability. [3,4] Finally, the results of research work carried out on this subject, including the fluorination of a solid electrolyte using xenon difluoride XeF_2, will be presented. The fluorination of two types of materials will be highlighted, a crystalline material and a glass-ceramic material.

References

[1] Zheng, F. et al., J. Power Sources 389, 198–213 (2018).
[2] Chen, R. et al., Chem. Rev. 120 (14), 6820–6877 (2020).
[3] Lu, Y. et al., ACS Appl. Mater. Interfaces 11 (2), 2042–2049 (2019).
[4] Gao, L. et al., J. Energy Chem. 77, 521–528 (2023).

Knot theory and knot invariants

Clément Legrand

Supervisors : Michael Heusener (LMBP)

Keywords: *knot theory; low dimensional topology; invariant; classification.*

Knot theory is a branch of mathematics which tries to understand how a string can be knotted in the space. This theory arose in the middle of the 19^{th} century with Gauss and Tait. During this time physicists thought that the structure of the atoms could be knots. In this context Tait decided to investigate the question of knots and created a table with all knots up to a certain number of crossings. It turns out that atoms are not knots, but knot theory is still an active research domain in mathematics because of its links with low dimensional topology and theoretical physics. In this talk we will first give a mathematical definition of a knot and try to understand how we can make a list of such objects.

References

[1] R. H. Crowell and R. H. Fox, *Introduction to knot theory*, Graduate Texts in Mathematics, Vol. 57, Springer-Verlag, New York-Heidelberg, 1977 (Reprint of the 1963 original).

[2] A. Kawauchi, *A survey of knot theory*, Birkhäuser Verlag, Basel, 1996 (translated and revised from the 1990 Japanese original by the author).

Study of anisotropic cosmic expansion with type Ia supernovae from the Zwicky Transient Facility

Chloé Barjou-Delayre

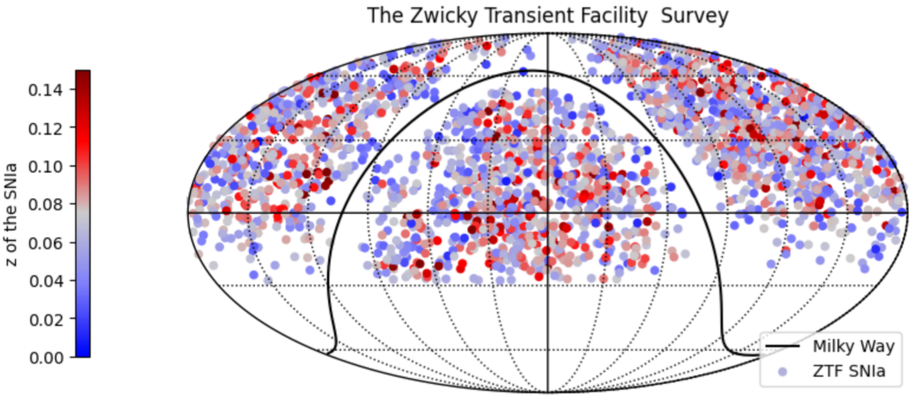
Supervisors : Philippe Rosnet (LPCA)

Keywords: *cosmology; supernovae; universe.*

The type Ia Supernovae (Sne Ia) are astronomical objects essential for cosmologist. Their common explosion mechanism produces almost the same luminosity which allows us to deduce their distance, making them "standards candles". By knowing their distance, we can study and characterize the Universe.

Indeed thanks to E. Hubble studies we know that the Universe is in expansion. A way to study it is to construct what we call in cosmology a Hubble diagram which represents the redshift of the SNe Ia as a function of their distances (the redshift, z, is an observational quantity used to describe the recessing velocity of astrophysical objects). From this diagram we can deduce several cosmological parameters describing the expansion of the Universe. Such as the Hubble constant, denoted H_0, which describe the current expansion rate of the Universe. Hoewever, the value of H_0 is still debated as the different methods to measure it lead to incompatible results. This tension questions the standard cosmological model, based on the cosmological principal stating that the Universe is homogeneous and isotropic.

The Zwicky Transient Facility (ZTF) telescope has detected more than 3000 Sne Ia in the nearby Universe during its first phase (2018-2020). This unique data sample allows to address new cosmological questions as potential anisotropy in the local Universe. My thesis subject is to try to test the expansion rate in the local Universe, i.e. verify if H_0 has the same value in any direction.



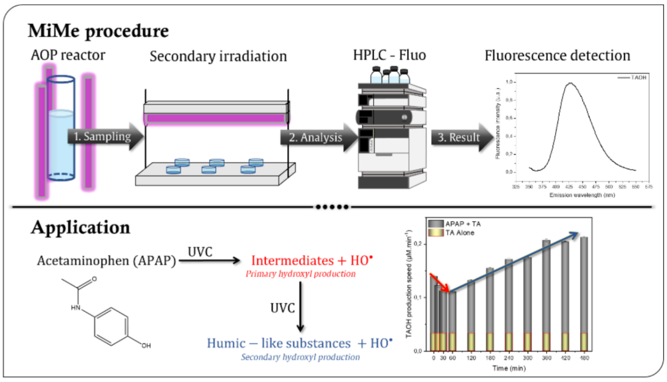
Development of a new method for temporal monitoring of hydroxyl radicals during UV-based AOPs

Hugo Clermont

Supervisors : Mohamad Sleiman (ICCF), Gilles Mailhot (ICCF, LaMP)

Keywords: *ROS; UVC; terephthalic Acid; photodegradation; acetaminophen; fluorescence*.

This research focus is the development of the Mirror Method (MiMe), a new methodology for monitoring the production of hydroxyl radicals ($HO^•$) during advanced oxidation processes (AOPs). The method provides a precise and non-invasive way to track $HO^•$ generation over time, enabling real-time assessment of the oxidative capacity of AOPs without interfering with the reaction dynamics. Terephthalic acid (TA) is used for the monitoring of $HO^•$ while 4-hydroxyphenylacetic acid (HPAA) coupled with horseradish peroxidase (HRP), is used for tracking H_2O_2. Detection is carried out using spectrofluorimetry and liquid chromatography coupled with fluorescence detection, following product generation in a mirrored setup of the main reactor.



Key parameters, including probe concentration, photon flux, total volume, and irradiation time, were systematically optimized to enhance the reliability and sensitivity for the MiMe. Using acetaminophen (APAP) degradation under UVC irradiation as a model system, the MiMe is used not only to quantify $HO^•$ production but also to uncover the critical role of reaction intermediates, such as oligomers and humic-like substances (HuLiS), in enhancing $HO^•$ generation in the later stages of degradation. The ability to use HPLC for separation and analysis of intermediates ensures accurate and interference-free monitoring of $HO^•$ production, even in the presence of fluorescent by-products.

The method's high sensitivity, reproducibility, and ability to assess the degradation of pollutants over time without disrupting the AOP make it a powerful tool for studying ROS dynamics in environmental processes. Furthermore, the MiMe procedure can be expanded to monitor multiple ROS species simultaneously, providing a comprehensive approach to understanding the intricacies of AOP degradation mechanisms.

Photobiological transformation of organic compounds in clouds

Pauline Nibert

Supervisors : Laurent Deguillaume (LaMP), Angelica Bianco (LaMP)

Keywords: *cloud; organic matter; mass spectrometry; photochemistry; microorganisms.*

Clouds cover almost 70% of the Earth's surface and are one of the greatest sources of uncertainty in climate models [1]. Due to their multiphasic nature, clouds are characterised as a complex, dynamic and transformative medium. While the relative composition of inorganic species in the aqueous phase of the cloud is fairly well-known, it is not the case for organic species, since in average 50–80% of these compounds remains unknown [2]. Recently, a new impetus in the analysis of organics has been given by the development in high resolution mass spectrometry, such as Fourier Transform Ion Cyclotron Resonance Mass Spectrometry analysis (FT-ICR MS), that have been used to explore the complexity of dissolved organic matter (DOM) in clouds at the molecular level. In addition to the chemical reactions that occur naturally in the cloud, microbiological processes can also influence the transformation of compounds in the cloud aqueous phase.

The goal of my work is to compare the impact of photochemistry and micro-organisms on DOM composition. In this frame, we carried out an incubation/irradiation of real in-situ collected cloud water (i.e. with the endogenous microorganisms and the natural DOM and oxidants). A cloud sample was collected on 04/09/2024 at the puy de Dôme observatory and then divided into five equal fractions: (0) analysed as time 0 of our experiment, (1) exposed to UV-vis light with microorganisms to study the synergy between photochemical and microbiological transformations, (2) exposed to UV-vis light without microorganisms to study the impact of photochemistry, (3) kept in the dark with microorganisms to study microbiological transformations and (4) kept in the dark without microorganisms to have a control experiment. Each sample was then incubated for 8h and aliquots were taken at intermediate times (2h and 4h). Previous to the FT-ICR MS analysis, the DOM contained in each aliquots was preconcentrated and desalted by solid phase extraction (SPE). Once the mass spectrum obtained, signal to noise correction, internal recalibration, formula assignment and data treatment are carried out using different software such as DataAnalysis, MFassignR [3, 4], and python programming. Statistical tools such as principal component analysis (PCA) or clustering allow us to find correlation and difference between the various aliquots. Further physicochemical and microbiological analysis were also performed on each aliquot. The results obtained show a significant variation of the DOM composition, even after only 8h of incubation/irradiation, and give us new hints for the future research in this field.

References

[1] H. Herrmann et al., Chem. Rev. 115(10), 4259–4334 (2015).

[2] P. Herckes, K. T. Valsaraj, J. L. Collett Jr., Atmos. Res. 132, 434–449 (2013).

[3] L. Pailler, P. Renard, E. Nicol, L. Deguillaume, A. Bianco, Molecules, 27(22), 7796 (2022).

[4] S. K. Schum, L. E. Brown, L. R. Mazzoleni, Environ. Res. 191, 110114 (2020).

Carbon origin of carbonatites: Constraints given by short-lived radioactive systems ^{146}Sm-^{142}Nd and ^{182}Hf-^{182}W

Thomas Rouyer

Supervisors : R. Doucelance (LMV), M. Boyet (LMV), H. Rizo (Carleton University)

Keywords: *isotopic geochemistry; carbonatites; TIMS.*

Carbonatites are magmatic rocks, which mean that they ascent from the Earth mantle as a magma. They are characterized by low silica (<20 weight %) but high carbonate contents (>50 weight %). Although uncommon, they are currently known at 609 locations on Earth which are both spatially and temporally widespread [1]. They range from 3 billion years old in Greenland to the present day at the Oldoinyo Lengaï volcano (Tanzania). Carbonatites are associated with very different geological settings including oceanic islands (Cape Verde), rift systems (Kaizerstuhl, Germany) and even large igneous provinces such as the Deccan Trapps (Amba Dongar, India). This long and extensive presence on Earth suggests that carbonatites play an important role in Earth's mantle dynamics.

However, the mechanisms behind their formation are still poorly constrained, and uncertainty remains about the origin of their carbon enrichment. Two main hypotheses currently address this question. The first suggests that carbon in carbonatites is primordial, originating directly from a mantle source, typically linked to a deep and isolated reservoir. The second proposes that carbon enrichment results from recycled carbon, either inherently present in the carbonatite source or introduced through contamination during its ascent. This recycling could be linked to processes such as subduction fluids and sediments being incorporated into the source, crustal delamination, or contamination during magma ascent.

Short-lived radioactive systems provide important insights into deep and early mantle dynamics. As all radioactive systems they have captured early Earth mantle processes that cause chemical fractionation, such as core and mantle-crust formation. However, due to their short half-life $(T_{1/2}^{^{182}\text{Hf}} = 8,9\ Ma\,;\ T_{1/2}^{^{146}\text{Sm}} = 103\ Ma)$ and because their radioactive decay has ceased, the snapshot they provide of early Earth mantle processes remained intact.

Here, I present the first results of the coupled use of the short-lived radioactive systems ^{146}Sm-^{142}Nd and ^{182}Hf-^{182}W to place constraints on carbonatite formation processes and sources, and to assess possible spatial and temporal variations.

References

[1] Humphreys-Williams and Zahirovic (2021), *Elements*, Vol. 17, 339–344.

Photochemical transformation of triphenyl phosphate with reactive species in cloud water

Yi Wu

Supervisors : Marcello Brigante (ICCF), Angelica Bianco (LaMP)

Keywords: *cloud water; reactive species; photooxidation; organic pollutant.*

Clouds, covering approximately 50% of the Earth's surface, can undergo various reactions due to contributing 7%–15% of atmospheric aqueous phase volume and the abundance of organic and inorganic matters, metals, microorganisms, etc., especially with solar irradiation, playing an important role in atmospheric chemical composition and fate of substances. Photogenerated reactive species (RS) from various precursors drive the oxidation capacity of cloud water, including hydroxyl radical ($HO^\bullet$), sulfate radical (SO_4^-), and also triplet state ($^3C^*$) [1]. In the natural environment, the physicochemical properties of cloud water from different air mass origins vary considerably, leading to variations in abundance of $HO^\bullet$, SO_4^-, and $^3C^*$. Organics are important sinks for RS in cloud water and 70%–90% of dissolved organic compounds remain uncharacterized. Recently, organic compounds from biogenic or anthropogenic origin, like phenolic compounds, pesticides, additives, etc., have been widely detected in the atmosphere. Triphenyl phosphate (TPHP), an organophosphate ester, is a semi-volatile organic compound, and its reaction with $HO^\bullet$ has been considered as the dominant sink process. Nevertheless, the transformation mechanism in cloud water, especially in the case of multiple RS under solar irradiation, has not yet been clearly clarified.

In this work, we used hydrogen peroxide (H_2O_2), persulfate (PS), and 2-benzoylbenzoic acid (BBA) as precursors, respectively, to yield $HO^\bullet$, SO_4^-, and $^3C^*$, to investigate their reactivity with TPHP under simulated solar illumination. Results showed that the phototransformation rate constants of TPHP increased with initial precursor concentration. Second-order reaction rate constants of $HO^\bullet$ and SO_4^- with TPHP ($k_{\text{TPHP},\text{HO}^\bullet} = 7.20 \times 10^9$ M^{-1} s^{-1} and $k_{\text{TPHP},\text{SO}_4^-} = 5.99 \times 10^9$ M^{-1} s^{-1}) were calculated by competitive kinetics with a reference compound, and for $^3\text{BBA}^*$ ($k_{\text{TPHP},^3\text{BBA}^*} = 1.73 \times 10^9$ M^{-1} s^{-1}) using transient absorption spectroscopy. Transformation pathways of TPHP in hv-H_2O_2, PS, or BBA reaction systems were proposed by identifying intermediates using HPLC-MS and IC-MS analysis. The contribution of the three RS to the transformation of TPHP was assessed based on $k_{\text{TPHP,active species}}$ and their abundance in cloud water from different air mass origins (urban, remote, marine). Furthermore, the lifetime of TPHP was calculated to better understand its fate in the atmospheric aqueous phase.

References

[1] Herrmann, H.; Hoffmann, D.; Schaefer, T.; Bräuer, P.; Tilgner, A., ChemPhysChem, 2010, 11 (18), 3796–3822.

Search for the coherent neutrinoless conversion of a muon bound to a nucleus into an electron at J-Parc

Thomas Clouvel

Supervisors : Cristina Cârloganu (LPCA)

Keywords: *particle physics; muon; cLFV; BSM physics.*

The Standard Model (SM) of particle physics provides a comprehensive description of the elementary particles and their interactions. Despite its remarkable success in providing experimental predictions, several phenomena remain to be explained. In particular, the results of neutrino oscillation experiments have shown flavor violation for neutral leptons [1]. However, flavor violation has not yet been observed in charged leptons. In the Standard Model, charged lepton flavor violation (cLFV) is strictly forbidden, and even in minimal extensions to account for neutrino oscillations, it is highly suppressed by the large mass of the W boson. The COMET experiment [2] aims to detect cLFV through a process involving new physics: the coherent neutrinoless conversion of a muon bound to a nucleus into an electron. The experiment is designed to achieve a single event sensitivity of 10^{-17} on this process branching ratio, representing an improvement by four orders of magnitude compared to the current world limit [3]. A significant challenge for COMET is the mitigation of background from cosmic rays. Atmospheric muons could enter the detector and produce electrons that mimic signal events or be misidentified as electron candidates. A subsystem known as the Cosmic Ray Veto (CRV) is designed to distinguish cosmic ray-induced events from genuine signal events. A comprehensive study of the radiation environment that affects the CRV has been conducted to optimize its efficiency, exploring various geometric configurations and shielding materials.

References

[1] The Super-Kamiokande Collaboration, *Evidence for oscillation of atmospheric neutrinos*, Phys. Rev. Lett., 81:1562–1567, 1998.

[2] The COMET Collaboration, *COMET Phase-I technical design report*, Prog. Theor. Exp. Phys., 033C01:102, 2020.

[3] The SINDRUM II Collaboration, *A search for μ–e conversion in muonic gold*, Eur. Phys. J. C, 47:337–346, 2006.

Spikes traps and geometry of numbers

Florian Tilliet

Supervisors : Eric Gaudron (LMBP)

Keywords: *geometry of numbers; Minkowski's theorem.*

Imagine that you are trapped in a room with a spiked wall closing in and threatening to crush you. If you are small enough, you might sneak between the spikes, but if you are too big, you will probably end up dead. Geometry of numbers is a branch of mathematics that allows us to estimate the maximal size you should not exceed to survive in this room. In this talk, I will present the fundamental result of this domain, known as Minkowski's theorem. It has numerous applications in other areas of mathematics, such as number theory, as well as in modern cryptographic systems.

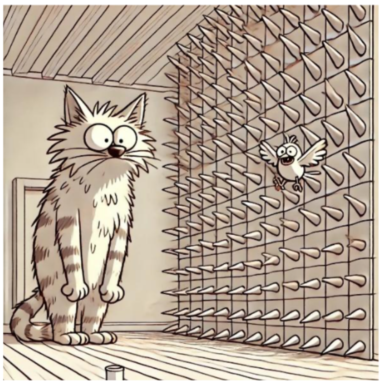


Image generated by Dall-E.

Investigation of sorption and photochemical capacity of sewage sludge derived materials for the removal of emerging contaminants

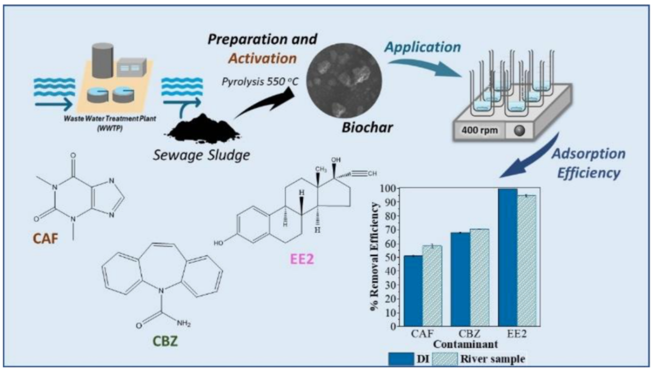
Marina Anastasiou

Supervisors : Vasilios Sakkas (University of Ioannina), Mohamad Sleiman (ICCF)

Keywords: *sewage sludge; biochar; caffeine; carbamazepine; 17-α-ethinylestradiol.*

Annually, wastewater treatment plants produce millions of tons of sewage sludge [1], which present the facilities with high disposal and processing costs [2]. An attractive alternative to common disposal methods is the thermochemical conversion of sludge into biochar, an activated carbon-like material with promising potential in water decontamination applications.

This study investigates materials derived from sludge and biochar for contaminant removal via sorption and photochemical processes. Sewage sludge and biochar pyrolyzed at 550°C were mechanically milled, activated, and characterized by an assortment of techniques before their application. Carboxylic groups and phenols were among the surface functional groups detected, with the materials presenting heterogeinity in their morphology.



Three organic pollutants with an increasing presence in wastewater effluents —caffeine (CAF), carbamazepine (CBZ) and 17-α-ethinylestradiol (EE2)—were selected for evaluation. Results showed effective removal of 17-α-ethinylestradiol (%R= 100%), followed by carbamazepine (%R= 68%) and caffeine (%R = 51%). Parameters affecting removal efficiency included among others, initial concentrations of biochar and the contaminants, along with temperature. For a better understanding of the system's dynamics, kinetic, adsorption equilibrium and thermodynamic studies were performed.

Under UVC irradiation, sludge was found to effectively degrade the studied contaminants indicating its potential use in photochemical water treatment processes. Furthermore, meassurements of reactive oxgen species (ROS) produced were conducted for the investigation of the undelying degradation pathways. Research is underway to explore the efficiency of biochar and sludge-derived composites with photcatalytic materials for effective, sustainable, and cost-efficient contaminant removal.

References

[1] Eurostat, 2022, https://ec.europa.eu/eurostat.

[2] Bondarczuk et al. (2016) Environment International, 87, 49–55.

Posters

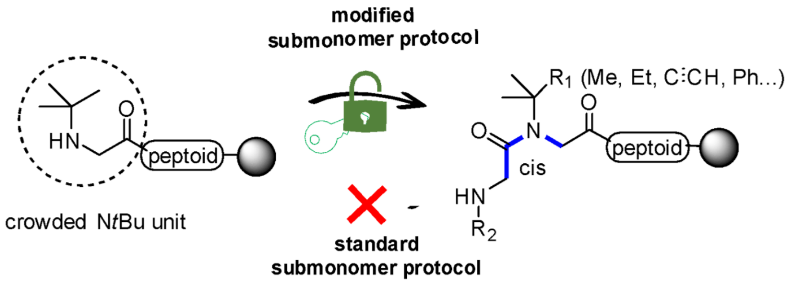
The difficulty of solid-phase synthesis of peptoid oligomers with bulky tert-butyl side chains has finally been tackled

Zacharie Bordas

Supervisors : Claude Taillefumier (ICCF), Sophie Faure (ICCF)

Keywords: *peptoid; peptide; solid-phase synthesis.*

In 1992, peptoids, a new class of biotic foldamers emerged [1]. Peptoids, i.e. N-substituted glycine oligomers, represent a unique class of protease-resistant peptidomimetics that closely resemble peptides. However, substitution of the amide nitrogen reduces the ability to form intramolecular hydrogen bonds and, consequently, the factors governing peptoid folding are different. Tertiary amide bonds in peptoids generally exist as cis- and trans-isomers in equilibrium. The adoption of stable secondary structures relies on the ability to control this equilibrium, which in turn depends to a very large extent on side chain chemistry (electronic factors, steric hindrance, ability to form hydrogen bonds). Our group has enriched the peptoid toolbox by proposing several cis-inductive side chains, and in particular the tert-butyl side chain [2]. Steric hindrance of the tert-butyl group allow the adoption of the cis amide. This side chain has already shown its ability to strongly stabilise polyproline I (PPI)-type helices. Here, we report the first solid-phase syntheses of peptoids containing NtBu units, using a modified submonomer protocol. To demonstrate the effectiveness of this new protocol, we synthesized a series of homooligomers with up to 12 NtBu units and applied it to the synthesis of various peptoid oligomers with sterically demanding NCα-gem-dimethyl side chains (mimics of proteinogenic side chains) [3].



References

[1] R.J. Simon, R.S. Kania, R.N. Zuckermann, et al., Proc Natl Acad Sci., 1992, 89, 9367-9371.

[2] O. Roy, C. Caumes, Y. Esvan, C. Didierjean, S. Faure, C. Taillefumier., Org Lett., 2013, 15, 2246-2249.

[3] R. Shyam, L. Nauton, G. Angelici, O. Roy, C. Taillefumier, S. Faure., Biopolymers, 2019, 110, e23273.

How to seek hydrogen in earth's mantle?

Jessy Dominique

Supervisors : Nathalie Bolfan-Casanova (LMV), Bertrand Moine (LMV)

Keywords: *mantle, hydrogen, water, experimental, xenoliths.*

Hydrogen, also referred as "water", is one of the most common element on Earth's surface and is essential for life. However, Earth's mantle is estimated to be the main hydrogen reservoir of the planet by storing the equivalent of several ocean masses. Though it is mostly composed of nominally anhydrous minerals (NAMs), hydrogen is stored as a trace element (part per million weight; ppm wt.) within mineral structure defects. Earth's mantle can be studied in two ways: either by analysing natural samples (xenoliths, peridotites massifs, melt inclusions) but this kind of method is generally limited to the uppermost part of the mantle except for rare superdeep minerals (majorite, diamond) going down to the transition zone (400-660 km depth). The second possibility is to use experiments to constraint as close as possible the physico-chemical behaviour of deep mantle lithologies. This study presents an overall view of the methods used to seek hydrogen in the minerals and the state of knowledge of hydrogen behaviour in the mantle. This will combine knowledge from experiments with recent contributions from natural samples to understand which processes favor hydrogen incorporation using various parameters such as hydrogen solubility in minerals, pressure, temperature, oxygen fugacity and species speciation (i.e., proportion of H_2-CH_4-OH-H_2O in the system).

Unravelling UV-induced photochemical mechanisms for nano-polystyrene pemoval from water

Yongrong Zou

Supervisors : Gilles Mailhot (ICCF, LaMP), Mohamad Sleiman (ICCF)

Keywords: *polystyrene nanoplastics; UV-based AOPs; hydroxyl radicals ($^{\bullet}OH$); photochemistry.*

During human-induced disposal or natural weathering, plastics undergo fragmentation or degradation into smaller particles, which can be defined as microplastics (MPs, 1 µm to 5 mm) or nanoplastics (NPs, 1 to 1000 nm) depending on their sizes [1]. The small-sized plastic fragments pose a greater threat to ecosystems and humans than larger plastic pieces, which has attracted global concern. Consequently, it is urgent to develop effective and environmentally sustainable methods for the removal of NPs from aquatic environments.

In this study, we focused on applying different homogenous advanced oxidation processes (AOPs) for the removal of polystyrene nanoplastics (PS-NPs) from water, evaluating the impact of different UV-induced oxidation processes on the apparent color and turbidity of the suspension, microscopic morphology, dynamic size, molar weight, UV characteristic absorption, and intermediate products. Specifically, the dynamic changes of reactive oxygen species (ROS) such as $^{\bullet}OH$, H_2O_2, and ROOH during the reaction process were monitored using fluorescence spectrophotometer and high-performance liquid chromatography (HPLC) techniques.

The photoaging of PS-NPs induced by photo-based AOPs is shown in the Fig.1. The UV irradiation could induce PS-NPs to generate ROS, which subsequently attack the surface of PS-NPs, resulting in the production of yellowing discoloration and humic-like components. These products are also precursors of ROS, ultimately contributing to the oxidative degradation of PS-NPs. Additionally, different light sources (UVA, UVB and UVC) could influence the composition and amount of ROS generated, thereby affecting the reaction time scale. Furthermore, the introduction of oxidants (H_2O_2) significantly impacts these photochemical processes, either positively or negatively depending on the light sources.

The qualitative and quantitative analysis of PS-NPs in the AOPs and quantitative monitoring of ROS can help us to understand the behavior of PS-NPs in the environment, which also provides a scientific basis for the development of effective nano-pollution control strategies.

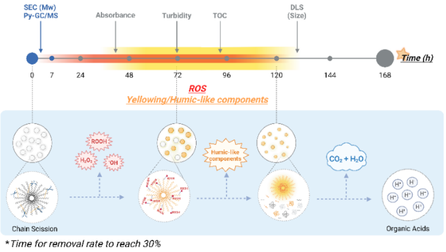


Figure 1. Schematic illustration of PS-NPs photoaging behavior in water.

References

[1] Junaid, M., Liu, S., Chen, G., et al., 2023, *Transgenerational impacts of micro(nano)plastics in the aquatic and terrestrial environment*, Journal of Hazardous Materials, 443(Pt B), 130274.

Institut de Chimie de
Clermont-Ferrand

Comparisons of radiosonde water vapor measurements with ECMWF ERA-5 and contrails observations above Clermont-Ferrand

Sidy Diarra

Supervisors : J.L. Baray (LaMP, OPGC), P. Keckhut (LaTMOS), N. Montoux (LaMP)

Keywords: *water vapour, cirrus, contrail, Lidar, full sky camera, ECMWF ERA5.*

Cirrus clouds significantly influence the radiation budget of the Earth, depending on their optical thickness and altitudes [1]. The contrails formed from aircraft emissions contribute also to this effect [2]. The formation of contrails and their potential evolution in cirrus clouds is linked to the fine scale thermodynamic state of the atmosphere, and to the supersaturation of water vapour with respect to ice. However, obtaining reliable measurements of water vapor at the the typical contrail altitude formation (10 km) remains challenging.

In this study, we combine different observations: Lidar is used to detect ice crystals [3], standard meteorological balloon soundings provide temperature, water vapor, and wind profiles [4], and meteorological reanalyses (ECMWF) is analyzed to better understand the overall context.

The first objective of this study is to assess the quality of the radiosondes humidity measurements from MeteoFrance network by comparing with the ERA-5 reanalysis at the aircraft cruise altitudes. The second objective focuses on documenting the formation and evolution of contrails. This is achieved using a combination of instruments: an ADS-B recorder to identify aircraft type and position, a full sky camera to detect the presence of contrails and a collocated lidar to retrieve macrophysical and optical properties of the contrail and water vapour concentration.

A case study which occurred on June 2, 2023, over the CO-PDD site (Clermont-Ferrand, France) reveals two distinct contrail categories: Persistent contrails (>2 hours) were observed under favorable conditions with with RHI of 107%-116%, temperatures of 217-223 K, and horizontal extensions up to 4.78 km. In contrast, non-persistent contrails (<3 minutes) formed under less favorable conditions, with RHI below 90% and temperatures above 214 K. This study is part of the European project BeCoM (101056885) whose objective is to reduce the contrail radiative forcing.

References

[1] Heymsfield et al., (2017). Meteorological Monographs, 58, 2-1.

[2] Kärcher et al., (2018). Nature communications, 9(1), 1824.

[3] Fréville et al. (2015). Sensors, 2015, 15, 3041-306

[4] Dupont et al., (2020). Journal of Atmospheric and Oceanic Technology, 37(5), 857-871

Study of charmless 3-body b-hadron decays with π^0 and assessment of the calorimeter reconstruction performance for the LHCb ECAL upgrade project

Laetitia Guerry

Supervisors : Vincent Tisserand (LPCA), Stéphane Monteil (LPCA)

Keywords: *LHCb detector, b-hadrons, picosecond timing detector.*

The Standard Model of Particle Physics explains successfully the fundamental interactions between particles of ordinary matter. However, it is incomplete, as it cannot explain neutrino masses nor cosmological observations such as matter-antimatter asymmetry in the Universe or the origin of dark matter. Physics beyond the Standard Model is either searched for production of new particles via high energy collisions or from physics happening at the intensity frontier. The indirect approach provides accurate measurements of the Standard Model parameters to confront theory and studied process where virtual new particles could contribute.

This analysis, carried out in collaboration with physicists from Pekin, UCAS and Wuhan universities will provide precise measurements of the branching fractions of b-hadron such as $B^0_{(s)}$ and Λ_b baryon into $h^+h^-\pi^0$ final states, where h can either be protons, pions or kaons. These chamless b-quark transitions are dominantly proceeding through loop diagrams in the SM and can embody in principle Beyond Standard Model amplitudes. The nature of a particle in LHCb is determined from the combination of information from the different particle's identification (PID) subdetectors [1]. PID variables are commonly used in particle physics analysis to fight against misidentification background, therefore these responses need to be precisely reproduced in the Monte Carlo (MC) simulation. The detector features are implemented in the simulation to mimic the DATA behaviour but corrections still need to be applied to MC samples to remove the imperfections of the simulation and reflect samples collected during data taking in the years 2016-2018 at LHC pp collider. Dedicated multivariate tools were designed to select signal candidates where each particle is correctly identified and reject combinatorial background coming from random combination of unrelated tracks or neutral pions.

Studying final states containing neutral pion is a challenge in LHCb due to the large amount of combinatorics coming from photons association. During the high luminosity phase of the LHC, the number of collisions per bunch crossing in LHCb will increase from $\mu = 5$ to $\mu = 50$. To be able to distinguish photons coming from the same pp collision and reduce the pileup, the SPIDER (Swift Pipelined DigitizER) ASIC is currently being designed. This new technology will bring the knowledge of the timing of the energy depositions in the electromagnetic calorimeter with tens of picosecond of resolution.

References

[1] A. Poluektov, ICHEP 2018.

Photostability of multilayer films containing recycled polyethylene

Alexy Duchamp

Supervisors : J. Christmann (ICCF), S. Therias (ICCF)

Keywords: *polyethylene, recycling, photoageing, durability*.

The use of Recycled Plastic Materials (RPM) is a major concern to improve our environmental impact in the production of new plastic products. The integration of these RPM, either alone or mixed with virgin material, raises major questions about the durability of the products under outdoor use conditions, with stress factors such as sunlight or heat causing photoageing.

To tackle these issues, Barbier Group (French company producing polyethylene – PE – films) and POPPI (POlymers, Photochemistry, Properties and Interfaces) group are working in close collaboration in the frame of the Common Laboratory POPBA. One of the main objectives of POPBA is to study the photoageing of PE films containing recycled materials.

A preliminary study showed that recycled PE (r-PE) films photooxidize faster than virgin PE (v-PE) ones, either without added stabilizer or in presence of HALS. The present study aims to study the effect of incorporating r-PE (in a blend or as a multilayersystem with v-PE) on the photostability of the obtained films. Non-stabilized and stabilized (with HALS type NH) systems were considered. A multiscale analysis was performed on these samples in order to link the modifications of the chemical structure and macromolecular architecture to that of the use properties, especially mechanical ones. It was shown that blend and multilayer systems have a photostability between that of v-PE and r-PE alone. Tensile tests and oxidation profiles within the film thickness will also be presented.

Institut de Chimie de
Clermont-Ferrand

Chromium oxidation strategies in YAG:Cr powders synthesized via Pechini process

Romain Thévenet

Supervisors : François Réveret (ICCF), Geneviève Chadeyron (ICCF), Audrey Potdevin (ICCF)

Keywords: *YAG:Cr^{4+}; lasers; Pechini synthesis.*

Cr^{4+}-doped $Y_3Al_5O_{12}$ crystals (YAG:Cr^{4+}) are currently a source of interest for laser fabrication due to both their saturable absorption and gain medium properties. The most common synthesis methods yield to the obtaining of bulk materials, transparent ceramics or monocrystals, which require an oxidation step of the dopant using a high-temperature thermal treatment [1].

This study presents the synthesis of YAG:Cr powders through Pechini process. The oxidation of chromium ions in the YAG matrix was achieved through a codoping with a charge compensator ion and/or the use of an oxidizing agent during the synthesis. The obtained powders were structurally and morphologically characterized through X-ray diffraction and microscopy. UV-visible spectroscopy of the obtained powders shows the appearance of absorption bands attributed to Cr^{4+} after optimization of the synthesis conditions (Figure 1a). Emission spectroscopy of these same powders confirms the presence of Cr^{4+} ions in the YAG matrix obtained under oxidizing conditions (Figure 1b). These optical characterizations demonstrate the efficiency of the oxidation treatment applied.

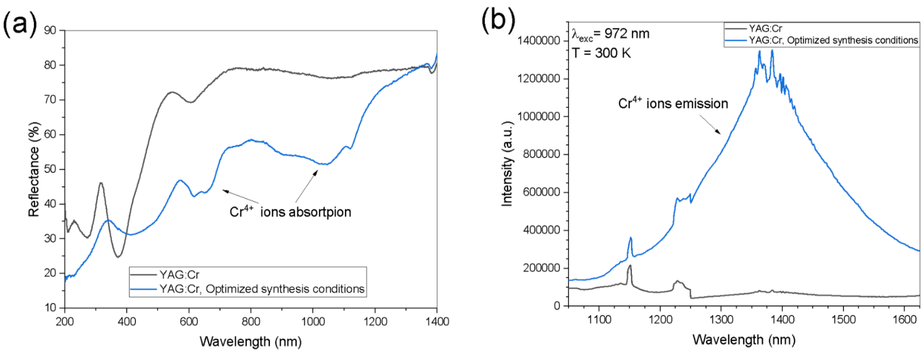


Figure 1. a) Diffuse refelectance UV-visible spectra of obtained YAG:Cr powders.
b) Emission spectroscopy of the same YAG:Cr powders.

References

[1] Perrière, C., et al., *Study of dopant distribution in Cr^{4+}:YAG transparent ceramics and its use as passively Q-switching media in Nd:YAG laser delivering 38 mJ per pulse*, Opt. Mater. X, vol. 12, p. 100107, 2021.

Institut de Chimie de
Clermont-Ferrand

Preparation and characterization of a monolithic composite composed of geopolymers and layered fouble hydroxides (LDH) for simultaneous immobilization of ions in an alkaline environment

Yunge Bai

Supervisors : Fabrice Leroux (ICCF), Guillaume Renaudin (ICCF)

Keywords: *geopolymer, layered double hydroxide, co-immobilisation.*

A geopolymer foam-based monolithic composite filter has been developed for the co-immobilisation of cationic and anionic pollutants. By combining geopolymer, which traps cations, with layered double hydroxides (LDH), known for their anion exchange properties, the filter enables simultaneous removal of both types of pollutants. A powder study demonstrated the synergistic effect of this combination for co-adsorption. [1] The proposed synthesis method allows the formation of monolithic filters suitable for pollutant immobilization in real case.

This work focuses on developing a geopolymer/LDH composite foam to optimize microstructure and ion exchange performance. Synthetic AFm phases (calcium-based LDH with enhanced alkaline stability) were incorporated during the alkaline activation of metakaolin-based geopolymer. Foaming, achieved using hydrogen peroxide and a surfactant, enables liquid percolation. The composites were characterized by XRD, Raman, and solid-state ^{27}Al NMR, revealing partial carbonation and degradation of the Ca_2Al-NO_3 AFm phase during alkaline activation. Synthesis parameters were optimized to stabilize the composite, paving the way for co-immobilisation tests on cation/anion pairs.

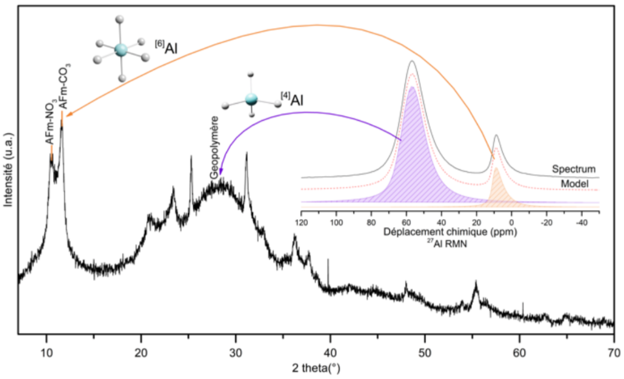


Figure 1. XRD and ^{27}Al NMR spectra of a monolithic geopolymer/40% Ca_2Al-NO_3 AFm composite activated by sodium silicate, showing aluminum in tetrahedral (geopolymer) and octahedral (LDH) coordination.

References

[1] Q. Tian, K. Sasaki, *A novel composite of layered double hydroxide/geopolymer for co-immobilization of* Cs^+ *and* SeO_4^{2-} *from aqueous solution*, Science of The Total Environment, 2019, 695, 133799.

Institut de Chimie de
Clermont-Ferrand

Rejuvenation of magmatic systems: Identification and quantification of recharge and mixing processes as eruption triggers

Nicole Vizuete

Supervisors : Etienne Médard (LMV), Pablo Samaniego (LMV)

Keywords: *magma stockage; magma recharge; eruption triggers; explosive volcanism; dacitic composition.*

Volcanic eruptions result from complex processes occurring within the Earth's lithosphere, including melt generation in the mantle, magma accumulation in crustal reservoirs, and magma ascent through the crust up to the surface. For an eruption to occur, magma stored at the trans crustal magmatic reservoirs should have the suitable viscosity and density to promote magma ascent while pressure gradients are developed in the upper reservoir and conduits. Highly explosive dacitic eruptions in arc systems frequently follow extended periods of quiescence, during which magma reservoirs undergo multiple recharge and reheating events. Understanding these pre-eruptive "priming" steps is essential for deciphering the behaviour of volcanic plumbing systems and the triggering mechanisms of large eruptions.

Magmatic reservoirs in the crust often develop mushy zones, i.e. partially crystallized regions that can be rejuvenated by the intrusion of hotter, volatile-rich magmas. Petrological evidence of such recharge includes mafic enclaves, mingling structures, and mineral textures indicative of chemical disequilibrium. Our study aims to identify and characterize magma recharge and mixing events, as these processes have triggered numerous highly explosive eruptions worldwide. Identifying the frequency and mechanisms of recharge events is crucial for volcanic hazard assessment. While macroscopic evidence of mixing may be absent, microscopic textural and compositional features, particularly in plagioclase crystals, reveal thermal cycling linked to successive, non-eruptive recharge events.

To investigate these processes, we analyze two dacitic eruptions: the 800 BP Plinian eruption of Quilotoa volcano (Ecuador) and the 1802 AD collapse-driven eruption of Tutupaca volcano (Peru). Despite differences in eruptive dynamics, both eruptions produced moderate-to large-volume dacitic deposits (64–66 wt.% SiO_2) with similar mineral assemblages composed by plagioclase, amphibole, biotite and Fe-To oxides. Our findings indicate disequilibrium features in plagioclase crystals, with variations in chemical composition and temperature reflected in their zoning patterns. Growth phases interrupted by dissolution suggest thermally induced fluctuations, indicative of multiple magma reinjections. These recharges may result from (1) convection within a chemically homogeneous magma reservoir (rejuvenation) and/or (2) mixing between resident and newly injected magma (mingling). To fully constrain the processes leading to these eruptions, further analysis of trace elements in plagioclase (e.g., Mg, Fe, Sr) and pre-eruptive conditions is required. Our ultimate goal is to construct thermal profiles of the magma reservoirs by correlating An content with thermometric calibrations and diffusion studies. These insights will enhance our understanding of magmatic rejuvenation and its role in triggering explosive eruptions.

Evaluation of machine learning models for forecasting the occurrence of occupational accidents using binary time series

Aho Yapi

Supervisors : Pierre Latouche (LMBP, X), Arnaud Guillin (LMBP, IUF), Yan Bailly (Cikaba)

Keywords: *occupational accident prevention, binary time series, machine learning*.

Occupational accidents represent a major challenge for companies and employees due to their significant human and economic costs. However, current prevention strategies struggle to proactively anticipate risks. Data from field reports, near-misses, and other organizational and human factors remain largely underutilized in existing accident prediction approaches. In this context, this study introduces a generic framework for short-term workplace accident forecasting, incorporating covariates and relying on binary time series. To ensure the robustness and operational applicability of the models, a cross-validation methodology specific to time series, combined with an optimisation and evaluation based on aggregated periods, is proposed. Several machine learning algorithms, including both traditional methods and deep learning approaches, were trained, evaluated, and compared within this framework. The results highlight the relevance of our approach and provide valuable insights for identifying the most effective models in occupational accident prediction.

Gas transport behaviour of isotactic-polypropylene and bio-banking: A molecular dynamics simulation approach

Ghazal Borhan

Supervisors : P. Malfreyt (ICCF)

Keywords: *isotactic polypropylene (i-PP), biobank, gas transport behavior, laboratory applications.*

Isotactic polypropylene (i-PP) is widely utilized in medical and laboratory applications, including syringes, pipette tips, microplates, and storage tubes, due to its high rigidity, good chemical resistance, and suitability for sterilization. [1] In addition to these properties, the gas penetration behavior of i-PP plays a crucial role in preserving the stability and integrity of biological samples, making it a valuable material for biobanking. [2]

A "biobank" is defined as an organized process for the long-term storage of biological samples and associated data to support diverse research purposes. [3] Optimizing biobanking processes—including sample collection, transportation, preservation, and storage—requires the selection of appropriate polymer materials for medical containers and laboratory devices. Since maintaining the stability of biological samples is essential, understanding the gas penetration behavior of i-PP is critical for its effective use in storage applications. This study investigates the transport behavior of four different gas penetrate molecules including O_2, N_2, H_2, and CO_2, in i-PP using molecular dynamics (MD) simulations.

We considered the mean squared displacement (MSD) of the gas molecules as a function of time to describe the gas diffusion(D). [4] Also solubility(S) were determined through the test particle insertion (TPI) method. [5] The calculations have been studied in four temperatures: 300 K, 350 K, 400 K, and 500 K.

The results indicate that (D) correlates with molecular effective size and increases with temperature, whereas (S) is more closely related to the condensability and decreases as temperature rises. Finally, our findings suggest that i-PP can be considered an effective gas barrier within a specific temperature range.

References

[1] Gai.K , Ren.X , Chen.J , Zhou.X , Wan.Q , Li.Y, Industrial & Engineering Chemistry Research /2022, 62(2)-971-981/ DOI: 10.1021/acs.iecr.2c03446.

[2] Knizhnik.A , Komarov.P , Potapkin.B , Shirabaykin.D , Sinitsa.A , Trepalin.S, Minerals, 2023, 13, 1151. DOI:10.3390/min13091151

[3] Hewitt.R , Watson.P, Biopreservation and Biobanking, 2013, 11(5) 309-315/ DOI:10.1089/bio.2013.0042.

[4] Muller-Plathe.F, Acta Polym., 1994 (45) 259–293. DIO:10.1002/actp.1994.010450401

[5] Widom.B , Chem.J Phys., 1963 (39) 2808–2812. DIO:10.1063/1.1734110.

Institut de Chimie de Clermont-Ferrand

Measuring the lifetime of a mixed light-matter quasi-particle: the Polariton

Loïc Méchin

Supervisors : Pierre Disseix (IP), François Médard (IP)

Keywords: *condensed matter physics; optics; light-matter interaction; experimental techniques*.

For fifty years, the improvement of electronic devices has been based on the miniaturization of components, following the well-known Moore's law. The use of electrons imposes intrinsic limits on the operation of theses devices due to the fermionic nature of these charge carriers, leading to energy losses through interactions between electrons and their environment. The photon, elementary particle of light, seems to be a good candidate to improve the energy efficiency and the operating frequency of these devices. However, the use of light is prevented by the impossibility of making interactions between two photons.

To address this issue, the scientific community has proposed to use a quasi-particle, named polariton, which results from the reversible exchange of energy between an elementary excitation of the material (named exciton), and a photonic mode propagating in the material. Polaritons have properties of both light (high velocity) and matter (strong interactions), which is useful to realize new optoelectronic devices. For potential applications and because polariton results from the strong coupling between exciton and photon, it is necessary to confine the light in the active material and to have robust excitons (electron-hole pairs in coulomb interaction), even at room temperature. The realization of an optical waveguide with gallium nitride (GaN) satisfies both conditions: (i) confinement of light by total internal reflections, and (ii) robust excitons thanks to the large bandgap of GaN.

Operation of optoelectronic devices based on polaritons depends strongly on the lifetime of this quasi-particle. In this work, we present an experimental technique to optically measure the lifetime of polaritons. This technique consists of extract the polaritonic guided mode using a grating coupler deposited on the surface of the waveguide and to image the focal plane (reciprocal space) on the entrance slit of a camera with a short temporal resolution (a few $10^{-}12$ s) to study the temporal decay of the luminescence of polariton states along their dispersion curve. The obtained experimental results are then analysed with theoretical models allowing to determine the polariton lifetime and are compared to the theoretical predictions of the coupled oscillators model [1] to confirm the findings. Our study also highlights several sources of feeding for the polaritonic guided mode, in particular through built-in electric field effects [2], intrinsic to polar materials such as GaN.

References

[1] J. J. Hopfield, *Theory of the Contribution of Excitons to the Complex Dielectric Constant of Crystals*, Phys. Rev. 112, 1555 (1958).

[2] L. Méchin et al., *Effects of the Built-in Electric Field on Free and Bound Excitons in a Polar GaN/AlGaN/GaN Based Heterostructure*, arXiv:2501.07164.

ZnAl-Cl LDH derived mixed oxides as photocatalysts for degradation of persistent herbicide in water

Hao Wang

Supervisors : Vanessa Prévot (ICCF), Mohamed Sarakha (ICCF), Claude Forano (ICCF)

Keywords: *ZnAl-Cl LDH, persulfate, photocatalysis.*

Layered Double Hydroxides (LDHs) containing transition metals, are materials with tunable chemical composition and unique lamellar structure, receiving extensive advertence in recent years because of their photoactivity, and particularly for the photocatalytic degradation of various pollutants, such as bisphenol A via Advanced Oxidation Processes (AOPs). Upon thermal treatment, the layered structures of LDHs collapse and transform into non-stoichiometric metastable mixed metal oxides with semiconducting properties. Such chemical transformation can enhance the photocatalytic activity by increasing surface area and improving redox properties [1].

In this study, we investigated the photocatalytic degradation of chloridazone (CLZ) as a model pollutant using calcined ZnAl-LDH as a photocatalyst combined with persulfate (PS) photocatalytic oxidation. CLZ is a selective herbicide belonging to the pyridazinone-derived pesticide class [2].

As a result, shown in the Fig.1, ZnAl-LDH-500°C exhibits highly efficient degradation activity for CLZ under the synergism of photocatalysis and PS oxidation, which is 1.72 higher than that in the photocatalytic systems, respectively. Simultaneously, we also studied the effects of different condition parameters on the photodegradation of CLZ in ZnAl-LDH /PS/light system, such as dosage of photocatalyst, concentration of PS, PH and so on. In addition, radical quenching experiments showed that $SO_4^{\cdot -}$ and $OH^{\cdot}$ jointly participated in the degradation of CLZ. A deep structural characterization (XPS, PL) of pristine LDH and calcined derivatives was performed in order to identify the catalytic active species. This study might provide an excellent reference for high-efficiency catal ysts for pollutant degradation in the actual environment.

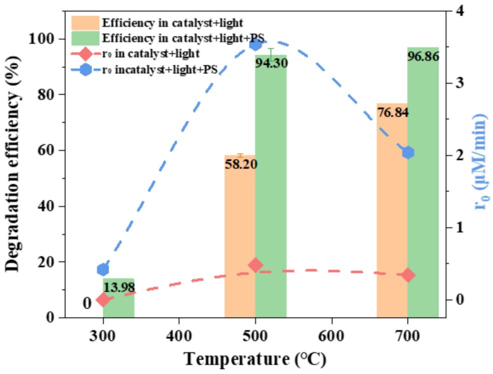


Figure 1. Degradation efficiency of CLZ and initial rate in different catalysts/light with or without PS system.

References

[1] Ali Khan et al., Journal of Energy Chemistry (2023), 84: 242-276.

[2] El-Said et al., Journal of Environmental Chemical Engineering (2018), 6(2): 2214-2221.

Institut de Chimie de
Clermont-Ferrand

Enhancing photovoltaic module efficiency and stability using phosphor/polymer composites as encapsulants

Hugo Lajoie

Supervisors : S. Thérias (ICCF)

Keywords: *phosphor; nanocomposites; fluorescence; dispersion; UV-downconversion; photovoltaic.*

Ultraviolet (UV) radiation is a major factor in the degradation of both polymer encapsulants and solar cells in photovoltaic (PV) modules. In polymer encapsulants, UV exposure accelerates yellowing due to the photo-aging of additives, particularly UV absorbers, leading to a loss of transparency that negatively impacts the efficiency of solar cells. Additionally, UV-induced degradation of the cells themselves contributes to decreased performance, while these high-energy photons are only minimally converted into electricity. Addressing both the degradation and underutilization of UV photons is critical to improving PV module performance and longevity.

This study investigates the integration of fluorescent down-converters particles into polymer encapsulants to tackle these issues, and to boost the efficiency of the solar module itself. Three types of fluorescent materials were studied : carbon quantum dots (CQDs) with red emission, quinine with blue emission, and "Alq3 complexes" with yellow-green emission. These phosphors with down-conversion properties were incorporated into industrial-grade ethylene-vinyl acetate (EVA) or in thermoplastic polyolefin (TPO) films, which are among the most commonly used polymer encapsulants in photovoltaic field. The phosphor/polymer composites were prepared in toluene solution to achieve homogeneous particle dispersion and prepration of thin films ($< 100\ \mu$m).

Films with different content of phosphors in the polymer composites were studied. Both fluorometric and transmission analyses were performed to study the optical properties of the films in terms of UV absorption and re-emission intensity. While increasing the phosphor concentration led to higher UV absorption, this did not always correlate with an improvement in re-emission efficiency. Through 2D emission maps in the visible range, we found that each type of particle exhibited distinct re-emission behavior in the same polymer matrix.

Further work is focused on optimizing the balance between UV absorption and re-emission efficiency by adjusting the particle concentration and film thickness. Additionally, these particles are expected to display different stability under environmental stresses due to their differing nature (organic or inorganic), spatial geometry, and fluorescence mechanisms. Current studies aim to evaluate their long-term stability under conditions such as UV exposure, thermal cycling or humidity environment to determine their viability in PV applications. Incorporating a functional polymer composite encapsulant into the PV structure has the potential to enhance module efficiency by simultaneously mitigating UV-induced degradation and increasing the conversion of usable light.

Institut de Chimie de
Clermont-Ferrand

Muckenhoupt weights

Jérémie Moukambi Moukambi

Supervisors : Christoph Kriegler (LMBP)

Keywords: *weighted L^p spaces; Hardy-Littlewood maximal operator; doubling measure.*

The class of Muckenhoupt weights A_p consists of those weights ω for which the Hardy-Littlewood maximal operator is bounded on $L^p(d\omega)$ (weighted L^p space). Specifically, we consider functions f on $\mathbb{R}^n$ (real space of dimension n) and their associated maximal function $M(f)$ defined as

$$M(f)(x) = \sup_{r>0} \frac{1}{r^n} \int_{B_r(x)} |f|,$$

where $B_r(x)$ is the ball in $\mathbb{R}^n$ with radius r and center at x. We wish to characterise the functions $\omega : \mathbb{R}^n \to [0, +\infty)$ for which we have a bound

$$\int |M(f)(x)|^p \omega(x)\, dx \leq C \int |f|^p \omega(x)\, dx,$$

where C depends only on p and ω.

In our presentation, we will first recall the definition of the Muckenhoupt class. Then, we will see some examples of functions belonging to this class. And we will end with a discussion of its properties.

References

[1] B. Muckenhoupt, *Weighted Norm Inequalities for the Hardy Maximal Function*, Transactions of the American Mathematical Society, 165: 207-226, 1972.

Synthesis of haspin Kinase inhibitors and development of PROTACs candidates for cancer therapy applications

Killian Malosse

Supervisors : Pascale Moreau (ICCF), Francis Giraud (ICCF)

Keywords: *organic chemistry; kinase inhibitors; PROTACs.*

Due to their crucial role in regulating cell signaling pathways, protein kinases can be implicated in a variety of pathologies. For example, many kinases are overexpressed in cancer. Among them, Haspin stands out as an essential mitotic kinase and a potential therapeutic target, particularly for developing new therapeutic strategies against triple-negative breast cancer and pancreatic cancer, which are associated with poor prognosis. In previous work, a structure-activity relationship study on a pyrroloisoquinoline backbone demonstrated the ability of various compounds to inhibit Haspin [1].

In parallel, a novel therapeutic strategy has emerged: PROTACs (PRoteolysis TArgeting Chimeras), which induce degradation of the targeted protein rather than simply inhibiting it. This intracellular degradation is achieved by hijacking the cell's natural protein degradation system to target the protein of interest (Fig. 1). PROTACs offer several advantages, including efficacy at low doses and a lasting effect even after the molecule has been eliminated from the body.

This work aims to integrate previously identified inhibitors with the PROTACs strategy to break down Haspin kinase, ultimately contributing to the development of novel anti-cancer therapies.

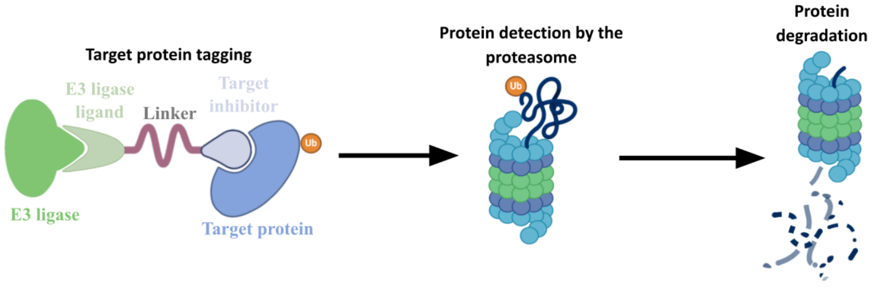


Figure 1. Schematic representation of the PROTAC mechanism.

References

[1] M. Defois, B. Josselin, P. Brindeau, A. Krämer, S. Knapp, F. Anizon, F. Giraud, S. Ruchaud, P. Moreau. *Synthesis and biological evaluation of 1H-pyrrolo[2,3-g]isoquinolines*, Bioorg. Med. Chem., 2024, 100, 117619.

Institut de Chimie de
Clermont-Ferrand

Study of overexpressed enzymes for elastomer degradation

Otmane Hammouti

Supervisors : Virgil Helaine (ICCF), Christine Guerard-Helaine (ICCF)

Keywords: *biocatalysis; biodegradation; enzyme; latex clearing protein; elastomers.*

Tire and road wear particles (TRWP) are small particles emitted by tire treads during use. They are generated by the phenomenon of abrasion, which can be defined as friction between the tire and the road surface. They have a complex composition, 50% of which comes from the tire and 50% from the road environment. The release of TRWPs into the environment is considered as a form of pollution, and is a major concern because of their dispersion in various environmental compartments, and their ability to release various contaminants into water, atmosphere and soil.

With the aim of understanding the environmental fate of TRWP and their degradation mechanisms, Michelin, the Centre National de la Recherche Scientifique (CNRS) and the Université Clermont Auvergne inaugurated a joint laboratory called "BioDLab" in 2023, dedicated to the investigation of abiotic and biotic degradation of tire constitutive dienic elastomers. To achieve this goal, the development of innovative analytical techniques will be an essential prerequisite to detect and characterize the transformation products resulting from the exposition of elastomers to abiotic stresses such as photooxidation or thermooxidation, and to microorganisms or over-expressed enzymes (biotic degradation).

In collaboration with Genoscope (Evry, France), our aim will be to explore the biodiversity for synthetic elastomers-degrading enzymes. A few enzyme families have already been identified in the literature for their ability to degrade hydrocarbon-based polymers. Among them, the latex clearing protein (Lcps) family consists of heme enzymes capable of degrading poly(cis-1,4-isoprene). They have been identified in several bacterial species like *Gordonia*, *Rhodococcus*, *Norcardia*, *Solimonas* and *Streptomyces* [1].

An overview of the production techniques implemented for studying them as well as the developed methods for their activity assessment will be presented herein. Their mechanisms of action and their substrate specificity will also be mentioned.

References

[1] Kasai, D., *Poly(cis-1,4-Isoprene)-Cleavage Enzymes from Natural Rubber-Utilizing Bacteria*, Biosci. Biotechnol. Biochem. 2020, 84 (6), 1089–1097.

Insights into the 2020 instability crisis of Mt Merapi through numerical modeling

Michael Galárraga

Supervisors : Karim Kelfoun (LMV)

Keywords: *discrete element method; magma pressure; flank instability; fracturing*.

The western flank of Mt Merapi (Indonesia), one of the most active volcanoes located in proximity to populated areas, became unstable in October 2020. Surveillance techniques such as Synthetic Aperture Radar (SAR) and Electronic Distance Measurements (EDM) give an idea of the displacement magnitude. However, these remote sensing methods are limited in providing information about subsurface processes and deformation mechanisms. This limitation is critical when assessing the potential for catastrophic flank failure (e.g., Mt. Saint Helens in 1980 [1]), which remains a significant concern.

Observations show a correlation between this flank movement, a NW-SE fracture crossing the entire summit, and the presence of magma within this discontinuity. In order to better understand this instability, we developed numerical models in an attempt to relate the magma pressure to the slope deformation at Mt. Merapi. In particular, relying on its ability to describe progressive failure mechanisms in elasto-plastic media, we use the Discrete Element Method (DEM) [2] to investigate the role of the NW-SE fracture pressurization on the deformation of Mt Merapi flanks.

We show here the main results of sensibility analyses performed to study the influence of the rock mechanical properties, fracture length, and magma pressure magnitude on the flank stability, comparing the resulting deformation with the 2020 Merapi crisis displacements. Despite assumptions such as material homogeneity and hydrostatic pressurization, our modeling approach allows us to make predictions not only on the potential for collapse and its kinematics, but also on the mobilized volumes, all critical for risk assessment.

References

[1] Voight, B., Janda, R. J. & Glicken, H., *Nature and mechanics of the Mount St Helens rockslide—avalanche of 18 May 1980*, Geotechnique 20, A176 (1983).

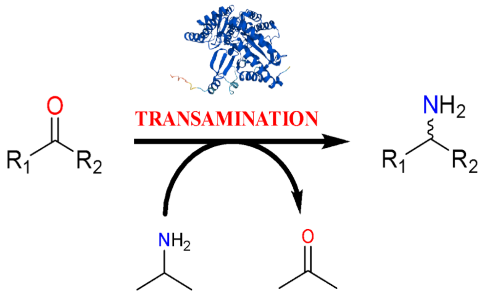
[2] Cundall, P. A. & Strack, O. D. L., *A discrete numerical model for granular assemblies*, Géotechnique 29, 47–65 (1979).

Innovative biocatalytic processes for the stereoselective synthesis of chiral amines and amino alcohols

Stéphany Bouzid

Supervisors : Thierry Gefflaut (ICCF), Virgil Helaine (ICCF)

Keywords: *biocatalysis; transaminases; chiral amines; thermostability; immobilisation*.



Chiral amines play an essential role in medicinal chemistry, and the highly stereoselective and eco-compatible synthesis of this class of molecules is a major challenge for the development of tomorrow's drugs. One of the most successful approaches developed to date involves catalysing the conversion of prochiral ketones to chiral amines using one family enzyme: transaminases (TA), which are abundant in biological systems.

For several years, our team has been researching and studying transaminases in order to develop novel synthetic processes with these enzymes [1,2]. Recently, we have built the largest collection of TAs described to date and identified within it numerous enzymes with high potential for application in organic synthesis [3].

In this presentation, we will highlight the characteristics of one of the best performing TAs in our collection. This enzyme has exceptional properties, such as a broad substrate spectrum and excellent thermostability. In addition, with the aim of purifying and recycling this enzyme, a high-performance immobilisation method will also be presented.

References

[1] Guérard-Hélaine, C. et al., *Stereoselective Synthesis of γ-Hydroxy-α-Amino Acids through Aldolase–Transaminase Recycling Cascades*, Chem. Commun., 2017, 53 (39), 5465–5468.

[2] Heuson, E.et al., *Enantioselective Synthesis of D- and L-α-Amino Acids by Enzymatic Transamination Using Glutamine as Smart Amine Donor.*, Adv. Synth. Catal., 2019, 361 (4), 778–785.

[3] Gourbeyre, L. et al., *Biocatalysed Synthesis of Chiral Amines: Continuous Colorimetric Assays for Mining Amine-Transaminases*, Catal. Sci. Technol., 2021, 11 (3), 904–911.

ÉCOLE DOCTORALE
DES SCIENCES FONDAMENTALES
Université Clermont Auvergne