



# SCIENTIFIC • DAYS •

Doctoral School of Fundamental Sciences

## CAMPUS DES CEZEAUX

Amphithéâtre recherche  
Pôle physique



Seminars

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MAY  
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Posters and talks  
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## WITH THE CONTRIBUTION OF



# GRAPHIC DESIGN

Special thanks to *Camille Valadeau* for, once again, handling the graphic design for the 2026 edition of the Scientific Days!

## CAMILLE VALADEAU

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.



## INVITED TALKS

### FLORE-ANNE PELLOQUET



*Science communication illustrator and designer trained in physical chemistry through the LUMOMAT Master's program (Light, Molecules, Matter). After working as a physical chemistry analyst at Michelin, she developed an illustration-based approach to scientific outreach focused on clarity, accessibility, and visual storytelling. Her experience with science mediation organizations, including Les Petits Débrouillards and AFEV, strengthened her ability to communicate complex scientific ideas to audiences of diverse ages and educational backgrounds while maintaining scientific precision and strong pedagogical engagement.*

### MOHAMED SARAKHA

*Researcher in physical chemistry and environmental photochemistry, specializing in the photocatalytic and photochemical transformation of organic pollutants in aquatic and atmospheric environments. His work focuses on advanced oxidation processes, UV-induced reaction mechanisms, and the environmental fate of emerging contaminants, including pharmaceuticals, pesticides, and industrial compounds. Through kinetic, mechanistic, and spectroscopic approaches, he contributes to the understanding of light-driven chemical dynamics and the development of sustainable strategies for pollutant degradation, water remediation, and environmental protection.*



# TUESDAY 26, MAY

08:30 - 08:45	<b>Reception</b>	
08:45 - 09:00	<b>Opening speech</b>	
09:00 - 09:20	Daeun Kwon (LPCA), <i>How can Monte Carlo simulation unravel the mysteries of the FLASH effect in ultra-high dose rate radiotherapy?</i>	p. 9
09:20 - 09:40	Adrian Darricau (LPCA), <i>An introduction to lepton flavours in particle physics</i>	p. 10
09:40 - 10:00	Thomas Erbland (ICCF), <i>Plasmonic Bi/BiOF heterostructures for CO<sub>2</sub> photoconversion</i>	p. 11
10:00 - 10:30	<b>Poster flash presentations:</b> Mathilde Guilleton (ICCF), Thomas Reggio (LPCA), Aymeric Dziduch (LaMP), Matthieu Finck (IP), Jérémie Moukambi (LMBP), Arthur Sauvagnat (IP)	p. 27–32
10:30 - 11:20	<b>Coffee break &amp; Poster session #1</b>	
11:20 - 11:40	Antoine Canzi (LaMP), <i>Impacts of dust, pollution, and biological particles on ice nucleation activity at the Puy de Dôme mountain station</i>	p. 12
11:40 - 12:00	Adrianna Dujardin (LMV), <i>Intergranular melt in natural peridotites: distribution, melt fraction, and composition</i>	p. 13
12:00 - 13:00	<b>Lunch break</b>	
13:00 - 13:20	Chloé Barjou-Delayre (LPCA), <i>Study of anisotropic cosmic expansion with type Ia supernovae</i>	p. 14
13:20 - 13:40	Abdelhamid Haddad (LPCA), <i>A journey within the ATLAS high-granularity timing detector</i>	p. 15
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15:40 - 16:00	Anne Dorval (LMBP), <i>Geometry, stability, and compression: compactness of composition operators on the polydisc</i>	p. 18
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09:20 - 09:40	Mathilde Torre (IMOST), <i>Development of new therapeutic agents targeting cancer-associated fibroblast</i>	p. 20
09:40 - 10:00	Augusto Misolas (ICCF), <i>Green syntheses of adsorbent and photocatalytic materials from lemon peel wastes for the removal of contaminants in water</i>	p. 21
10:00 - 10:30	<b>Poster flash presentations:</b> Louise Burreler (ICCF), Helena Fest (LMV), Léo Ceremonie (ICCF), Elhadji Mountaga Diallo (LMV), Marion Schmitt (LPCA), Manon Pouget (LMV)	p. 39–44
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# TALKS



# How can Monte Carlo simulation unravel the mysteries of the FLASH effect in ultra-high dose rate radiotherapy?

Daeun Kwon

Supervisors: Lydia Maigne

**Keywords:** *ultra-high dose rate, H<sub>2</sub>O<sub>2</sub>, water radiolysis, Monte Carlo simulation.*

Since 2014, high-dose-rate radiotherapy (> 40 Gy/s) has gained significant momentum due to its ability to spare normal tissue while maintaining an effective tumour control [1]. The prescribed dose is delivered within an extremely short time, from microseconds to milliseconds, but the mechanisms underlying normal tissue protection remain unclear and require understanding, beyond physical interactions, the chemical and biological processes involved. Ionizing radiation induces water radiolysis, producing reactive oxygen species (e.g., •OH, H<sub>2</sub>O<sub>2</sub>) that oxidize DNA, causing strand breaks and chemical modifications critical to radiation-induced cell death. To investigate these mechanisms, using the GATE platform and the Geant4-DNA library, we developed a multi-scale digital twin of a ultra-high dose rate 67.5 MeV proton beam (ARRONAX, IBA Cyclone 70XP, Nantes) impinging a ultra-pure water sample (pH=5.5) and compared our simulations with water radiolysis chemistry experiments handled by radiochemists from the Subatech laboratory. We could reproduce various oxygen levels, CO<sub>2</sub> contents, and dose-rates conditions to follow species along time (from 10<sup>-12</sup> to 15 min after irradiation). We extended the study until the evaluation of DNA strand breaks using a clustering algorithm to be compared in a near future with biological experiments on cell populations. Overall, simulation shows a good agreement with measurements. As perspectives, future work will investigate the role of hydrated electrons in understanding CO<sub>2</sub> and O<sub>2</sub> effects through time resolved radicals' measurement.

## References

- [1] Favaudon, V., Caplier, L., Monceau, V., et al. Ultrahigh dose-rate FLASH irradiation increases the differential response between normal and tumor tissue in mice. *Sci. Transl. Med.* 2014, 6(245):245ra93. doi:10.1126/scitranslmed.3008973.

# An introduction to lepton flavours in particle physics

Adrian Darricau

Supervisors: Jean Orloff, Ana M. Teixeira

**Keywords:** *particle physics, neutrino physics, flavour physics, phenomenology.*

Particle physics aims at describing the fundamental building blocks of matter and their interactions. So far, the Standard Model of particle physics (SM) [1] has shown great success in describing nature at this scale, even predicting numerous phenomena. However, experimental observations offer compelling evidence to the fact that the SM cannot provide the ultimate description of Nature; at the very least, it is incomplete, and further ingredients must be necessarily present to explain neutrino oscillations (massive neutrinos and leptonic mixing) [2], the abundance of a form of non-luminous, dark matter in the Universe, and the matter-antimatter asymmetry of the Universe [3].

In recent years, many well-motivated extensions of the SM have emerged, aiming at addressing (some of) these problems. Some of these New Physics (NP) models exhibit the appealing feature of being testable (and thus falsifiable) by current and future experiments, be it at high-energy colliders or then at the so-called high-intensity frontier. Comprehensive phenomenological studies of these NP models thus include direct searches at colliders, precision observables, flavoured signatures, as well as implications for neutrino phenomena and dark matter observables.

Neutrino oscillations necessarily imply the violation of the so-called “lepton-flavours” in the neutral lepton sector, which are strictly conserved in the SM. In turn this opens the door to a generalised violation of lepton flavours in the charged sector (cLFV) [3]. Some NP models have the interesting feature of predicting cLFV decays which would be within future experimental reach. Such an observation would correspond to a discovery of New Physics!

In this talk, I will introduce the SM and its current limitations, and briefly outline some interesting extensions allowing to overcome the latter issues. Following a presentation of several cLFV transitions and decays which are the object of dedicated searches, I will subsequently illustrate how one can use these observables to test NP models in view of future measurements.

## References

- [1] R. L. Workman et al. (Particle Data Group), *Review of Particle Physics*, *Prog. Theor. Exp. Phys.* 2022, 083C01.
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- [3] Lepton Flavor and Number Conservation, and Physics Beyond the Standard Model, *Prog. Part. Nucl. Phys.* 2013, 71, 75.

# Plasmonic Bi/BiOF heterostructures for CO<sub>2</sub> photoconversion

Thomas Erbland

Supervisors: Pierre Bonnet, Angélique Bousquet

**Keywords:** photocatalysis, bismuth oxyfluorides, plasmonic nanoparticles, CO<sub>2</sub> photoconversion, heterostructures.

Addressing the environmental emergency requires advanced photocatalysts for clean energy production and pollutant remediation. Among Bi-based semiconductors, bismuth oxyfluorides BiO<sub>x</sub>F<sub>3-2x</sub> are promising materials due to their low charge recombination rates, although their activity remains mainly limited to the UV range [1]. In this regard, enhancing their performance through coupling with plasmonic metals is an attractive strategy. Since metallic bismuth exhibits localized surface plasmon resonance (LSPR), integrating Bi nanoparticles with BiOF offers a fully Bi-based and compatible approach.

In this work, we developed a novel synthesis of Bi-NPs/BiOF nanostructures with controlled compositions via in situ exsolution of metallic bismuth using hydrazine hydrate. The materials were characterized structurally, morphologically and optically. Bi/BiOF with optimal composition of 10w% metallic Bi shows best performances for CO<sub>2</sub> selective photoconversion to CO and methyl orange degradation under UV-visible light. The enhancement arises from improved charge separation and extended light absorption induced by plasmonic Bi nanoparticles. This study demonstrates that exsolution is an effective route to engineer efficient LSPR-active photocatalysts for environmental applications.

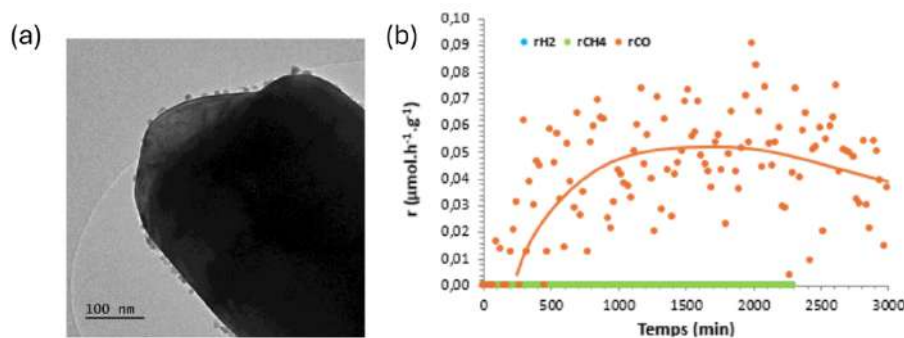


Figure1: (a) TEM image of Bi/BiOF, (b) CO<sub>2</sub> photoconversion under UV-vis light.

## References

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# Impacts of dust, pollution, and biological particles on ice nucleation activity at the Puy de Dôme mountain station

Antoine Canzi

Supervisors: Céline Planche, Evelyn Freney

**Keywords:** *ice nucleating particle, biological aerosols, in situ.*

In this work, we investigate how different aerosol types contribute to ice nucleation (IN) activity at the Puy de Dôme station (PUY, France; 1465 m a.s.l.; [1]) during the RACLET field campaign conducted in April 2024 [2]. PUY observatory is known for its exposure to a wide diversity of air masses and atmospheric conditions, and previous work [3] has shown that the resulting variability in air mass origin strongly influences the IN activity observed at the site. The RACLET campaign provided one month of continuous high-resolution measurements of aerosol properties under contrasting meteorological and air mass conditions. The dataset includes two Saharan dust events, clean and polluted continental air masses, and an unseasonably warm period. INP concentrations were measured with the PINE-c instrument, complemented by fluorescence data from a WIBS-5 and aerosol vertical profiling by LIDAR. This unique combination of in situ and remote sensing observations enables us to assess the influence of particle type, source region, and atmospheric processing on INP concentrations and variability at a mid-tropospheric site. A comparative analysis of the two dust events allows us to investigate the potential effect of dust particle aging on their ice nucleation efficiency. In addition, the combination of in situ and remote sensing measurements enables the reconstruction of vertical INP concentration profiles during these events. The high-temperature period reveals a marked day/night contrast in aerosol properties, notably associated with an increased presence of large biological particles. During the continental polluted air mass event, a strong enhancement in IN activity was observed, correlated with elevated concentrations of submicron particles, suggesting a possible contribution from secondary aerosol components. We will present the results of this study, along with the method used to speciate INP concentrations into contributions from different particle types and origins.

## References

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# Intergranular melt in natural peridotites: distribution, melt fraction, and composition

Adrianna Dujardin

Supervisors: Sylvie Demouchy, Emmanuel Gardés

**Keywords:** *peridotites, intergranular melts, volumic fraction, SEM, EDS.*

Data on melt distribution and composition in natural partially molten peridotites remain either incomplete or contradictory, or even entirely lacking. In this study, we characterize the distribution and composition of the intergranular melt/liquids in several peridotites from the Borée Maar (Massif Central, France). The aim is to quantify the melt fraction and calculate their chemical compositions focusing on major elements and a few minor elements to determine potential equilibrium conditions and condition for melt formation. The observed melt films have thickness ranging from a few tens of nanometers to a few micrometers. These melt films were examined using scanning electron microscope (SEM) and energy-dispersive spectroscopy (EDS) maps. The raw EDS spectra were treated using a new MATLAB macro that we developed. It enables quantitative EDS-based composition determination (down to 0.1 wt.%) for most major and minor elements. Furthermore, our results evidence the presence of different intergranular phases: two melts with distinct textures and compositions, microcrystals of clinopyroxene growing within the intergranular melt films, and bubbles. We also demonstrate that these melts did not originate from infiltration of the host basalt of Borée. To conclude, we also discuss the role and consequences of these melt films as geochemical reservoirs and their impact on geophysical properties.



# Study of anisotropic cosmic expansion with type Ia supernovae

Chloé Barjou-Delayre

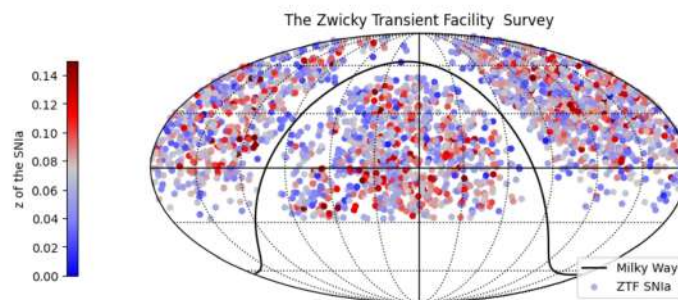
Supervisors: Philippe Rosnet

**Keywords:** *cosmology, supernovae, universe.*

The type Ia Supernovae (Sne Ia) are astronomical objects essential for cosmologists. Their common explosion mechanism produces almost the same luminosity which allows us to deduce their distance, making them 'standard 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 receding 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 describes the current expansion rate of the Universe. However, the value of  $H_0$  is still debated as different methods to measure it lead to incompatible results. This tension questions the standard cosmological model, based on the cosmological principle 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., to verify whether  $H_0$  has the same value in any direction.



# A journey within the ATLAS high-granularity timing detector

Abdelhamid Haddad

Supervisors: Louie Corpe

**Keywords:** *particle physics, Large Hadron Collider, ATLAS experiment, upgrades, high granularity, timing detector, data acquisition software, calibration.*

Particle physics seeks to understand the fundamental building blocks of matter and their interactions. At the forefront of this exploration is the CERN's Large Hadron Collider (LHC) [1]. At the LHC, protons are accelerated and collided at extremely high energies, recreating conditions approaching those after the Big Bang. These collisions allow experiments, such as the ATLAS experiment, which I am part-of, to test theoretical models with unprecedented precisions.

The upcoming High-Luminosity LHC (HL-LHC) [2] upgrade will increase the amount of collected data by roughly a factor of ten by cranking up the number of collisions per unit time, which in turn poses significant challenges for particle reconstruction in the much denser collision environment. To preserve excellent tracking performance, the ATLAS experiment is developing the High-Granularity Timing Detector (HGTD) [3], a precision timing layer capable of measuring particle arrival times with a resolution of about 50 picoseconds.

In this talk, I will introduce you to the LHC and HL-LHC, discuss the role of HGTD within ATLAS and present my contributions to the data acquisition software and detector calibration.

## References

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# A deep crustal effect on the genesis of Peruvian magmas

Tristan Chaptal

Supervisors: Gannoun Mouhcine, Nauret François, Samaniego Pablo

**Keywords:** *subduction zone, central volcanic zone, Peru, garnet signature, isotopy.*

The formation of mountains and volcanism is caused by the mobility of tectonic plates. In the case of the Andes, the Nazca plate undergoes subduction beneath the South American plate, resulting in explosive volcanism that can be seen in Peru. The magmas that feed the volcanoes are produced at the deep mantle and pass through the continental crust. These magmas undergo processes that modify their physico-chemical properties, and these modifications have repercussions on the eruptive dynamics at the surface. To understand the volcanic activity, it is necessary to understand the formation of magmas at depth. I am interested in the contribution of the continental crust to these magmas as they rise to the surface.

Following field missions, laboratory work enables the chemical and isotopic compositions of lava to be analysed. We are able to retrace the history of the magmas and to quantify the effect of the continental crust. My thesis work focuses on Peruvian volcanism because it is located in the subduction zone with the thickest continental crust (70 km). The second part of this study focuses on the analysis of products emitted by the Peruvian monogenic volcanoes, located near the city of Arequipa. Approximately 30 edifices were sampled during a two-week mission in May-June 2024. These volcanoes are doubly interesting: they are located at the boundary between two large crustal provinces and have some of the most primitive compositions in the region. They are therefore ideal for trying to better understand the processes involved in the early stages of magma formation.

Using the geochemical compositions of my samples, I show that a group of products emitted by these volcanoes (those that have undergone the least differentiation) exhibit a certain heterogeneity but acquire a common signature during their differentiation: the garnet signature. This term refers to high element ratios present in magmas, induced by the presence of garnet, a high-pressure mineral. Through various models, we show that this signature is acquired through ternary mixing processes at the base of the crust, with magmas resulting from the partial melting of lithologies with residual garnet. We also show that the isotopic compositions of our samples are strongly controlled by the location of each volcano, and therefore controlled by local heterogeneities in the basement.



# Eu<sup>3+</sup>-doped YVO<sub>4</sub> materials synthesized via sol-gel for luminescent coatings

Fernanda Garcia De La Cruz

Supervisors: Audrey Potdevin, Damien Boyer

**Keywords:** YVO<sub>4</sub>:Eu<sup>3+</sup>, sol-gel process, dip-coating, luminescent materials.

Recent progress in optical and photonic technologies has intensified the need for high-performance luminescent materials, particularly as size-controlled powders and homogeneous thin films [1]. Consequently, current research is largely directed toward optimizing synthesis strategies and processing techniques for established host matrices instead of introducing entirely new material systems [2]. Among vanadate-based phosphors, europium-doped yttrium orthovanadate (YVO<sub>4</sub>:Eu<sup>3+</sup>) continues to stand out due to its strong red emission under UV excitation and remarkable chemical stability [3]. In this work, YVO<sub>4</sub>:Eu<sup>3+</sup> materials were synthesized by an original sol-gel route using vanadium oxytrisopropoxide as the vanadium precursor and yttrium and europium chlorides as rare-earth sources. The resulting sols were either dried and sintered to result in crystallized powders or subsequently used to fabricate highly luminescent coatings by dip-coating deposition technique, allowing the preparation of uniform and well-adherent thin films on glass substrate. The sol-gel method proves to be a highly promising technique, offering additional benefits such as low-temperature synthesis, uniform powder morphology, and homogeneous multicomponent coatings. The structural and morphological studies of powders and coatings were conducted using X-ray diffraction (XRD), FT-IR and Raman spectroscopies as well as scanning electron microscopy (SEM). The XRD patterns confirm the formation of crystalline YVO<sub>4</sub>:Eu<sup>3+</sup> in all the case (Fig. 1a), while the visual appearance of the coating under daylight and UV light are shown in Fig. 1b and Fig.1c, respectively. Finally, the optical properties were recorded by photoluminescence and UV-visible spectroscopies. These results highlight the versatility of the sol-gel approach for producing YVO<sub>4</sub>:Eu<sup>3+</sup> luminescent powders and coatings.

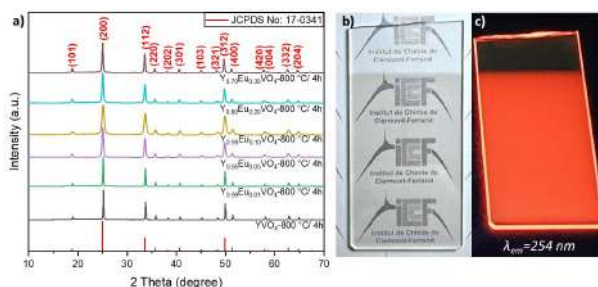


Fig. a) XRD patterns of YVO<sub>4</sub> with different Eu<sup>3+</sup> concentrations, picture of prepared coating upon b) daylight, and c) UV light.

## References

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- [3] Piz, M. *Journal of Thermal Analysis and Calorimetry* 2025, 150, 19823

# Geometry, stability, and compression: compactness of composition operators on the polydisc

Anne Dorval

Supervisors: Frédéric Bayart

**Keywords:** *complex analysis, composition operators.*

Composition operators arise from a simple idea: first deform a space, then observe how functions defined on that space are affected by this deformation. In this talk, I investigate this phenomenon in Bergman spaces on the polydisc, a multidimensional domain from complex analysis. The central question is: when does a geometric deformation not only preserve stability, but also enforce a form of concentration or simplification? This property, known as compactness, can be viewed as a mathematical notion of compression: families of potentially complex functions become, after transformation, automatically more regular or more concentrated. I will present the geometric intuition behind the phenomenon, the underlying analytical mechanisms and the precise criteria connecting boundary behaviour and compactness.



# Accelerating the search for new physics at the LHC using BumpNet

Eva Mayer

Supervisors: Julien Donini, Manon Michel, Samuel Calvet

**Keywords:** *machine learning, ATLAS, bump hunt, new physics, data analysis, LHC.*

Particle physics aims to understand the fundamental constituents of matter and the forces governing them. While the current theoretical framework, the Standard Model, successfully explains a wide range of experimental observations, several phenomena, such as dark matter, remain unexplained. This motivates the search for previously unknown particles at the Large Hadron Collider (LHC) at CERN.

At the LHC, protons are accelerated to nearly the speed of light and collided at extremely high energies, producing a wide variety of particles that are recorded by large detectors such as ATLAS. If a new particle is produced and rapidly decays into known particles, it may appear as a small excess of events at a particular value in a reconstructed mass distribution. Identifying such signals within enormous datasets is challenging and traditionally requires highly specialized analyses targeting specific theoretical scenarios, often taking years of work.

In this project, a machine-learning method designed to search for these signals more efficiently is developed. The approach uses a convolutional neural network, called BumpNet, to automatically identify statistically significant excesses in particle mass distributions without requiring detailed background modelling for each case. This enables a broad, model-independent scan of many possible signatures in the data within a fraction of the time required for traditional analyses.

Initial studies using simulated data show promising results, including successfully reproducing known experimental signals and identifying potential new-physics scenarios. Such approaches could significantly accelerate the exploration of the vast datasets produced by the LHC and help ensure that no unexpected discoveries remain hidden in the data.

## References

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# Development of new therapeutic agents targeting cancer-associated fibroblast

Mathilde Torre

Supervisors: Emmanuelle Moreau, Sébastien Schmitt

**Keywords:** *tumour targeting, cancer, fibroblast, chemotherapy, tumour microenvironment.*

Nowadays, one of the major challenges in oncology is the lack of selectivity of therapeutic agents, which leads to significant side-effects and limited therapeutic efficacy. An emerging strategy to overcome this involves targeting specific components of the tumour microenvironment (TME) [1]. Indeed, TME accounts for approximately 40 to 50% of the tumour mass and is composed of various cell types that interact in a complementary and complex manner. Among these, cancer-associated fibroblasts (CAFs) represent a major cellular component of the TME. CAFs express on their surface a specific marker known as Fibroblast Activation Protein (FAP $\alpha$ ), a type II transmembrane serine protease. More than 90% of solid tumours express FAP $\alpha$ , whereas its expression is almost undetectable in healthy tissues, except in granulation tissue during wound healing [2]. FAP $\alpha$  therefore emerges as a highly attractive target for tumour-specific drug delivery. Our objective is to design and optimize vectors targeting FAP $\alpha$  that can be conjugated to therapeutic agents, thereby enhancing both tumour selectivity and therapeutic index. Drawing inspiration from vectors successfully employed in nuclear medicine [3], we have synthesized new analogues and functionalized them with various hydrophilic or lipophilic linkers, to modulate their hydrophilic-lipophilic balance. The enzymatic activity of these analogues will be evaluated against FAP $\alpha$  and related enzymes such as DPPs or PREP. This comprehensive screening approach will enable us to identify vectors with optimal selectivity profiles [4]. In the subsequent stage, the most promising vectors will be conjugated with therapeutic agent, with the ultimate goal of improving treatment efficacy while significantly reducing systemic toxicity. This targeted approach represents a compelling strategy for precision cancer therapy, specifically designed to exploit the unique characteristics of the tumour microenvironment.

## References

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- [4] Poplawski, S. E., et al. *J. Nucl. Med.* 2024, 65, 100.



# Green syntheses of adsorbent and photocatalytic materials from lemon peel wastes for the removal of contaminants in water

Augusto Misolas

Supervisors: Mohamad Sleiman, Vasilios Sakkas

**Keywords:** *lemon peel, green synthesis, adsorbent, photocatalysis, contaminants.*

Emerging contaminants particularly pharmaceuticals when not efficiently treated contribute to the aquatic and environmental toxicities. During water treatment, different materials have been utilized for the removal of these contaminants. The synthesis of these materials may also have an environmental impact when hazardous and large volume of chemicals are used. This study explores the synthesis of different materials from a waste material using green and sustainable routes. Lemon peel wastes were obtained from lemon processing plant in Chalkida, Greece. They were cleaned, dried, and pulverized. Biochar was produced by pyrolyzing dried lemon peel powder at different temperatures and was characterized using different analytical methods. Biochar are carbon-rich materials with exposed functional groups capable as adsorbent of contaminants. Next, carbon quantum dots (CQDs) were synthesized from biochar at different conditions (dose, temperature, time) using hydrothermal method, eliminating the use of any solvent. The CQDs were combined with graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) to improve its photocatalytic efficiency in different water matrices. Further, silver nanoparticles (AgNP) were synthesized in a microwave reactor (< 5 min) using lemon peel powder extracts as reductant. UV-Vis measurements confirmed the successful synthesis of nanoparticles. Lastly, zinc oxide (ZnO) nanoparticles were also synthesized following an optimized microwave conditions (3 min, 300 W) using Zinc (II) solution and lemon peel powder extracts. The lemon peel extracts acted as stabilizers of ZnO particles increasing the production of ZnO particles. UV-Vis measurements confirmed the synthesis of ZnO. The adsorption efficiencies and the photocatalytic activities of the different materials produced were tested for the removal of emerging contaminants in water like anti-convulsive drug- carbamazepine and anti-diabetic drugs- gliclazide and repaglinide.

# Engineering light-matter coupling in TMD-based optical microcavities: from free excitons to Moiré exciton-polaritons

Maria Vittoria Maggi

Supervisors: Dmitry Solnyshkov, Guillaume Malpuech

**Keywords:** *cavity quantum electrodynamics, moiré lattice, quantum blockade, optical spin Hall effect, corner-space renormalization algorithm.*

The exciting new research field called Cavity Quantum Electrodynamics of Quantum Materials, an emerging area at the interface between quantum condensed matter physics and photonics, studies how confined electromagnetic fields can modify collective states of matter, such as in Bose-Einstein condensation or superconductivity. Indeed, strong light-matter coupling allows electronic degrees of freedom to acquire new symmetries and topological properties from the photonic environment.

Our work is focuses on excitons in twisted bilayer transition metal dichalcogenides (TMDs), which form a moiré superlattice with a nanometer-scale primitive vector. Embedding these structures into optical microcavities enables the engineering of light-matter interactions toward the quantum blockade regime [1], a nonlinear regime relevant for quantum memory and computing applications.

The first part of my work is devoted to the Optical Spin Hall Effect under non-resonant excitation in  $WS_2$  monolayers on a planar waveguide with distributed Bragg reflectors. Dark excitons with out-of-plane dipoles coherently excite both polarization modes, which acquire an out-of-plane electric field projection due to TE-TM mixing, revealing a novel exciton-photon coupling mechanism. The second part models light interacting with the TMDs lattice using a many-body Bose-Hubbard approach. It identifies optimal parameters for quantum blockade: intra- and inter-site correlations and hopping amplitudes. Dissipative processes are explicitly included through the Master Equation formalism. To address the computational challenges of many-body open systems, simulations are performed using the Monte Carlo wavefunction method combined with a corner-space renormalization algorithm [2], enabling tractable simulations in regimes that would otherwise be computationally prohibitive.

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# Sensitivity of the FCC-ee to the tau lepton forward-backward asymmetry in Z decays

Willy Weber

Supervisors: Romain Madar

**Keywords:** *FCC-ee, tau leptons, electroweak interactions, forward-backward asymmetry.*

The Future Circular Collider in its electron-positron phase (FCC-ee), proposed at CERN, is designed to produce large numbers of well-controlled particle collisions. This offers a unique opportunity to precisely test the Standard Model (SM) of particle physics [1].

The study presented at the 2026 Scientific Days of the Ecole Doctorale des Sciences Fondamentales (EDSF) focuses on tau leptons, heavier relatives of electrons that are produced in these collisions. Tau leptons decay almost immediately into lighter particles, including at least one neutrino, which cannot be directly detected. As a result, part of the information about the original tau is always missing, making its reconstruction a significant experimental challenge.

Using detailed computer simulations of both the particle collisions and the detector response, it is studied how accurately the original direction of a tau lepton can be inferred from its visible decay products. By analyzing the angular distribution of reconstructed tau leptons, asymmetries in their production predicted by the SM are probed.

A central observable in this context is the forward-backward asymmetry, the tendency of particles to be produced more frequently in one direction relative to the direction of the incoming electron beam. This asymmetry is highly sensitive to the structure of the electroweak interaction and provides a precise test of the fundamental symmetries described by the SM.

This work helps determine how precisely such measurements can be performed at the FCC-ee and defines important performance requirements for future detector systems. In doing so, it contributes to preparing the next generation of precision experiments aimed at testing the fundamental structure of matter.

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# POSTERS



# The unloved tagatose-1,6-bisphosphate aldolase proves to be of interest

Mathilde Guilleton

Supervisors: Christine Guérard-Hélaine, Virgil Hélaine

**Keywords:** *aldolase, biocatalysis, stereoselective synthesis.*

In the context of green chemistry, which promotes the use of selective catalysts and waste-minimizing processes, enzymes are valuable tools for the synthesis of complex molecules.

The aldol reaction is a key transformation for forming carbon-carbon bonds, enabling the construction of elaborated molecular frameworks and the introduction of new functional groups in a single step, often generating one or two stereogenic centers. Aldolases provide precise control over stereoselectivity, regio-, and chemoselectivity under mild and environmentally friendly conditions.

Among DHAP-dependent aldolases, four enzymes allow access to the four possible stereochemical configurations. However, selective access to the (S,S) configuration remains limited. The tagatose-1,6-bisphosphate aldolase (TagA), the enzyme associated with this configuration, is not strictly stereoselective and produces a mixture of D-tagatose-1,6-bisphosphate and D-fructose-1,6-bisphosphate [1,2].

This low selectivity has likely limited interest in TagA, leaving its catalytic potential largely unexplored [3]. Selective formation of (S,S) products is crucial for bioactive compounds such as D-tagatose, a low-glycemic sweetener with favorable nutritional and metabolic properties. Producing its phosphorylated precursor, D-tagatose-1,6-bisphosphate, is therefore a strategic step. Screening 200 aldolases led to the discovery of a new TagA capable of selectively generating pure D-tagatose-1,6-bisphosphate. Exploration of its substrate scope subsequently enabled the synthesis of several (S,S) compounds obtained pure or highly enriched.

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# Dark matter phenomenology: from feeble to stronger coupling

Thomas Reggio

Supervisors: Andreas Goudelis

**Keywords:** *particle physics, phenomenology, dark matter, freeze-in, freeze-out, cosmology.*

Since several decades, the question of the nature of dark matter has been a major motivation for the construction of a vast number of theories Beyond the Standard Model of particle physics. The most important observation that all dark matter models try to answer is why there is as much dark matter in the Universe as is inferred from Cosmic Microwave Background observations.

In order to do so we need to consider a production mechanism associated with a dark matter model. One of those mechanisms is the so called freeze-in. Within this framework, the cosmic density of dark matter depends on the initial temperature of the early Universe. Usually taken to be effectively infinite it is, nevertheless, a poorly constrained quantity and can assume relatively small values.

In this talk I will introduce the evidence for the existence of dark matter as well as different production mechanisms, then present how a low initial cosmic temperature can drastically change the predictions of a concrete dark matter model.

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# Ice crystal morphology and microphysical properties of low-level Arctic mixed-phase clouds from four airborne campaigns near Svalbard

Aymeric Dziduch

Supervisors: Olivier Jourdan, Guillaume Mioche

**Keywords:** *Arctic, cloud microphysics.*

The Arctic is warming at a rate approximately four times faster than the global average, a phenomenon known as Arctic amplification, accompanied by a rapid decline in sea ice extent and profound changes in surface-atmosphere exchanges. These transformations strongly influence cloud properties and radiative feedbacks, making Arctic clouds a key component of the regional climate system. Among the wide variety of cloud types, the Arctic provides particularly favorable conditions for the formation of mixed-phase clouds (MPCs), characterized by the coexistence of supercooled liquid droplets and ice crystals. The structure of these clouds, their links with environmental conditions, and their impact on the radiative budget remain insufficiently understood, partly due to limited in situ observations. This lack of knowledge contributes to persistent uncertainties in their representation in climate and weather models.

This study presents an extensive characterization of the microphysical and ice crystal morphological properties of low-level Arctic MPCs, based on in situ observations from four airborne campaigns conducted around Svalbard. The in situ dataset comprises 46 hours of cloud sampling. During these flights, 731,600 ice crystal images were collected and classified using a convolutional neural network, providing an unprecedented statistical view of Arctic ice crystal habits. Using the Marine Cold Air Outbreak index, four meteorological regimes were identified-Cold Air Outbreak (CAO), Warm Air Advection (WAA), and two transitional states-revealing strong contrasts in cloud structure and phase partitioning. CAO conditions are characterized by cold and moist environments supporting well-developed mixed-phase layers with enhanced riming and precipitation, while WAA conditions produce thinner, mostly liquid layers capped by strong temperature inversions. Weak inversions favor deeper, more turbulent clouds with larger droplets and higher ice water contents. Surface conditions also exert a major control: over open ocean, enhanced heat and moisture fluxes promote turbulence and glaciation efficiency, leading to higher ice water content and rimed ice crystals, whereas over sea ice, clouds remain shallower and are dominated by pristine or aggregated crystals. This work provides the first large-scale statistical analysis of ice crystal habits in Arctic MPCs. The results show that rimed particles dominate during CAO, while columnar and aggregated habits prevail during WAA. Over open ocean, stronger vertical motions further enhance riming efficiency. These findings highlight the strong coupling between surface fluxes, thermodynamic stability, and synoptic forcing in controlling the structure and evolution of Arctic mixed-phase clouds.



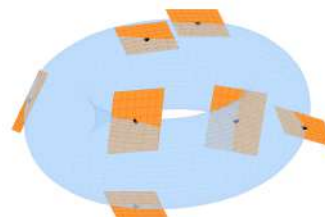
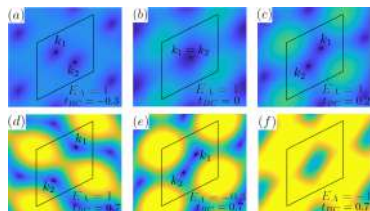
# Bundles in solid state physics

Matthieu Finck

Supervisors: Dmitry Solnyshkov

**Keywords:** *topology, quantum mechanics, solid state physics.*

In crystals, the behaviour of electrons is governed by the Schrödinger equation, whose solutions organize into energy bands. The shape of bands can inform us about the properties of the materials (conductor, insulator, semi-conductor). Sometimes, there are points at which the bands meet: Dirac points. We studied Dirac points in a material called the kagome lattice. It is a simple 2D lattice which can be implemented in many physical platforms, including photonic systems. Its band structure has Dirac points which can be moved by tuning the system's parameters. An interesting phenomenon occurs: two Dirac points can sometimes annihilate in pairs, opening a gap between the bands. But physicists have noticed that, in certain configurations, two Dirac points collide without annihilating. They wanted to know when the annihilation occurs, and when it does not. It turns out that this is a topological phenomenon. Topology is a domain of mathematics which plays an important role in many areas of physics. In our work, we study a topological object called "fiber bundle". One can obtain a fiber bundle by attaching fibers on an object. For example, a Möbius band is a fiber bundle, that you can obtain by attaching segments on a circle. But you can also get a cylinder by attaching little segments on a circle. The difference between these two: the Möbius band is twisted! In the same way, in quantum mechanics, one is interested in quantum states. The collection of all quantum states forms a fiber bundle structure. If it is twisted, then many interesting phenomena can occur. For the annihilation of Dirac points, we proved that if the bundle was twisted, then there was a sort of invisible force that prevented points from annihilating when they collide.



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# Local weights for the Ornstein–Uhlenbeck semigroup

Jérémie Moukambi

Supervisors: Christoph Kriegler

**Keywords:** *semigroup, weight, maximal operator, Ornstein–Uhlenbeck operator.*

Let

$$L = -\Delta + 2x \cdot \nabla$$

be the Ornstein–Uhlenbeck operator acting on  $L^2(\mathbb{R}^d, d\gamma)$ , and let  $\exp(-tL)$  be its associated semigroup. It is known that  $\exp(-tL)$  is contractive on  $L^p(d\gamma)$ , for  $1 \leq p \leq \infty$ . Moreover, several operators derived from this semigroup, such as the maximal operator, the Riesz transforms, the Littlewood–Paley functional, and holomorphic spectral multipliers, are bounded on  $L^p(d\gamma)$  for  $1 < p < \infty$ .

A natural question is whether these boundedness properties remain valid when the Gaussian measure is modified by a weight, that is, by a positive measurable function. More precisely, we study weighted  $L^p$  spaces associated with measures of the form  $w d\gamma$ , where  $w$  is a weight, and ask under which conditions operators related to the Ornstein–Uhlenbeck semigroup remain bounded.

In this poster, we present a class of weights, larger than the Muckenhoupt class, which is necessary and sufficient to ensure the weighted  $L^p$  boundedness of the maximal operator

$$\sup_{t>0} e^{-tL}|f|.$$

This result is obtained when the maximal operator associated with the Ornstein–Uhlenbeck semigroup is restricted to the local region of the Gaussian grid introduced in [1].

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# Toward the realization of InGaN micro-substrates for efficient red-emitting micro-LEDs

Arthur Sauvagnat

Supervisors: Agnès Trassoudaine, Yamina André, Geoffrey Avit

**Keywords:** *HVPE, nanowires, InGaN, micro-substrates, red micro-LEDs.*

InGaN is a key material for high-performance optoelectronic devices, due to its tunable bandgap from infrared to ultraviolet depending on indium content. However, growing high-quality InGaN layers on low-cost substrates remains challenging because of compressive strain, indium segregation, and thermal instability, which reduce the EQE, especially for red emission. Nanowire (NW) architectures offer a promising solution by enabling strain relaxation and nearly defect-free growth. InGaN NWs are also good candidates as seeds for micro-substrates, while hydride vapor phase epitaxy (HVPE) provides high growth rates and composition control, making it a promising approach for InGaN micro-substrate fabrication [1,2].

This work demonstrates the selective area growth (SAG) by HVPE of well-ordered InGaN NWs with indium compositions spanning 0–100% on apertures varying from 200 to 500 nm. By using chlorinated precursors and optimizing III-element partial pressures (InCl<sub>3</sub>, GaCl), we achieve high-quality NW arrays. PL and TEM measurements reveal their optical properties, composition and crystalline quality. A phenomenological growth model taking into account III-element adsorption, diffusion, and chlorine-induced desorption provides further insight into InGaN NWs composition. We also demonstrate the MOVPE regrowth of InGaN on relaxed HVPE-GaN nanopillars [3], in an attempt to produce micro-substrates using this hybrid MOVPE/HVPE process. These findings and experiments should pave the way for InGaN micro-domains fabrication and RGB nitride-based pixel applications.

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# From photography to cinematography in particle physics: ATLAS high-granularity timing detector at CERN

Nicolas Cartalade

Supervisors: Boumediene Djamel, D'Eramo Louis

**Keywords:** *particle physics, detector instrumentation, timing calibration, HGTD, ATLAS, CERN.*

Understanding the fundamental components of matter requires detectors capable of reconstructing the thousands of particles produced every 25 nanoseconds at the Large Hadron Collider (LHC). The ATLAS detector, one of the four major experiments at CERN, works like a huge 3D camera measuring the energy and trajectories (tracks) of particles emerging from proton–proton collisions. We then use these “images” to identify known particles and search for new ones. However, with the increasingly dense environment expected at the HighLuminosity LHC (HLLHC), spatial measurements alone will no longer be sufficient. In the presence of up to 200 simultaneous collisions per event (5 times more than today), different particle tracks may overlap in space, making them indistinguishable. We need a new dimension of information : precise timing.

To meet this challenge, the HighGranularity Timing Detector (HGTD) will be installed in ATLAS around 2029. By measuring the time of arrival of particles with a below 50-picoseconds precision, the HGTD will separate particles that overlap in space but not in time. Adding this precise “time stamp” transforms event reconstruction, indeed, instead of a single static final picture, ATLAS will obtain multiple timeresolved frames, turning particle detection from a picture into a short film.

In this presentation, I will first summarize my firstyear PhD work, which focused on investigating and identifying the main effects that can degrade timing performance such as clockdistribution fluctuations and electronic jitter. Then, using detailed simulations, I worked on the development of calibration strategies to reach the required sub50picosecond precision. These efforts contribute directly to preparing ATLAS for the highprecision measurement needed during the HLLHC Run4 and to enhancing our ability to explore physics beyond the Standard Model.

# Thermodynamic study of an adsorption in heterogeneous system using isothermal titration calorimetry

Jean Duprat

Supervisors: Christine Bonal, Jean-Michel Andanson

**Keywords:** *thermodynamic, adsorption, isothermal titration calorimetry.*

Adsorption is a process where molecules, known as the adsorbate, adhere to a surface, the adsorbent. To fully understand this phenomenon, three fundamental thermodynamic parameters allow us to describe the nature of the interaction [1]. The first is the enthalpy change, which represents the energetic strength of the interactions between the adsorbate and the adsorbent. The second is the entropy change, which describes the organization of the molecules on the surface and the change in disorder of the system. Finally, the Gibbs free energy change is the resultant of these two terms; it is the essential value that tells us the spontaneity of the adsorption, whether the process occurs naturally or under specific conditions.

Traditionally, these values are estimated indirectly through different models of adsorption isotherms, but this method can be induced to model dependent errors. To achieve a more direct and rigorous characterization, we utilize Isothermal Titration Calorimetry (ITC) [2]. This technique measures the heat released or absorbed when the adsorbate is injected step-by-step into a cell containing the adsorbent. In an ideal scenario, ITC allows the determination of the three thermodynamic parameters from a single experiment. However, the reliability of the resulting titration isotherm can only be obtained in an optimal experimental window [3]. Unfortunately, in heterogeneous systems, low solubility and limited surface site density often push the experiment outside of these optimal conditions

In this work, we developed a hybrid methodology to overcome these limitations by combining ITC with a complementary analytical technic. UV-visible spectroscopy allows us to quantify the exact amount of molecules adsorbed at each injection. Therefore, we provide the missing variable needed. This allows us to calculate the enthalpy change directly from the measured heat. Once the enthalpy is determined, it becomes possible to determine the other thermodynamic parameters. We applied this approach to study the paracetamol adsorption onto a pure graphite surface.

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# Enzymatic degradation of elastomers: development of a screening test for the detection of elastomer-degrading laccases

Ana Julia Antunes Souza

Supervisors: Marielle Lemaire, Thierry Gefflaut

**Keywords:** *biocatalysis, biodegradation, laccase, polymer.*

During their use and aging, and due to friction with the road, tires release agglomerates composed of a mixture of materials from the tire and minerals from the road. These particles, known as Tire and Road Wear Particles (TRWP), represent a significant environmental concern, as they constitute an important source of microplastic pollution [1].

In this context, the present project focuses on the enzymatic biodegradation of elastomers, which are the main component of TRWP. More specifically, we are interested in enzymes from the laccase family, a group of oxidoreductases that catalyze the oxidation of a great variety of substrates while reducing molecular oxygen. These enzymes can also act via a redox mediator, which allows the oxidation of various substrates that are not directly oxidized within the enzyme active site, because of steric hindrance or inadequate redox potential [2]. Accordingly, the main objective of this study is to identify laccases or Laccase-Mediator Systems (LMS) capable of participating in the initial steps of elastomer biodegradation.

As a first step, we have focused on the development of a screening test suitable for demonstrating the oxidation of elastomers by certain laccases. This assay is based on the quantification of dissolved oxygen in the reaction medium, given that oxygen acts as a co-substrate for laccases and its consumption can be correlated to enzyme activity. In this presentation, the validation of the test through comparison to classical assays will be highlighted, as well as the application to LMS and to the oxidation of model substrates.

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# From Rubin-LSST to dark matter understanding

Théotime Hallouin

Supervisors: Johann Cohen-Tanugi

**Keywords:** *cosmology, Rubin/LSST, stellar streams, dark matter, star-galaxy.*

Stellar streams are long trails of stars comoving in the sky (see the joint figure for visualization and the Gaia paper [1] for more details). They are substructures of galaxies and are ideal for studying the intrinsic gravitational properties of the latter. With the upcoming Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST), the stellar stream branch of Dark Energy Survey Collaboration (DESC) is planning to use these structures for cosmology. The goal is to observe stellar streams within the Milky Way as precisely as possible and to study their internal structure in order to detect dark matter subhalos, i.e., invisible structures within the galaxy. Further work will allow us to constrain the composition of dark matter itself.

In this work, I present what we are planning to do with stellar streams in the context of Rubin/LSST and my contribution to this effort. I begin with a few words about the transition from previous surveys to LSST. Then, I discuss the first part of my work: the identification of stars and galaxies in the survey. Next, I present the main part of my work: the detection of stellar streams in early LSST data. Finally, I conclude with the future goals of stellar stream studies, namely the detection and characterization of dark matter subhalos.



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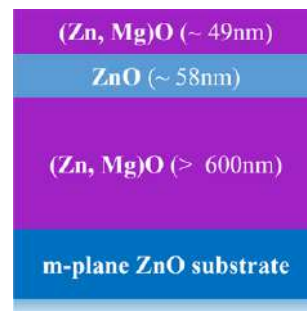
# Polariton lasing in ZnO waveguide

Nizar Riachi

Supervisors: Pierre Disseix, Joël Leymarie

**Keywords:** *excitons, semiconductors, photoluminescence, laser, polariton.*

Polaritons are composite particles product of the strong light interaction in a semiconducting material. Due to their bosonic nature, these particles can condense under optical excitation and generate a laser effect with a reduced threshold. However, this regime is only viable below the critical Mott density, beyond which a transition to a conventional laser occurs [1]. In this work, we try to explore the intermediate regime between polaritonic and conventional laser where light emission originates from electron-hole pairs [2]. Using microphotoluminescence spectroscopy and its time resolved version on a 20  $\mu\text{m}$  cavity in a ZnO based waveguide shown in the figure below, we study the optical gain as a function of the injected carrier density and the temperature in the final goal of having a phase diagram of the electron-hole behavior in the material. Using two types of optical excitation, CW laser emitting at 320 nm and Q-switch laser emitting at 266 nm, we identified the main transitions occurring in the material and we observed the lasing evolution with excitation intensity while also varying the temperature from 5 Kelvin until room temperature. A time resolved analysis using a femtosecond pulse laser helped determine the lifetime of the excitons and therefore the number of injected carriers. We observed a redshift of the lasing energy with increasing temperature. The possible gain mechanisms like exciton-electron and exciton exciton interaction already discussed in literature do not exactly fit with our experimental results suggesting other interactions may be considered.



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# A-polynomial and T-polynomial for knots, classical and quantum aspects

Thomas Alberge

Supervisors: Jérôme Dubois

**Keywords:** *Low-dimensional topology, Knot theory, Algebraic topology, Group representation, Reidemeister Torsion.*

The field of knot theory studies the different ways a knot, which is to say a circle, can be embedded into either our 3-dimensional euclidean space, or the 3-sphere. The classical approach consists of studying what is called the exterior of the knot, a topological space which can be described as a cube with a knotted hole inside, connecting two opposite faces. On the other hand the quantum approach, spearheaded by the discovery of the Jones polynomial in the 1970s, focuses on diagrammatic representations of knots and the so-called skein relations. A classical algebraic invariant of topological spaces is their fundamental group. Looking at the fundamental group of the exterior of a knot gives rise to an old and well-known invariant, simply called the group of the knot. In the 1930s, Reidemeister studied and classified the lens spaces – a family of 3-dimensional manifolds – using another invariant based on their fundamental group, the now called Franz-Reidemeister torsion. The idea was to produce a numerical invariant by looking at the different representations of their group and the way this group naturally acts on the universal covering of these spaces. But could this tool also be used for knots and knot groups ? In the 1960s, Milnor investigated in [2] the maximal abelian covering of the exterior of knots through a torsion invariant and recovered from there the Alexander polynomial of the knot, an older invariant with both a classical and quantum flavour. From this point on many other kinds of torsion were studied (like Kitano's polynomial torsion or the L2-Alexander torsion), among which the non-abelian Reidemeister torsion. The main difference with Milnor's torsion lies in the fact it looks at the universal covering – not the maximal abelian covering – and thus allows representations of the knot group to be non-abelian, in the hope to obtain more information. In fact, in the very important family of hyperbolic knots, everyone has a distinguished (non-abelian !) representation from which it is possible to recover all the geometrical structure of the exterior, further motivating this broader approach.

The goal of my thesis is to investigate a number of questions one may ask regarding non-abelian Reidemeister torsion. First of all, how would one go about actually computing these values ? If some specific families of knots have already been dealt with, fibered and twist knots being an example, there are still other families of interest to look at, like satellite knots among others. Further, it has been shown in [1] that torsion can also be understood as an algebraic element over a specific field. This expands the range of the study by allowing methods from algebraic geometry to come into play, possibly shedding a new light on the properties of Reidemeister torsion.

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# Doping of metal organic frameworks (MOF) by organic BODIPY luminophores.

Louise Burreler

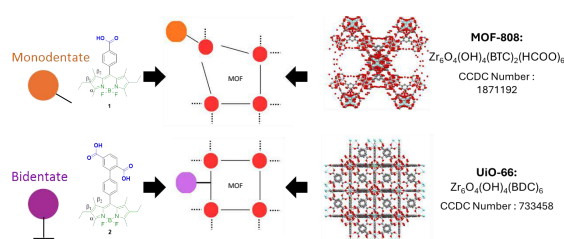
Supervisors: Federico Cisnetti, Clément Michelin

**Keywords:** *synthesis, BODIPYs, MOFs, fluorescent.*

BODIPYs are organic fluorophores that can be modified chemically at several specific positions, called  $\alpha$ ,  $\beta$ , meso, in particular by complexing functions, such as carboxylic acids. This would enable to obtain BODIPY-doped MOFs (Metal-Organic Frameworks). MOFs are porous hybrid materials belonging to the family of coordination polymers, composed of metal clusters linked by organic ligands (linkers). The dilution and organization by the MOF could solve the problem of Aggregation-Caused Quenching (ACQ), strongly reducing BODIPYs' photoluminescence in the solid state.

To achieve this, different ways of integration have been designed. The first one, is a monodentate pathway (see scheme). It requires functionalizing a BODIPY with one complexing function by a facile synthetic sequence. However, as a monodentate BODIPY would replace a bidentate linker of the MOF limited integration and reduced stability of the material are possible. The second one is a bidentate pathway: by connecting the meso position of the BODIPY to a moiety identical to a MOF linker a better stability of the doped MOF would be expected. However, more synthetic steps are required. For both approaches, there is also a challenge of finding MOF synthetic conditions compatible with BODIPYs (avoid temperatures and strong acidity).

A BODIPY carrying a carboxylate group in meso 1 was synthesized [1] for the monodentate route. Then, a second BODIPY functionalized with a terephthalic acid 2 was synthesized, to investigate the bidentate approach. These syntheses will be described in this communication as well as their results of integration of such BODIPYs into MOF-808 [2] and UiO-66 [3] (see scheme), under mild conditions. This integration was studied by XRD, IR etc. Photophysical analyses like excitation and emission spectra, quantum yields, luminescence decay allowed to assess the performance of the doped MOFs as luminescent materials.



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# K-feldspar phenocrysts as records of magma evolution and potential timescale constraints in post-orogenic magmatic systems

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**Keywords:** *K-feldspar, granitoids, magma differentiation, magma recharge, Ba zoning.*

Large K-feldspar phenocrysts are a common yet enigmatic feature of many granitoid magmatic systems, as their origin and petrogenetic significance remain debated. Due to their capacity to preserve textural and chemical evidence of crystal growth, resorption, and overgrowth, they have a great potential to provide valuable records of magma evolution and may ultimately permit timescale constraints on the governing processes. This study focuses on the investigation of K-feldspar phenocrysts from post-orogenic plutonic to subvolcanic rocks of the southeastern French Massif Central using optical microscopy, scanning electron microscopy (SEM), electron probe microanalysis (EPMA), laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), and micro X-ray fluorescence ( $\mu$ XRF).

The studied rocks range from mafic to granitic in compositions and are predominantly porphyritic, containing K-feldspar phenocrysts up to 5 cm in size. In granitic samples, phenocrysts are typically subhedral to euhedral and commonly display concentrically arranged inclusion trails, often restricted to outer crystal domains. Ba traverse analyses reveal both relatively homogeneous domains, interpreted to reflect partial diffusive equilibration, and normally zoned domains characterised by progressively decreasing Ba concentrations, consistent with crystallisation during magma differentiation. In contrast, phenocrysts from associated mafic dykes are rounded to anhedral, as a result of resorption, and contain abundant randomly distributed inclusions and embayments. Intermediate plutonic rocks and dyke samples contain predominantly euhedral phenocrysts that locally preserve resorption surfaces, (anti-)rapakivi textures, aligned inclusion trails, and poikilitic outer overgrowth rims.

Ba zoning in phenocrysts from the mafic dykes and quartz monzonitic samples also record multiple sharp stepped zones defined by abrupt increases in Ba content, indicating repeated perturbations in the magmatic system. Considered together with preserved resorption surfaces and (anti-)rapakivi textures, these features are most likely consistent with recharge by a more Ba-rich magma. Overall, the textural and chemical characteristics preserved in these K-feldspar phenocrysts indicate that they record key stages of magma differentiation and recharge, and highlight their potential for evaluating the evolution, and potential timescales, of post-orogenic magmatic systems.



# Fluorinated nanodiamonds: structural evolution and surface grafting

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**Keywords:** *nanodiamonds, structural transitions, thermal treatment, mechanochemistry.*

Diamond material is a metastable allotropic form of carbon under standard conditions leading to a slow transition toward graphite. The nanoscale of nanodiamond (ND) decreases the material stability, involving the formation at their surface of a disordered  $sp^2$  carbon shell rich in uncontrolled chemical functions. The fluorination treatment of NDs leads to a cleaner and stabilized surface through the elimination of residual amorphous  $sp^2$  carbon and surface functional groups (mainly C-H, COH, COOH) [1]. By using a high temperature thermal treatment, a progressive and controlled transition occurs from the surface of the ND, toward a conductive form of carbon. The carbon nano-onions (CNO) then obtained exhibit high surface area and high conductivity making them a promising candidate for energy storage applications [2]. The transition from ND toward CNO is a well-known process, however the thermal evolution of cleaned fluorinated nanodiamond (FND) has not been really studied yet. We study the structural evolution of FND under an inert atmosphere thermal treatment compared with ND's transition. We observed a transition at lower temperature for fluorinated materials, associated with a defluorination process, and a lower decomposition rate at high temperature indicating the formation of a stabilized outer conductive layer for FND.

Moreover, a mechanical treatment provides high energy on the material surface allowing the initiation of chemical reactions. Previous work in the laboratory determined that the ball-milling of FND leads to a defluorination and a surface reconstruction, developing surface defects that could be available as reactive sites for molecular grafting. We target the grafting of methacrylate molecules on the nanodiamond surface through a ball-milling process. Then we study a two step functionalization process based on a first activation treatment followed by a grafting step. Optimisation of the milling parameters allows both the defluorination, the surface reconstruction and the monomer grafting to be tailored.

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# Health impact of long-term exposure to volcanic particle deposits

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**Keywords:** *volcanic ash, long-term exposure, reprotoxicity, metallomics, oxidative stress.*

Some volcanic eruptions are associated with widespread and impacting tephra deposits that might affect the health of humans and animals up to many years after the eruption.

Since the eruption of Mount St. Helens in the 1980s, many studies investigated the acute respiratory health hazard of fine inhalable volcanic ash [1] but knowledge gaps remain whether long-term exposure can trigger the development of respiratory as well more systemic diseases.

In recent studies [2,3], it has been demonstrated that mice chronically exposed to artificial laboratory-crushed and metal-rich volcanic ash deposits from La Soufrière de Guadeloupe volcano (proof-of concept study) by multiple exposure pathways present an organ-specific and isotopically-typified metallomic deregulations associated with pathophysiological changes. These alterations preferentially impact the reproductive system and question about the impact of ash on male fertility.

Based on a comparative *in-vivo* approach, this study aims to further investigate the long-term reprotoxic effect of volcanic ash. For that, the elemental concentrations of potentially toxic elements (PTEs) and Cu-Zn-Fe isotope measurements coupled to histochemical, proteomic and transcriptomic analyses were measured in blood, liver and two organs of the male reproductive system (testis, seminal vesicle). The samples were collected on wild-type and mice exposed over two months to volcanic ash samples from the Tajogaite and Ubinas volcanoes, two ash samples with distinct health-relevant physico-chemical properties.

Our results confirm that prolonged exposure to metal-rich volcanic ash might contribute to testicular toxicity, likely mediated by altered oxidative stress status. The ash reprotoxicity is sample-dependent, with greater effects observed in cristobalite-rich and fine-grained samples that release higher content of potentially toxic and reactive oxygen species (ROS)-inducer elements (e.g., Fe and Cu). Our results also open perspectives for using redox-sensitive isotope tools as early signs of oxidative stress.

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# Characterization of a passive neutron counting device

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**Keywords:** *neutron detection, nuclear measurement, characterization, MCNP6.2©.*

At the CEA's Valduc center, accurately estimating nuclear material production is essential. To complement gamma spectrometry, we are developing a passive neutron counting method, focusing on Kromek's TN15 device [1]. Due to limited technical data, we first characterized the sensor to study its potential applications for quantification and localization of nuclear material.

Experiments involved measurement campaigns, initially using a source of  $^{252}\text{Cf}$  [2], then using plutonium standard masses. Experimental measurements are then compared to corresponding numerical simulations. For each configuration, different models and parameters are tested with MCNP6.2 code. Thus, the resulting discrepancies enabled the implementation and adjustment of an equivalent numerical model of the sensor for further digital investigation.

We observed a correlation with LiF/ZnS scintillator model and estimated key parameters such as the  $^6\text{Li}$  sensitive volume and  $^6\text{Li}$  enrichment of the scintillator but also moderation and efficiency of the device. This numerical model led to discrepancies around 9% for  $^{252}\text{Cf}$  and greater variations for plutonium standards depending on the mass.

Ongoing work aims to refine the sensor's characterization and develop a fully operational counting station.

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# Origin and evolution of late discrete eruptive activity in long dormant volcanic province: the case of the Monts Dore stratovolcano (France)

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Supervisors: Guillaume Boudoire

**Keywords:** *long-dormant volcanic province, magma storage, clinopyroxene barometry.*

In a world where volcanic eruptions are among the most significant natural hazards to humanity, quiescent volcanic provinces play a unique role. The lack of a collective memory of past eruptions often encourages local populations to settle in these areas. However, long periods of quiescence can lead to the accumulation of energy at depth, potentially resulting in violent eruptions. To mitigate disaster risks and detect potential changes in activity, it is crucial to understand the past behavior of these currently quiescent volcanic provinces and develop effective monitoring strategies. Although the last major phase of activity in the Mont Dore volcanic province (France) occurred approximately 200,000 years ago, discrete eruptive events took place sparsely until 7,000 years ago. An unusual seismic swarm in 2021-2022 highlighted the gaps in knowledge regarding these late eruptive events, particularly in the vicinity of the seismic activity.

To address this, a multidisciplinary approach combining the study of magmatic inclusions and pyroxene crystals is employed to constrain the architecture of the underlying magmatic system and to understand the evolution of magmas and fluids within it. Using this model, the chemistry of surface gaseous emissions is analysed to provide insights into the current state of the volcanic province. Seven sites were sampled, as well as two in the Chaîne des Puys (France) for comparison purposes. Whole-rock compositions range from basanite to trachybasalt (43.0-46.8 wt.% SiO<sub>2</sub>; 4.2-6.5 wt.% Na<sub>2</sub>O+K<sub>2</sub>O). First analyses of the melt inclusions seem to show a diversity of compositions that is at least as great.











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