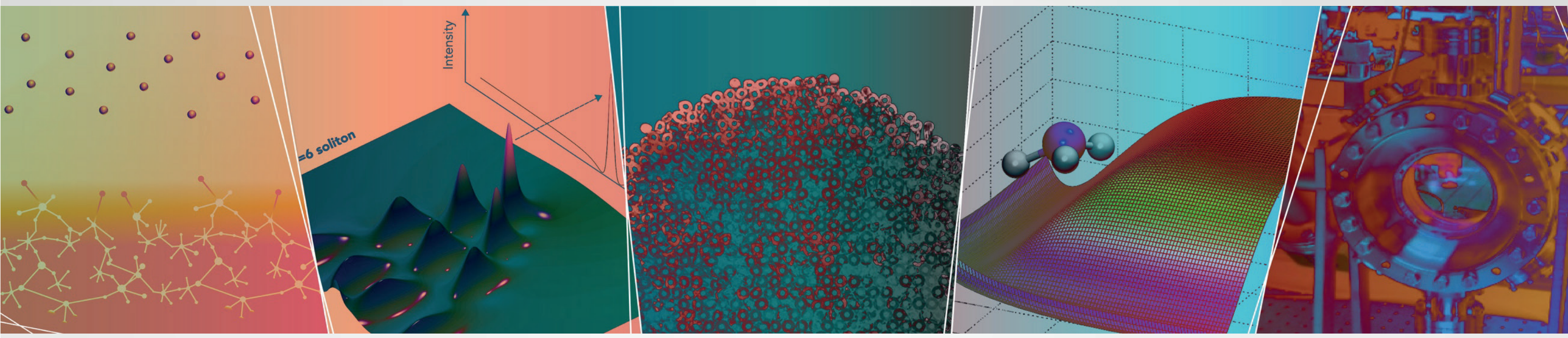
Les journées des doctorants du PhLAM 2022

Le **25 mars** à l'amphithéâtre Pierre Glorieux du **CERLA**
et le **30 mars** à l'amphithéâtre de l'**IRCICA**

PhLAM
Physique des Lasers
Atomes et Molécules



Université de Lille

Laboratoire PhLAM Bâtiment P5 campus Cité Scientifique 2 Avenue Jean Perrin 59655 Villeneuve d'Ascq cedex

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Programme

PHLAM DOCTORAL DAYS / JOURNÉES DES DOCTORANTS DU PHLAM 25 & 30 MARS 2022	
CERLA - Ampithéâtre Pierre Glorieux 25 mars	
9:00	***Introduction by the PhLAM director***
9:10	**HURBAIN Julien :** Modelling investigation of metabolic adaptation to oxidative stress.
9:30	**VANDENBERGHE Alan :** Deciphering circadian clock coupling with cell metabolism by fluorescence and bioluminescence.
9:50	**SEPTIER Dylan :** Double clad hollow core fibers for nonlinear microendoscopy.
10:10	**VANDERHAEGEN Guillaume :** Multiple Fermi Pasta Ulam Tsingou recurrences in uniform and dispersion oscillating fibers.
10:30	***Coffee Break & Posters by the 3rd year PhDs @ Cerla Hall***
11:00	**TOMBOZA Wendy :** Development of high temperature fiber optic pressure sensor for aircraft engines instrumentation. *Zoom*
11:20	**LECHEVALIER Corentin :** Measurement of the band dispersions of a Floquet-Bloch lattice realised with coupled fiber rings.
11:40	**YUAN Xiang :** Molecular properties in the linear response regime and beyond with relativistic equation of motion coupled cluster.
12:00	**HAIDER Kawssar Mujtaba :** Role of the organic waste products reactivity on secondary organic aerosol formation.
12:20	***Lunch break & posters by the 3rd year PhDs @ Cerla Hall***
14:25	**SAWAGODO Alfred :** MT 180s.
14:30	**CLAUS Jordan :** Characterization, microsolvation and reativity of aerosol precursors by microwave and infrared spectroscopy, supported by quantum calculations.
14:50	**BARRELLON—VERNAY Rafaël :** Unveiling Nucleation mechanism in aiRcraft Engine exhAust and its link with fuel composition (UNREAL).
15:10	**DELPIERRE Pauline :** Mathematical modeling of the synchronization of the liver circadian clock with metabolism – Application to the design of chronotherapeutic protocols targeting metabolic deseases.
15:30	***Coffee Break & Posters by the 3rd year PhDs @ Cerla Hall***
15:50	**BAYDI Brahim :** Peigne de fréquence et nouvelle dynamique paramétrique non linéaire en cavité optique.
16:10	**INFUSO Maxime :** Unravelling the atmospheric iodine chemistry using molecular simulations.
16:30	***Closing remarks***

Programme

PHLAM DOCTORAL DAYS / JOURNÉES DES DOCTORANTS DU PHLAM 25 & 30 MARS 2022	
IRCICA - Ampithéâtre IRCICA 30 mars	
9:00	**SRIVASTAVA Shivang :** Characterization and manipulation of quantum states of the light with highdimensional encoding.
9:20	**ALDAIR MISAEL Wilken :** Simulating Resonant Inelastic X-ray Scattering Across the Whole Periodic Table.
9:40	**ZAFAR Sadain :** CO2 hydrates as an alternative solution to water desalination and greenhouse gas mitigation.
10:00	**MADHUR Vikas :** Development of a new instrument coupling mass spectroscopy and optical diagnostics for the analysis of environmental samples at atmospheric pressure.
10:20	***Coffee Break & posters by the 1st year PhDs @ IRCICA***
10:50	**AL ASEEL Joelle :** Experimental and Theoretical studies on a new laser method to determine the adsorption energy on carbonaceous surfaces.
11:10	**GYAWALI Prakash :** Studies of the physico-chemical properties of water complexes in the terahertz domain.
11:30	**OUARKOUB Cecilia :** Ultrafast measurement of topological excitations in a polariton gas.
11:50	**DUFOUR Martin :** Encodage, Décodage, multiplexage non-linéaires et applications aux télécommunications optiques.
12:10	***Lunch break & posters by the 1st year PhDs @ IRCICA***
14:25	**BADIN Sylvain :** Theoretical study of iodine plasma for spacecraft propulsion. *Zoom*
14:30	**LERNER Alexandre :** High temperature Fiber Bragg Gratings embedding in metallic structures produced by additive manufacturing.
14:50	**LAFARGUE Léa :** High energy, ultrashort fiber laser system at 1053 nm for ultrahigh intensity laser frontend improvement.
15:10	**BANCEL Eve-Line :** Frequency combs in multi-core optical fibers for precision spectroscopy.
15:30	***Coffee Break & posters by the 1st year PhDs @ IRCICA***
15:50	**NEGRINI Stefano :** Gain Though Loss in passive fiber cavities.
16:10	**HANOUN Christelle :** Ultrafast measurements in synchrotron radiation sources and free electron lasers.
16:30	***Closing remarks***

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Abstracts des 3èmes années

Abstracts des 1ères années

PhD student name / Nom de l'étudiant: **Rawan Abouhaidar**

PhD year (1/2/3/…) / Année du doctorat: **First year**

Thesis title / Titre de la thèse: **Molecular dynamics investigation of the influence of surfactants on halogens propensity at the air-water interface**

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations: **Cèline Toubin**

Keywords (max. 5) / Mots-clés: **Air-water interface, surfactants, molecular modeling, surface propensity, physical chemistry.**

Abstract / Résumé

In the atmospheric environment, both organic and inorganic compounds are present and have a strong influence on the chemical composition of the troposphere. On the other side, the ocean surface water and sea mist spray are enriched with surface active organic compounds, which may have a significant effect on the distribution of halide ions at the interface (Ekholm V et al., 2018; Prisle NL et al., 2012). For instance, the abundance of bromide (Br^-) ions at the interface is implicated in halogen activation processes relevant for the ozone budget in the troposphere (Simpson WR et al., 2015). In this context, we evaluate the surface affinity of cationic hexylammonium, neutral hexylamine, and anionic propylsulfate at the air/liquid interface, and the effect of these ionic surfactants on the abundance of bromide at interfaces. Inspired by liquid X-ray Photoelectron Spectroscopy (XPS) experiments, we conducted Molecular Dynamics (MD) simulations and we were able to speculate about the distribution of these species between bulk and surface area in aqueous systems. Here, the results are in good agreement with the experimental ones, which clearly advocate that those organic molecules dislike the bulk and prefer to reside near the free surface; indicating the effect of salting. In contrast, both solutions containing hexylammonium and hexylamine show an enhancement of the surfactant bromide concentration while the propylsulfate solution do not alter the bromide concentration. In parallel, the same results were observed in the presence of NaCl. These results demonstrate that molecular level properties bring valuable insights on the interfacial behavior of organic and inorganic species on water films, that can be transposed to aerosol particles.

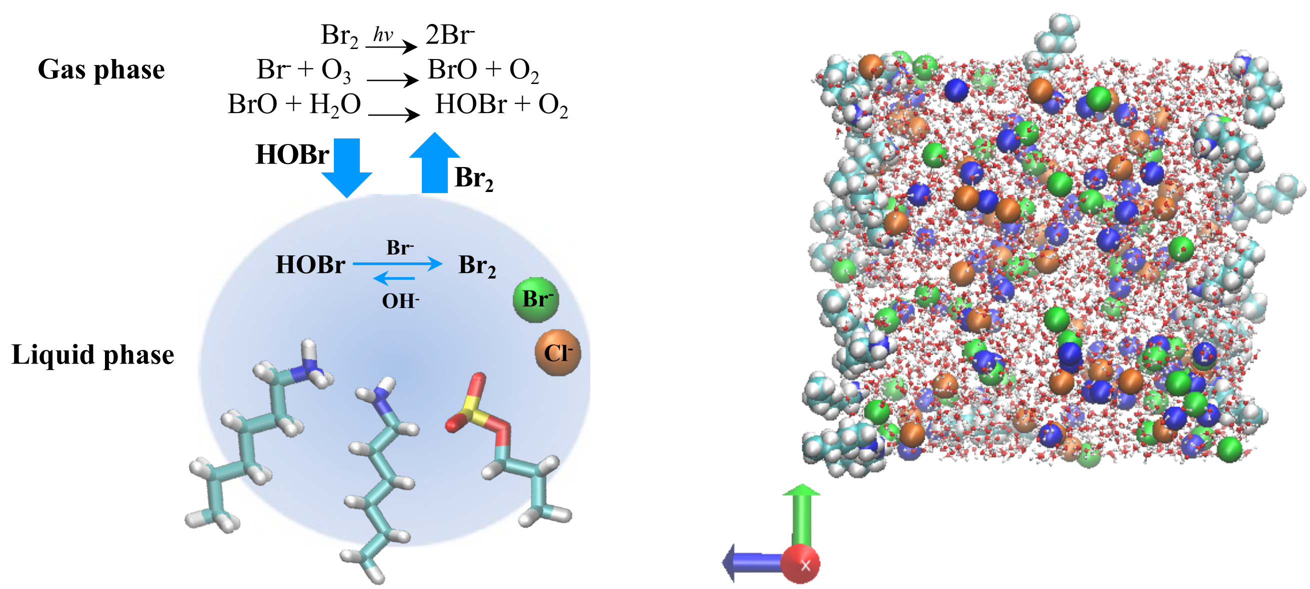

Figure 1: (a) The influence of surfactants on halogen propensity at the air-water interface. (b) Molecular view of a hexylammonium bromide with NaCl aqueous solution. Color code for the ions: Br: green, Cl-: orange, and Na+: blue.

PhLAM Doctoral Days / Journées des doctorants du PhLAM

25 & 30 Mars 2022

PhD student name / Nom de l’étudiant : Sylvain Badin

PhD year (1/2/3/…) / Année du doctorat : 1

Thesis title / Titre de la thèse : Theoretical study of iodine plasma for spacecraft propulsion

Cotutelle (Y/N): Y

Supervisors & affiliations / Encadrement et affiliations :

Andre Severo Pereira Gomes, Phlam, Université de Lille

Nicolas Sisourat, LCPMR, Sorbonne université

Keywords (max. 5) / Mots-clés :

theoretical chemistry
ion-ion collision
spacecraft propulsion
relativistic electronic structure calculations
semi classical dynamics

<u>Abstract / Résumé</u>

The development of low power electrical thruster is an important step in the field of satellite propulsion. In this context, iodine is a promising candidate to replace the propellant currently used in those thrusters, mostly xenon which is costly and hard to store. However, the chemistry of iodine for electric propulsion is not well known, due to the lack of knowledge about the elementary electronic processes occurring inside the thruster. The aim of the PhD project is to establish the first complete model of iodine chemistry in thruster operating conditions. For that, a combination of high-end relativistic electronic structure calculations, molecular and atomic collision simulations and chemical kinetics modeling will be implemented and used.

In order to compute the reaction rates between the most common species of iodine present in an electrical thruster (I^+,I^-,I,I_2,I_2^+,I_2^-,…), potential energy surfaces will be calculated with the Diarc software and be used for semi classical dynamics calculation.

PhD student name: Bon Mathilde

PhD year (1/2/3/…): 1

Thesis title: **Molecular characterization of *G. Prisca* microfossils by mass spectrometry at the cellular scale**

Cotutelle (Y/N): Ghent University (Belgium)

Supervisors & affiliations: Kevin Lepot[2, 3], Yvain Carpentier[1] and Thijs R.A. Vandenbroucke[4]

[1] Univ. Lille, CNRS, UMR 8523 - PhLAM - Physique des Lasers Atomes et Molécules, F-59000 Lille, France
[2] Univ. Lille, CNRS, Univ. Littoral Côte d'Opale, UMR 8187 - LOG – Laboratoire d'Océanologie et de Géosciences, F-59000 Lille, France [3] Institut Universitaire de France (IUF) [4]Department of Geology and Soil Sciences (WE13), Ghent University, Krijgslaan 281/S8, Ghent, 9000, Belgium

Keywords (max. 5): paleontology, biogeochemistry, mass spectrometry, phylogeny

Abstract

The objective of my research is to decipher the composition of individual (micro)fossils cells in terms of biomacromolecule derivatives (such as algenan, cellulose, peptidoglycan, chitin or collagen) and biomarker signatures (e.g., porphyrins from chlorophyl) using novel methods for microscale molecular characterization. Here, we focus on cells of « *Gloeocapsomorpha prisca* », a model fossil microorganism extracted from a sedimentary rock called « **kukersite** »; the samples originated from Estonia where they were collected from **Upper Ordovician (460 Ma)** strata. Kukersite comprises >99% of this *G. Prisca* species, thus allowing us to correlate the extensive existing bulk-rock molecular data (Derenne et al. 1990) and our novel microanalyses. This organism is likely a **photosynthetic bacterium** or a **microalga** (Derenne et al. 1992; Blokker et al. 2001), and our data may help clarify its **biological affinity**. We develop protocols for low-contaminant fossil sample preparation (demineralization, **organic solvent extraction** of solubles) in order to analyze the matured (bio)polymer forming the insoluble macromolecular organic matter.

Rock-Eval 7 S allows us to quantify H, O, S (as well as S speciation) during bulk-sample pyrolysis along temperature ramps, using flame ionization and IR detectors. This helps us to assess the source of the **organic matter**, its thermal maturity, and efficiency of solvent-extraction of the macromolecular fraction. Secondary ion time-of-flight **mass spectrometry** (**ToF-SIMS**) is used to resolve molecular compositions in the extracted biopolymer and to assess sample preparation protocols, owing to its extreme surface sensitivity and sub-micrometer scale resolution. Microscale two-step laser **mass spectrometry** (**µL2MS**) is used to characterize fossils at the micrometric scale with controlled fragmentation using various desorption and ionization wavelengths. Laser desorption-ionization Fourier-transform ion cyclotron resonance **mass spectrometry** (**LDI-FT-ICR-MS**), provides sub-ppm mass accuracies**,** is used to assist in molecular identification (Gross 2017) at the sub-millimetric scale. The analytical parameters of all three types of instruments are fine-tuned to maximize the **molecular information** obtained in the mass spectra. The goal of this novel analytical approach is to create a **molecular identity** sheet of target microorganisms, which will allow to better constrain and assign their **phylogeny**. Ultimately, it could help us know more about the appearance and early **evolution of life** on Earth. The techniques applied here to **paleontology** can be transposed to **exobiology** (for example, a laser desorption-ionization mass spectrometer will be sent to Mars, a ToF-SIMS has been sent to a comet (Fray et al. 2016 ; Goesmann et al. 2017).

PhD student name: Thomas Bunel

PhD year (1/2/3/…): First

Thesis title: Generation of multiple frequency combs in few mode passive fiber resonators

Cotutelle (Y/N): No but collaboration with the Hong Kong university

Supervisors & affiliations: Arnaud Mussot and Matteo Conforti (Ulille/PhLAM/Photonics team); Kenneth Wong (Hong Kong)

Keywords (max. 5): Optical frequency combs, nonlinear optic, optical fiber, Fabry-Perot cavity

Abstract

Optical frequency combs are light sources that revolutionized the science of precision measurements in the beginning of the 21st century. The applications extend to different fields of the detection of pollutants by measuring distances for autonomous cars or the detection of exoplanets. More recently, implementing multiple frequency combs has added speed and precision, making it possible to gain several orders of magnitude in the speed of analysis compared to single comb systems to access ultra-precise dynamic characterizations.

The objective of this project is to develop multiple frequency comb light sources from simple short fiber resonators supporting several transverse modes. This additional degree of freedom generates a rich and original dynamic to be studied from a fundamental point of view before being able to optimize these sources for one of the aforementioned applications. Then, the first part is devoted to the sizing and characterization of sources and the second will take place in Hong-Kong for implementation in biomedical imaging systems.

The used resonators are Fabry-Perot cavities made from optical fibers with a fiber length of around 6cm. Both fiber ends are mounted in ceramic ferrules and Bragg mirrors are deposited at each extremity. These cavities were made in collaboration with the LAAS (Toulouse) and the Fresnel Institute (Marseille). Their linear characterization reveals a high finesse.

For the moment the used optical fibers are single-mode to learn to generate our firsts optical frequency combs. For that, optical train pulse pump was developed in a way to inject a maximum of light in the cavity. Thanks to this setup, we were able to observe the first nonlinear effects that occur in cavities. Effects which allow to generate cavity solitons and frequency combs.

PhD student name / Nom de l'étudiant : **DEL FRÉ Samuel**

PhD year (1/2/3/…) / Année du doctorat : **1**

Thesis title / Titre de la thèse :

FR: **Études théoriques de la photodésorption de glaces moléculaires d'intérêt interstellaire**

EN: **Theoretical studies of photodesorption of molecular interstellar ices**

Cotutelle (Y/N) : **N**

Supervisors & affiliations / Encadrement et affiliations : **Maurice MONNERVILLE** (directeur de thèse)**, Denis DUFLOT** (co-directeur)**, Alejandro RIVERO SANTAMARIA** (co-encadrant)

Keywords (max. 5) / Mots-clés: **photodesorption, interstellar ice, classical molecular dynamics, carbon monoxide**

Abstract / Résumé

In the coldest parts (~10K) of the interstellar medium (ISM), most of the molecular species except H_2 accrete onto dust grains leading to the formation of chemically rich physisorbed molecular ice mantles, referred to as molecular ices. However, surprisingly large abundances of gas phase molecules are also observed in these cold regions. Due to the cold temperature, the existence of these gaseous species is naturally suggested to be the result of non-thermal desorption processes at the ice surfaces. One of these processes is the desorption induced by UV photons, namely UV photodesorption, which has been studied for various molecular ices including CO (e.g., [1],[2]) for which it has been shown that the UV photodesorption follows a "Desorption Induced by Electronic Transition (DIET)" mechanism [3]. In this astrochemical context and in the framework of the ANR PIXyES *(Photodesorption Induced by UV-X-rays and Electrons on ice Surfaces)*, this study aims at understanding, at the molecular level, the energy redistribution after VUV excitation in pure CO ice by means of molecular dynamics using a classical force field [4]. The focus is on the end of the DIET mechanism where the electronic energy of the excited molecule redistributes on the vibrational states of its electronic ground state which leads to photodesorption of a neighbouring molecule from the ice surface. To do so, a cluster approach is used to model the ice amorphous structure. The obtention, optimization and characterization of the theoretical samples is detailed in this work. Then, the energy profile to observe the desorption of a CO molecule from the cluster surface is presented using different approximations. These preliminary results show that the energy required to desorb a CO molecule from the cluster surface is much lower (≈ 60 meV) than the vibrational energy acquired by the excited CO molecule after the VUV irradiation (≈ 8 eV). This observation suggests that the CO photodesorption should be highly probable as has been reported in the experimental works.

[1] M. Bertin *et al.*, « UV photodesorption of interstellar CO ice analogues: from subsurface excitation to surface desorption », *Phys. Chem. Chem. Phys.*, vol. 14, nº 28, p. 9929, 2012, doi: 10.1039/c2cp41177f.

[2] E. C. Fayolle *et al.*, « CO ICE PHOTODESORPTION: A WAVELENGTH-DEPENDENT STUDY », *Astrophys. J.*, vol. 739, nº 2, p. L36, oct. 2011, doi: 10.1088/2041-8205/739/2/L36.

[3] M. Bertin *et al.*, « INDIRECT ULTRAVIOLET PHOTODESORPTION FROM CO:N_2 BINARY ICES — AN EFFICIENT GRAIN-GAS PROCESS », *Astrophys. J.*, vol. 779, nº 2, p. 120, déc. 2013, doi: 10.1088/0004-637X/779/2/120.

[4] M. C. van Hemert, J. Takahashi, et E. F. van Dishoeck, « Molecular Dynamics Study of the Photodesorption of CO Ice », *J. Phys. Chem. A*, vol. 119, nº 24, p. 6354-6369, juin 2015, doi: 10.1021/acs.jpca.5b02611.

PhD student name / Nom de l'étudiant : Bakhao DIOUM

PhD year (1/2/3/...) / Année du doctorat : 1

Thesis title / Titre de la thèse : Manipulation of quantum pulses

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Majid TAKI, Giuseppe PATERA (University of Lille, PG IKS)

Keywords (max. 5) / Mots-clés : Quantum Optics, Ultrashort Pulses, Nonlinear Optics

Abstract / Résumé

Quantum information science offers multiple possibilities for encoding, transmitting and manipulating information in ways not possible with classical technologies. In particular, quantum communication and the distribution of information in a quantum network can be implemented efficiently by the use of an orthogonal set of broadband optical pulses: Photonic Temporal Modes (PTM). PTMs are particularly suitable because we can prepare quantum states with good quality, reliability and flexibility. But manipulating them efficiently, meaning without destroying the encoded quantum information, presents some challenges: efficient detection schemes need to be implemented either with single pass or frequency combs.

For single pass detection, I am considering strategies based on nonlinear optical processes for the manipulation of PTMs that does not destroy the encoded quantum information. The work consists on a protocol which includes Sum Frequency Generations (SFGs) presenting an imperfect conversion efficiency (<100%) interspersed by a parametric amplification process. By adequately adjusting the interference between these processes, it is possible to select a desired PTM from a multimode input pulse.

Using frequency combs also, it is possible to use the analogy between the spatial and temporal degrees of freedom to translate time imaging schemes that have been originally conceived in spatial domain allowing us to implement a scheme for demultiplexing multimode frequency combs. This was done by implementing temporal cavities based on temporal imaging mainly time-lenses. It is a highly desirable functionality of any platform based on the basis of Gauss-Hermite modes allowing for the possibility to separate or mix them in highly efficient way.

PhLAM Doctoral Days / Journées des doctorants du PhLAM
25 & 30 Mars 2022

PhD student name / Nom de l'étudiant : Rabih El Sokhen.

PhD year (1/2/3/…) / Année du doctorat : 1

Thesis title / Titre de la thèse : Topological photonics in coupled fibre rings.

Cotutelle (Y/N): Non

Supervisors & affiliations / Encadrement et affiliations : PhD Supervisor: Pr Stéphane Randoux
Co-Supervisor: Pr Alberto Amo Garcia

Keywords (max. 5) / Mots-clés: photonic lattice, coupled fiber ring, topological properties, non-linear effects.

Abstract

This thesis aims to study experimentally a photonic lattice formed by two coupled fiber ring system and explore new topological properties of light i.e. geometrical features that remain unchanged under deformations of the system. These ideas have been employed in the context of photonics in which light propagates with unprecedented efficiency.
This system will make it possible to access unexplored regimes and unveil new topological phases of light in 1D and 2D multiplexed networks, and to study the robustness of these topological phases in the presence of optical non-linear effects.

Résumé.

La thèse vise à étudier expérimentalement un système photonique formé de deux boucles de fibres optiques couplées et explorer de nouvelles propriétés topologiques de la lumière, c'est-à-dire des caractéristiques géométriques qui restent inchangées sous les déformations du système. Ces idées ont été utilisées dans le contexte de la photonique dans lesquels la lumière se propage avec une efficacité sans précédent.
Ce système permettra d'accéder à un régime peu exploré et de dévoiler des nouvelles phases topologiques pour la lumière dans des réseaux multiplexés à 1D et 2D, et étudier la robustesse de ces phases topologiques en présence d'effets non-linéaires de la lumière.

PhD student name: Eden Haseeb

PhD year (1/2/3/…): First year

Thesis title: Rewiring programmed cell death and inflammation via modulation of ERK signaling dynamics

Cotutelle (Y/N): N

Supervisors & affiliations: Franck Riquet & Benjamin Pfeuty

Université de Lille, CNRS, UMR 8523-PhLAM-Physique des Lasers Atomes et Molécules, 59000 Lille, France

Keywords (max. 5): ERK, Signaling dynamics, Immunogenic Cell Deaths, Modelisation, HCS

Abstract

Cellular stress can promote responses *via* the activation of signaling pathways ranging from survival to eliciting the initiation of programmed cell deaths (PCDs) such as necroptosis and apoptosis. While necroptosis is more inflammatory, due to the release of cytokines, chemokines, and damage-associated molecular patterns, apoptosis is considered as a less immunogenic cell death modality. The main challenge in this context is to identify modulators that can dampen the immunogenic signature associated with PCDs and especially in necroptosis conditions.

The recent findings from the Death Dynamics Team (DDT) and that of others show that ERK is involved in necroptosis-activated cell-autonomous functions *via* the increase of pro-inflammatory cytokines gene expression. Using quantitative ERK signaling dynamics analysis via biosensor imaging, the DDT revealed distinct amplitude- and frequency-modulated (AM/FM) ERK activity signaling dynamics in L929 depending on the triggered cellular process: survival, apoptosis, or necroptosis. We propose that (AM/FM) ERK signaling dynamics would mediate proinflammatory cytokine gene expression increase during TNF-induced necroptosis in L929.

To test this hypothesis, we need to establish the causality link by investigating the origin of ERK signaling dynamics (pulse generator) and the correlation between ERK signaling dynamics and pro-inflammatory gene expression patterns at the single-cell level during necroptosis. i) To identify the origin of ERK pulsatile activity, we are running a screening for the modulator of necroptosis using an FDA-approved library of 1500 compounds that will maximize the repurposing of hits. ii) to assess the relevance of those hits we will implement combined biosensing imaging with pro-inflammatory gene expression levels (i.e. layered immunofluorescence) at the single-cell level for correlation purposes. This unique project is meshing cellular and molecular biologists, theoretical physicists, live-cell imaging and compound screening specialists, and computer scientists (machine learning for data analysis and processing).

PhLAM Doctoral Days
March - April 2022

PhD student name / Nom de l'étudiant : Farid MADANI

PhD year (1/2/3/…) / Année du doctorat : 1st year.

Thesis title / Titre de la thèse : Experimental study of disordered quantum systems in the presence of interactions with a Bose-Einstein condensate.
Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Radu CHICIREANU, Pascal SZRIFTGISER

Keywords (max. 5) / Mots-clés : Quantum Chaos, Bose Einstein Condensate, Quasi 1D-gas, Kicked Bose gas, Fabry–Perot cavity.

Abstract / Résumé

I am performing my PhD in the "Quantum Chaos" group on the subject of quantum simulation of Anderson localization using ultra-cold atomic gases. The goal of our experiment is to study new quantum disorder and localization effects in the presence of controllable interactions. For this, in the past 3 years, the group has built a new experimental setup, which produces potassium Bose-Einstein condensates (BEC). From a technical point of view, the originality of the setup, is in that it is almost entirely based on telecom fiber laser technology, which increases its robustness and reliability. We so manage to a create BEC of the ^{41}K isotope with typically 4.10^5 atoms, and fast repetition rates of ~16 s, for which low-field Feshbach resonances are available, and can be used to tune inter-atomic resonances.

We are currently implementing 2D optical lattices, which will help us to create quasi-1D gases in the strongly-correlated (Tonks-Girardeau) quantum-gas regime. This systems can be mapped on a free-fermion system, for which dynamical localization has been predicted (dubbed "Many-Body Dynamical Localization"). However, the analogy with free fermions is only partial, and interesting unique features of the strongly-interacting bosonic systems are expected.

Since the beginning of my PhD, I also implemented a new laser frequency stabilization system for the experiment. The idea is to lock the frequency of the laser using an ultra-stable Fabry-Perot cavity, which consists of two parallel mirrors, mounted inside a vacuum chamber (10^{-7} mBar) on an Ultra-Low Expansion (ULE) glass rod. The stability of such cavities match that of atomic references, traditionally used in our experiments. Once the laser is mode matched and tuned in resonance with the cavity fundamental mode, light can enter the cavity, by effect of interference. The stabilization of the laser frequency is performed using the Pound-Drever-Hall method, which consists in applying a phase modulation of the light, detecting the cavity reflection and demodulating it to generate the error signal. A PID controller is then used to cancel the laser frequency fluctuations around the cavity resonance.

PhD student name / Nom de l'étudiant : Mucci Alexandre

PhD year (1/2/3/…) / Année du doctorat : 1er année

Thesis title / Titre de la thèse : Gaz de solitons optiques

Cotutelle (Y/N): Non

Supervisors & affiliations / Encadrement et affiliations : Pierre Suret, François Copie

Keywords (max. 5) / Mots-clés : Soliton, Optique, Gaz de soliton

Abstract / Résumé

The nonlinear Schrödinger equation (NLSE) is a central model of nonlinear science, applying to many different fields of study such as hydrodynamics, plasma physics, molecular biology and optics[1]. In particular optical fiber are a favorable environment for experiments like the propagation of coherent or incoherent waves.

Recently our group has developped an experimental setup known as a Recirculation Optical Fiber Loop (ROFL) that allows us to record in single shot the complex behavior of light over large distances (several hundreds km) and with a temporal resolution of a few picosecond[2].

Through a mathematical tool called the Inverse Scattering Transform (IST) also called nonlinear Fourier transform (NFT) which is a analogue to the classical Fourier transform (FT) but for nonlinear integrable evolutionary equations we are able to decompose light pulses into nonlinear spectral data called solitonic part (soliton) and radiative/dispersive part[3].

In this work, we are currently studying the propagation of square shaped light pulses that are composed for the most part of solitons and observe how a phase modulation can affect the spatio-temporal dynamics thus indicating a modification brought upon the nonlinear spectral data.

[1] Agrawal, G. P. (2000). Nonlinear fiber optics. In *Nonlinear Science at the Dawn of the 21st Century* (pp. 195-211). Springer, Berlin, Heidelberg.

[2] Kraych, A. E., Agafontsev, D., Randoux, S., & Suret, P. (2019). Statistical properties of the nonlinear stage of modulation instability in fiber optics. *Physical review letters*, *123*(9), 093902.

[3] Shabat, A., & Zakharov, V. (1972). Exact theory of two-dimensional self-focusing and one-dimensional self-modulation of waves in nonlinear media. *Sov. Phys. JETP*, *34*(1), 62.

PhLAM Doctoral Days / Journées des doctorants du PhLAM
25 & 30 Mars 2022

PhD student name: MURR Georges

PhD year (1/2/3/…): 1

Thesis title: Optimisation de l’horizon de prédictibilité des évènements extrêmes par « deep learning »

Cotutelle (Y/N): N

Supervisors & affiliations: COULIBALY Saliya

Keywords (max. 5): Spatiotemporal chaos - Machine Learning - Neural Networks - LSTM - GRU

Abstract

The long term prediction of extreme events like ocean rogue waves, heat waves, floods, earthquakes, has been always difficult to achieve because of their high complex dynamics. The observations and predictions of chaotic systems are ubiquitous in optics because it offers a great advantage related to the significantly faster field evolution and to the higher number of events that can be recorded in a reasonable amount of time. In our work, we used a passive Kerr resonator; this cavity is made of a synchronously pumped highly nonlinear fiber loop. The emission of the cavity can be highly chaotic with the generation of large amplitude peaks. We aim to predict these pulses before they occur by looking for their precursors. The study is performed using the mean-field approximation of the intracavity dynamics. The prediction of high dimensional chaotic systems took a big step forward after the improvements of machine learning algorithms, especially artificially neural networks. At the center of chaos theory is the discovery that hidden within the unpredictability of chaotic systems are deep structures of order. Chaos denotes not true randomness but the orderly disorder characteristic of these systems. The ability of neural networks to find these hidden correlations in data helped in performing forecasting of spatiotemporal complex dynamics. In our study, we implemented several recurrent neural network architectures to perform sequence to sequence forecasting and we have been able to predict the profile of the pulse.

Nom de l'étudiant : Ismail ZGHARI

Année du doctorat : 1

Titre de la thèse : Silice dopée et fibre optique pour la dosimétrie en radiothérapie pulsée

Cotutelle (Y/N): N

Encadrement et affiliations : Prof. Bruno CAPOEN et Dr. Hicham EL HAMZAOUI

Mots-clés : fibres optiques, cérium/gadolinium, dosimétrie, rayons X, protons

Résumé

La radiothérapie a connu plusieurs progrès ces dernières années concernant la taille et l'intensité des faisceaux de rayonnement X. Ceci a donné lieu à l'apparition de nouvelles techniques telles que la radiothérapie conventionnelle par modulation de l'intensité, basée sur l'adaptation du volume irradié au volume à traiter. L'objectif de ces nouvelles techniques est de contrôler la distribution spatiale de la dose délivrée aux cellules cancéreuses et réduire ainsi les effets secondaires aux organes à risque (organes sains proches des tumeurs cancéreuses). Par ailleurs, on peut aussi aujourd'hui réduire les effets secondaires de la radiothérapie en délivrant la dose sous forme d'impulsions X très brèves (flash-thérapie) ou en utilisant des faisceaux de particules (par exemple, en protonthérapie).

Ces techniques exigent des mesures in vivo et en temps réel de la dose absorbée avec une grande précision spatiale et temporelle. Pour cela, plusieurs recherches ont été menées pour réaliser des détecteurs permettant une dosimétrie en temps réel, ces détecteurs devant être à la fois sensibles aux faibles doses et résistants aux fortes irradiations. Dans ce contexte, nous proposons l'étude de dosimètres à fibre scintillante, basés sur la radioluminescence (RL) de verres de silice dopée. La sensibilité élevée de ces barreaux et fibres optiques, leurs dimensions submillimétriques et leur réponse linéaire dans une large gamme de dose font de ces matériaux des objets d'étude très pertinents.

Le projet ANR FIDELIO (**F**iber-based **I**n-vivo realtime **D**osim**e**try for Pu**l**sed Rad**io**therapy) vise à développer des dosimètres à base de fibres optiques scintillantes sensibles aux rayons X et aux protons, permettant de suivre des impulsions courtes (µs), notamment pour la caractérisation des faisceaux pulsés employés dans les techniques Flash-RT et HEPT (Protonthérapie à haute énergie). Pour ce type de dosimétrie, la silice dopée par des ions Ce^{3+} est pleine de promesses au vu de ses caractéristiques (matrice durcie, fort rendement de luminescence, temps de réponse). Les ions Gd^{3+}, quant à eux, se sont avérés particulièrement sensibles aux protons. C'est pourquoi un co-dopage de la silice par le couple Ce/Gd est envisagé.

L'objectif de la thèse est d'étudier les caractéristiques optiques et structurales de ces matériaux, sous forme de barreaux et de fibres, par les méthodes spectroscopiques (Raman, absorption, photoluminescence) ainsi que leurs caractéristiques dosimétriques (en RL) sous faisceaux de rayons X et de protons. De plus, une partie très importante de la thèse est consacrée aux modélisations des signaux de RL pour reproduire leur évolution temporelle dans ses matériaux, l'objectif étant de comprendre les mécanismes mis en jeu et leurs comportements en fonction de la dose ou du débit de dose.

Abstracts des 2èmes années

PhD student name: Joelle Al Aseel

PhD year (1/2/3/…): 2nd year PhD student

Thesis title: Experimental and Theoretical studies on a new laser method to determine the adsorption energy on carbonaceous surfaces.

Cotutelle (Y/N): N

Supervisors & affiliations: Cristian Focsa (PhLAM, CNRS, UMR 8523, Univ. Lille), Céline Toubin (PhLAM, CNRS, UMR 8523, Univ. Lille), Claire Pirim ((PhLAM, CNRS, UMR 8523, Univ. Lille).

Keywords (max. 5): Adsorption energy, laser induced thermal desorption, classical molecular dynamics, polycyclic aromatic hydrocarbons, carbonaceous surfaces.

Abstract

The reactivity of carbonaceous surfaces bears a fundamental role in various fields, from atmospheric chemistry and catalysis to graphene and nanoparticles. This reactivity is mainly driven by the surface chemical composition and by the strength of the interaction between the adsorbates and the surface (physi-/chemi-sorption). In order to study complex real-world mixtures, adsorption energies were determined by a combined theoretical and experimental method. Classical molecular dynamics (MD) based on a force-field approach was used to determine the adsorption energies of different adsorbate-surface systems theoretically. The system studied consists of a 4-sheet carbon slab (graphite or HOPG) and a PAH molecule. The results of these simulations show a good agreement with literature values. These simulations are used to complement the laser-assisted mass spectrometry that was recently proposed by Duca et al., 2021 as an original method to retrieve adsorption energies of organic and inorganic adsorbates on carbonaceous surfaces. This method consists of laser-induced thermal desorption (LITD) followed by resonance enhanced multiphoton ionization (REMPI) and reflectron time-of-flight mass spectrometry, which ensures high sensitivity to investigate low surface coverages. Well-characterized, laboratory-generated samples prepared by adsorbing a well-known concentration of PAHs on different carbon surfaces (soot, graphite and HOPG) were initially analyzed by this method. Mass spectra are recorded for successive laser pulses where the signal of the adsorbate is plotted as a function of the applied laser pulses. The pseudo-exponential decay is fitted by two mathematical models: Effective temperature and Transient temperature models. The first represents a steady state approach of the process, considering a constant temperature, while the second is more elaborated and accounts for the fast change in the surface temperature upon a laser pulse that triggers the desorption of molecules present on the surface. Temporal and spatial temperature profiles of the sample are simulated to better model the LITD process. Another approach is introduced to determine the temperature distribution experimentally. This will be done using a fast pyrometer to follow the change of the surface temperature upon heating with a continuous wave laser. Once the temperature profile is determined, the adsorption energy of the adsorbates can be retrieved.

PhLAM Doctoral Days
March - April 2022

PhD student name: Wilken Aldair Misael

PhD year (1/2/3/…): 2nd year

Thesis title: Simulating Resonant Inelastic X-ray Scattering Across the Whole Periodic Table

Cotutelle (Y/N): N

Supervisors & affiliations: André Severo Pereira Gomes

Keywords (max. 5): Actinides, Core Spectroscopy, Quantum Embedding Theories , Relativistic Quantum Chemistry, Theoretical Chemistry.

Abstract

Actinides are broadly used in several fields of science and technology, among other as catalysts in chemical processes. To characterize their behavior, one often employs spectroscopic techniques, and among existing methods X-ray spectroscopy is particularly promising in the context of actinides given its great sensitivity and selectivity. With the introduction of advanced X-ray spectroscopy techniques and light sources in recent years, it has recently become possible to investigate different core states of uranium-containing complexes [1]. Analyzing such spectra requires theoretical models capable of describing the electronic structure of actinide species in the ground and excited states [2]. This, in turn requires the use of approaches describing both electron correlation and relativistic effects. In this work we employ the Core–Valence-Separated Equation-of-Motion Coupled-Cluster Singles and Doubles (CVS-EOM-CCSD) framework [3] recently implemented in the DIRAC code [4] and Time-Dependent Density Functional Theory (TD-DFT) calculations to investigate the core excited and ionized states of the uranyl ion (UO_2^{2+}) in the gas phase and at in $Cs_2UO_2Cl_4$ crystal, the latter being treated with the frozen density embedding (FDE) method, as previously done for valence processes [5]. Our calculations are in accordance with previous experimental and theoretical reports, showing first the importance of the Hamiltonian in order to obtain qualitative results at U L_3- and M_4-edges, and second that embedded models can adequately reproduce the interaction of the uranyl ion and its equatorial ligands in the crystal environment for core states.

References

[2] JG Tobin et al. In: Surface Science 698 (2020), p. 121607.

[3] RG Denning. In: The Journal of Physical Chemistry A 111.20 (2007), pp. 4125–4143.

[5] Loıc Halbert et al. In: Journal of Chemical Theory and Computation 17.6 (2021), pp. 3583–3598.

[6] Trond Saue et al. In: The Journal of Chemical Physics 152.20 (2020), p. 204104.

[7] ASP Gomes et al. In: Physical Chemistry Chemical Physics 15.36 (2013), pp. 15153–15162.

PhLAM Doctoral Days
March - April 2022

PhD student name : BANCEL Eve-Line

PhD year (1/2/3/…) : 2^{e} année

Thesis title: Frequency combs in multi-core optical fibers for precision spectroscopy

Cotutelle (Y/N): N

Supervisors & affiliations : Arnaud Mussot (PhLAM) and Rosa SANTAGATA (ONERA)

Keywords (max. 5): Laser / Frequency comb / Fiber optics / Electro-optical modulation / Spectroscopy

Abstract / Résumé

Historically, frequency combs have been generated from mode-locked lasers. Since then, other technologies have emerged, such as soliton generation in micro-resonators, or electro-optical modulation. The latter offers the possibility to fully adapt the parameters. The performance of a set-up with a single comb is limited by the detection systems (bandwidth, spectral resolution, speed). One way to overcome this limitation is to use a second frequency comb to sample the first. Multi-heterodyne detection allows a transfer from optical frequencies to microwave frequencies, leading to easier detection and acquisition. Thus, ultra-fast and accurate measurements using dual frequency combs have recently been demonstrated, with distance measurement, spectroscopy, or optical frequency synthesis. The future trend is to increase the complexity of the systems with not only two, but three frequency combs to further improve the measurement performance (speed, resolution, new measurable parameters).

The thesis has as an objective the development of a new class of laser sources, with multiple frequency combs, all- fibered, versatile and tunable. The underlying technology is the generation of combs from a continuous source at 1.5 µm by electro-optical modulation. The combs are then spectrally expanded in a non-linear fiber which has the particularity of having 3 cores. This technological choice allows the generation of more than two combs from a single source, while maintaining a good coherence between the combs. Its use leads to the exploration of fields that are still relatively unknown to date, such as three-comb frequency spectroscopy [1].

The first part of my thesis took place at ONERA. It was devoted to the training in the use of a commercial dual frequency comb system. I studied in particular the influence of the comb parameters and the acquisition parameters during a double comb spectroscopy experiment, in order to define measurement and pre/post-processing protocols of the acquired spectra.

The second part of the thesis is devoted to the development of the three-comb electro-optical source. We have implemented the intensity modulation of the continuous laser at 1.5µm to obtain 3 coherent pulsed lasers. We then broaden these pulsed lasers, in the three-core fiber (fabricated on the FiberTechLille platform). We obtain 3 coherent combs of different repetition rates. Their output spectra are flat-top, spanning over 8 nm, with a SNR around 30dB, and an energy around 1 nJ at 500 MHz. The next step is to fully characterize the system, and implement dual-comb dispersion measurements.

[1] B. Lomsadze, B. C. Smith et S. T. Cundiff, Tri-comb spectroscopy, Nature Photonics (2018).

PhLAM Doctoral Days / Journées des doctorants du PhLAM
25 & 30 Mars 2022

PhD student name: Barrellon—Vernay Rafaël

PhD year: 3

Thesis title: Unveiling Nucleation mechanism in aiRcraft Engine exhAust and its Link with fuel composition (UNREAL)

Cotutelle (Y/N): N

Supervisors & affiliations: Thesis Director: Cristian Focsa (Phlam, Lille University)
Thesis Supervisors: David Delhaye, Ismael Ortega (ONERA, Paris)

Keywords: Atmospheric chamber, Oxidation Flow Reactor (OFR), Sustainable Aviation Fuel (SAF), Nucleation, nvPM.

Abstract

Unveiling Nucleation mechanism in aiRcraft Engine exhAust and its Link with fuel composition: UNREAL project and campaign at the CESAM atmospheric chamber

R. Barrellon-Vernay[1,2], I.K. Ortega[1], D. Delhaye[1], C. Focsa[2]
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[2]Univ. Lille, CNRS, UMR 8523, PhLAM – Physique des Lasers, Atomes et Molécules, F-59000 Lille, France

Aviation is actually one of the strongest growing transport sectors, and this trend is predicted to continue (IATA 2021). Aeronautics Emissions are numerous: greenhouse gases (CO_2, water), nitrogen oxides, sulfur oxides.... This thesis focuses on volatile particulate matter (vPM) and non-volatile particulate matter (nvPM). This is especially important given the actual concern of aviation industry to reduce the impact of aviation on climate and air quality (Neu 2020). vPM is formed by nucleation from gaseous precursors in the cooling exhaust gas downstream the engine. The molecular mechanism behind formation of these particles is still unknown. nvPM are essentially soot particles produced by the incomplete combustion of the fuel. They are present in the engine exhaust at temperatures higher than 350°C.

The UNREAL project aims at studying at the molecular level the different mechanisms of new vPM formation from the exhausts of aircraft engines fed by different fuel composition from the standard Jet A-1 to 100 % SAF (Alcohol to Jet, AtJ). Diluted fuel emissions produced from a liquid CAST burner (Jing 2003) were simultaneously injected, after particle filtration, into the CESAM atmospheric chamber (LISA, Créteil) and a Potential Aerosol Mass Oxidation Flow Reactor (PAM-OFR), for aging. A particular attention was given to the formation of new particles and notably organic matter.

In addition to on-line characterization techniques (particle size distribution, number concentration and chemical composition), different filter samples were collected to study the particle chemical composition in laboratory by Two Step Laser Mass Spectrometry and Secondary Ion Mass Spectrometry techniques (Ngo et al., 2020).

This work benefited from the support of the project UNREAL ANR-18-CE22-0019 of the French National Research Agency (ANR). PhLAM participate in the Labex CaPPA (ANR-11-LABX-0005-01) and the CLIMIBIO projects.

IATA (2021), *IATA Economics using data from IATA*, Monthly Statistics and from ICAO.
Neu U. (2020) *The impact of emissions from aviation on the climate*. Swiss Academies Communications 15 (9).
Jing, L. (2003), *7th ETH Conference on Nanoparticle Measurement*, ETH Hönggerberg, Zürich.
Ngo L. D. et al. (2020), *Atmos. Meas. Tech.* **13**, 951-967.

PhD student name / Nom de l'étudiant : Brahim BAYDI
PhD year /Année du doctorat : 2 ème année

Thesis title / titre de la thèse: Peigne de fréquence et nouvelle dynamique paramétrique non linéaire en cavité optique.
Cotutelle (Y/N): oui

Supervisors & affiliations/ Encadrement et affiliations : Saliya COULIBALY, Abdelmajid TAKI, PHLAM -Université de Lille, et François LEO, Mustapha TLIDI, OPERA-photonique – Université Libre de Bruxelles.

Keywords/ Mots-clés : optique non linéaire, dynamique non linéaire, oscillateur paramétrique optique et soliton paramétrique.

Abstract / Résumé

Les structures temporelles dans les résonateurs optiques attirent de plus en plus d'attention, notamment pour la génération des peignes de fréquences. Dans le domaine temporel, ces peignes sont constitués d'impulsions régulièrement espacées appelées solitons de cavité (CS). Ces impulsions se propagent sans se déformer grâce à la compensation de la dispersion par la non-linéarité d'un côté, et de la dissipation par le pompage externe, de l'autre. Jusqu'à présent, la grande majorité des études se concentre sur des solitons temporels générés à la même fréquence que celle de la porteuse permettant de pomper la cavité. Cependant, il est désormais possible de générer des solitons de cavité dont la fréquence est la moitié de celle de l'onde de pompe. Ce type de forçage dit paramétrique permet d'obtenir une dynamique proche de celle des oscillateurs paramétriques optiques.

Les oscillateurs paramétriques optiques (OPOs) sont des sources optiques susceptibles de produire, par interaction non-linéaire dans des milieux à forte susceptibilité non-linéaire d'ordre deux, deux ondes cohérentes "signal" et "complémentaire" (ou "idler") à partir d'un faisceau laser de forte puissance appelé "pompe". Ici, on étudie les solitons dans des cavités optiques en présence de non-linéarité du deuxième ordre (forçage paramétrique) et troisième ordre (fibre optique). Cette configuration présente une dynamique avec des avantages importants par rapport à ceux d'un résonateur de type Kerr (non-linéarité cubique). Des résultats expérimentaux récents démontrent l'intérêt pour ces structures solitoniques. L'objectif est d'étudier les conditions d'apparition et de stabilité des solitons paramétriques dans des cavités optiques en présence de non-linéarité quadratique et cubique. L'influence de la dérive temporelle ou walkoff sur la dynamique et la stabilité de ces nouvelles structures solitoniques est aussi considérée.

PhD student name: Jordan Claus

PhD year (1/2/3/…): 2nd year

Thesis title: Caractérisation, microsolvatation et réactivité de précurseurs d'aérosols par spectroscopie microonde, infrarouge et calculs quantiques / Characterization, microsolvation and reativity of aerosol precursors by microwave and infrared spectroscopy, supported by quantum calculations

Cotutelle (Y/N): N

Supervisors & affiliations: Laurent Margulès, Manuel Goubet (Université de Lille, CNRS, UMR 8523-PhLAM, Physique des Laser Atomes et Molécules F-59000 Lille, France)

Keywords (max. 5): microwave spectroscopy, aerosol precursors, polycyclic aromatic hydrocarbons, hydration

Abstract

Polycyclic aromatic hydrocarbons (PAHs) and their oxygenated products (oxi-PAH) are considered as important pollutants of the Earth's atmosphere since they are emitted by the combustion of fuels.[1] The study of their intermolecular interactions is essential to understand the formation of their aerosols. In this work, we have studied at molecular level the interactions present in the hydration of the oxi-PAH, α- and β-naphthaldehyde. This study has been performed using a supersonic jet Fourier transform microwave (FTMW) spectrometer in the 4-15 GHz range, with the support of theoretical calculations. Both isolated α- and β-naphthaldehyde species could present two possible structures: *cis,* the most stable one for α, and *trans* for β.[2] Our calculations show that there are three low energy monohydrates predicted for each conformer, *cis*/*trans*, in a range of 1500 cm^{-1}. Experimentally, one conformer has been observed in gas phase for α and two for β, corresponding to the most stable structures. All species are stabilized by intermolecular H-bonds between the water molecule and the aldehyde group of naphthaldehyde: for the first case, the oxygen of the aldehyde acts as proton acceptor and the aldehyde hydrogen as proton donor; for the second case, the oxygen of the aldehyde acts as proton acceptor and one of the ring hydrogens as a proton donor.[3]

[1] Karavalakis G. *et al. Sci. Tot. Environ.*, 409, 4, 738, **2011**.

[2] Goubet M., *et al. J. Phys. Chem. A*, 124, 4484, **2020**.

[3] This work is supported by the CaPPA project and by the CPER ClimiBio funded by the French National Research Agency (ANR) through the PIA 11-LABX-0005-01, the I-SITE ULNE/ANR-16-IDEX-0004 ULNE, the Regional Council Hauts-de-France and the European Funds for Regional Economic Development (FEDER).

PhLAM Doctoral Days
March - April 2022

PhD student name / Nom de l'étudiant : Delpierre Pauline

PhD year (1/2/3/…) / Année du doctorat : 2

Thesis title / Titre de la thèse : Mathematical modeling of the synchronization of the liver circadian clock with metabolism – Application to the design of chronotherapeutic protocols targeting metabolic deseases

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Marc Lefranc

Keywords (max. 5) / Mots-clés : Mathematical modeling, circadian clock, metabolism, biological systems, liver

Abstract / Résumé :

Living organisms orchestrate their physiology throughout the days thanks to a biological clock called *circadian clock*. In mammals, the liver maintains its homeostasis along the day/night cycle with a clock that is synchronized with the feeding/fasting cycle.

Circadian clocks are made up of networks of genes and proteins, which regulate reciprocally via feedback loops. Disruption of the liver clock due to a perturbation of the feeding and fasting rhythms, which synchronize the clock, can lead to metabolic diseases like obesity or type 2 diabetes. The increasing in the incidence of these diseases in recent years make it important to understand how the liver clock synchronizes to the metabolism in order to clarify the origin of these pathologies. Solving this problem requires quantitative approaches based on modeling.

To answer this question, we use mathematical modeling and experimental data to study how a change from a normal diet to high-fat diet disrupts the clock, by identifying the kinetic parameters that are sensitive to this change in diet, casting light on the involved input pathways of the clock. For this purpose, we have constructed a reduced mathematical model of the hepatic clock. This model is based on a systematic reduction of a larger model that reproduces accurately experimental data. The main interest of this approach is that no assumption on the input pathways is made.

Remarkably, we find that data for the normal and high-fat diets can be reproduced very well by the minimal model by making only one parameter diet-dependent. These parameters can be traced back to putative inputs.

PhLAM Doctoral Days / Journées des doctorants du PhLAM
25 & 30 Mars 2022

PhD student name / Nom de l'étudiant : DUFOUR Martin

PhD year (1/2/3/…) / Année du doctorat : 2ème

Thesis title / Titre de la thèse : Encodage, Décodage, multiplexage non-linéaires et applications aux télécommunications optiques

Titre de la présentation : Ultrafast single-shot measurement of optical solitons collisions.

Cotutelle (Y/N):N

Supervisors & affiliations / Encadrement et affiliations : Pierre Suret, Stéphane Randoux, François Copie

Keywords (max. 5) / Mots-clés : Solitons, Soliton gas, non-linear optics, fiber optics, Nonlinear Shrödinger Equation

Abstract / Résumé

In integrable systems the collision of solitons is elastic and is characterized by a phase and time shift in the propagation. This phenomenon has been widely studied in the 80's [2]. Recent applied mathematical work has been devoted to the collision of arbitrary pulses described both by solitonic and dispersive waves [3].

Here we describe preliminary results on picosecond light pulses collisions in optical fibers. By using a spectral filter made of a stretcher and a slit on an 80nm wide modelocked laser, we design controlled spectral width and central wavelength (I.e group volocity) of two pulses. The two pulses are launched into a single mode polarization maintaining fiber. We record in single-shot phase and amplitude of pulses before and after collision. Our preliminary observations reveal the influence of high order effects such as Raman scattering.

References

[1] A. Tikan, S. Bielawski, C. Szwaj, S. Randoux, P. Suret, "Single-shot measurement of phase and amplitude by using a heterodyne time-lens system and ultrafast digital time-holography" Nature Photon 12 228-234, 2018.

[2] F. M. Mitschke and L. F. Mollenauer, "Experimental observation of interaction forces between solitons in optical fibers," Opt. Lett. 12, 355-357, 1987

[3] M. Borghese, R. Jenkins, and K. D. T.-R. McLaughlin. Long Time Asymptotic Behavior of the Focusing Nonlinear Schrodinger Equation. ArXiv eprints, April 2016.

PhLAM Doctoral Days / Journées des doctorants du PhLAM
25 & 30 Mars 2022

PhD student name / Nom de l'étudiant : Prakash GYAWALI

PhD year (1/2/3/…) / Année du doctorat : 2nd year

Thesis title / Titre de la thèse : **Studies of the physico-chemical properties of water complexes in the terahertz domain**

Cotutelle (Y/N): No

Supervisors & affiliations / Encadrement et affiliations : Roman Motiyenko , Université de Lille (SMRE)

Keywords (max. 5) / Mots-clés : *Water complexes, DDS, Chirp-pulse, Large-amplitude motion, Rotational spectra*

Abstract / Résumé

Water vapour is the most abundant greenhouse gas in the atmosphere and plays a pivotal role in climate change and global warming. Also, the contribution of their complexes is noteworthy. However, there are no sufficient experiments of the latter in the THz region. The main challenge is to record high-resolution spectra of such weakly bonded complexes. The analysis is also not straightforward due to the presence of large amplitude motions. The supersonic-jet technique is a unique tool to record high-resolution spectra of molecular complexes. I present a recently developed chirped-pulse supersonic-jet spectrometer based on DDS radiofrequency up-converter. The spectrometer allows us to record broadband emission spectra of molecular complexes and radicals from 50 GHz to 500 GHz with a chirp-pulse of bandwidth up to 500 MHz.

The spectroscopic analysis of molecular complexes can be quite complicated due to the presence of large amplitude motions. I present the new assignments of the pure rotational transitions in $v_t=1$ and $v_t=2$ state of methylamine (CH_3NH_2) as a model prototype for ammonia-water complex (NH_3-H_2O). Methylamine exhibits two large amplitude motions. The methyl group CH_3 is associated with internal-rotation large-amplitude motion and amine group NH_2 is associated with inversion large-amplitude motion. The analysis is based on the "hybrid" model [1] that can fit rotational levels in molecules with two large–amplitude motions. The dataset used to calculate the predictions already contains around 3000 MW and 26848 FIR transitions of $v_t = 0$, 1 and 2 of CH_3NH_2, which are fit to a weighted standard deviation of 1.75 using 102 parameters. In the THz spectra, the rotational transitions of v_t=1-1 state were easily located within few MHz vicinity of their predicted positions. The assignment of the rotational transitions in v_t=2-2 state was more complicated due to somewhat higher shifts between predicted and measured frequencies. In this case, to confirm the assignments we used Loomis-Wood type diagrams. In total, more than 3500 new rotational transitions of methylamine in v_t=1-1 and around 2200 new rotational transitions v_t=2-2 states were assigned and added to the existing dataset. The latest results of the global fitting of MW and FIR data will be presented.

[1] I. Kleiner and J. T. Hougen, J. Mol. Spectrosc., 368, 111255 (2020)

PhD student name: Christelle HANOUN

PhD year (1/2/3/…): 2nd year

Thesis title: Ultrafast measurements in synchrotron radiation sources and free electron lasers

Cotutelle (Y/N): N

Supervisors & affiliations: Serge BIELAWSKI, Eléonore ROUSSEL [PhLAM, DYSCO team].

Keywords (max. 5): Terahertz, Ultra-fast measurements, Electro-optic sampling, Single-shot.

Abstract

Synchrotron radiation sources and free electron lasers are accelerator-based light sources that emit intense radiation at various wavelengths from the terahertz to the X-ray range, provided for scientists in various research fields (material science, medicine, chemistry, …). The optimization and stabilization of these sources require the development of single shot and ultra-fast detectors in the THz range. A popular method for recording THz signals in single-shot consists in imprinting, by electro-optic (EO) effect, the THz pulse under interest on a chirped laser pulse and analyzing the output laser spectrum. Nevertheless, the short-time scales involved and the speed of commercials cameras restrain the simplicity of extracting the information from the output signal. The latest was upgraded by associating it with the so-called photonic time-stretch technique[1] in which the modulated signal is slowed down in time by sending it in a long fiber (few kilometers) and then record it with a photodiode and an oscilloscope. This technique permited to achieve high repetition rates but still problematic for broadband THz signals where the temporal resolution limits the retrieval of the input signal. On the other side, a novel technique, called phase diversity[2], showed its ability to overcome the temporal resolution limitation and retrieve the input THz signal with unprecedented resolution. This work aims to develop a setup that combines these existing photonic techniques together in order to perform single-shot measurement at high repetition rates with a sufficient temporal resolution. First tests were done at the linear accelerator ELBE at Helmholtz-Zentrum Dresden-Rossedorf (HZDR) in order to measure the coherent diffration radiation (CDR) THz source, shot-to-shot with a sub-ps resolution in real time.

[1] Roussel, E., Evain, C., Le Parquier, M. *et al.* Observing microscopic structures of a relativistic object using a time-stretch strategy. *Sci Rep* 5, 10330 (2015).

[2] Roussel, E., Szwaj, C., Evain, C. *et al.* Phase Diversity Electro-optic Sampling: A new approach to single-shot terahertz waveform recording. *Light Sci Appl* 11, 14 (2022).

PhLAM Doctoral Days
March - April 2022

PhD student name: **Léa LAFARGUE**

PhD year (1/2/3/…): **2nd**

Thesis title: **High energy, ultrashort fiber laser system at 1053 nm for ultrahigh intensity laser front-end improvement**

Cotutelle (Y/N): **No**

Supervisors & affiliations: **Géraud BOUWMANS (PhLAM), Emmanuel HUGONNOT (CEA CESTA), Florent SCOL (CEA CESTA)**

Keywords (max. 5): **FOPCPA (fiber optical parametric chirped-pulse amplification), polarization-maintaining hybrid fiber, high energy**

Abstract:

Fiber Optical Parametric Amplification (FOPA) is a well-known process that consists of amplifying a weak signal beam by a high-intensity pump beam through a four wave mixing process thanks to the third-order nonlinearity of silica. Owing to striking characteristics of this approach such as high gain, low thermal effects, wavelength broad flexibility and tunability, adaptation of this technique to high-energy ultrashort pulses amplification has been proposed and demonstrated over time [1-3]. It is called Fiber-Optical Parametric Chirped-Pulse Amplification (FOPCPA) and gathered the extensive benefits' list of fiber systems. Phase matching conditions and fiber dispersion properties are critical for this outstanding method. Recently, we have demonstrated the amplification of ultrashort pulses at 1053 nm up to 1 µJ in an FOPCPA architecture in a specially designed solid core photonic bandgap [4]. This fiber has allowed us to get broad gain bandwidth around 1053 nm (related to zero dispersion wavelength position) associated with single-mode operation despite its 10 µm core diameter. However, this fiber was not a polarization maintaining (PM) one and the polarization of the output beam was slightly elliptical which is not well adapted for ultrahigh intensity laser beamline seeding.

In this talk, I will present an all-polarization maintaining FOPCPA system based on a specifically designed and realized solid core PM photonic hybrid fiber. This system produce µJ-range 10-nm-FWHM spectral bandwidth pulses at 1053 nm associated with single-mode linearly polarized (20 dB) beam. This energy is achieved thanks to 45 dB signal gain of the parametric amplifier. Compression of chirped pulses and characterization (pulse duration, temporal contrast) are ongoing.

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PhD student name / Nom de l'étudiant : Alexandre LERNER

PhD year (1/2/3/…) / Année du doctorat : 2

Thesis title / Titre de la thèse : High temperature Fiber Bragg Gratings embedding in metallic structures produced by additive manufacturing

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations :

- Géraud BOUWMANS (PhLAM)
- Guillaume LAFFONT (CEA List)

Keywords (max. 5) / Mots-clés : Optical fiber sensors, Fiber Bragg Gratings, Additive Manufacturing, Embedding

Abstract / Résumé

Additive manufacturing (AM) allows complex structures building layer by layer with a high control of the material parameters and geometry. This approach allows the embedding of optical fiber sensors (OFS) inside the manufactured parts during the fabrication process.

OFS present low intrusivity inside the monitored structures, high chemical and electrical resistance, and low susceptibility to electromagnetic fields. They hence are of high interest in the aerospace, spatial and nuclear fields. Fiber Bragg Gratings (FBGs) written using femtoseconds lasers allow high temperature – typically 1000°C – and strain measurements. Embedding these sensors by AM will allow distributed sensing inside complex structures during their manufacturing (process monitoring) and also while operating in harsh environments (Structural Health Monitoring)

The primary objective of the thesis is to embed fs-written FBGs in AM metallic structures (first stainless steel (SS), then aerospace-grade light alloys as titanium-based ones for example) for high temperature monitoring. The AM process is Selective Laser Melting (SLM), where a laser beam melts the surface of a powder bed allowing layer-by-layer consolidation of metallic parts.

In this context, we manufactured femtosecond written FBG arrays in polyimide coated optical fibers. Protected by a stainless steel capillary, these sensors were embedded in a SS 316L specimen by SLM. High frequency interrogation of the optical fiber sensors allowed to monitor the temperature along the specimen throughout its manufacturing.

We also present preliminary works about fs-written FBGs embedded in ceramic materials deposited layer-by-layer using plasma spraying. Process monitoring was realized as well as high temperature (400°C) characterization of the instrumented specimen.

Future works include special fibers embedding by SLM needing thinner metallic coating than the ones reported in the literature, and thermo-mechanical tests performed on instrumented ceramic specimen manufactured by plasma spraying.

PhD student name: Vikas Madhur

PhD year (1/2/3): 2nd

Thesis title: Development of a new instrument coupling mass spectroscopy and optical diagnostics for the analysis of environmental samples at atmospheric pressure
Cotutelle (Y/N): N

Supervisors & affiliations: Michael Ziskind[a], Yvain Carpentier[a], Sébastien Legendre[b]

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[b]HORIBA Scientific, F-59120 Loos, France

Keywords (max. 5): Mass Spectrometry, Laser desorption, Transfer line

Abstract

Two-step Laser Mass Spectrometry (L2MS) is widely used in our group for the surface chemical analysis of various types of samples (ice, soot, fossil, polymers, ...) as it can be tailored to reach ultra-sensitive detection limit toward specific classes of molecules. However, this technique commonly operates under ultra-high vacuum (UHV) and therefore necessitates the sample to support such environment. Here, we are aiming at analyzing samples at atmospheric pressure, allowing a much faster analysis without complex handling of the sample. A dedicated chamber is being build, which will also allow the coupling of ToF-MS to other analytical techniques, *e.g.* Raman spectroscopy and Laser-induced breakdown spectroscopy.
One of the major challenge in this work is to optimize the transfer of analytes from atmospheric pressure chamber to the ionization region of MS. This step is achieved with a capillary and a system of solenoid micro-valves which are aiming to inject a N_2 carrier gas seeded with the analytes. Various configurations are used to optimize the MS pressure and the flow of N_2 carrier gas to be able to analyze the ablated sample. Currently tested one or two valve system to be able to create differential pressure in the capillary, which helps to inject the analytes to the chamber.
First tests of the injection line were carried out utilizing the vapor pressure of kerosene, placing the liquid sample into a flask upstream the inlet valve. Optimum parameters that maximize the total ion count were determined, especially the duration of intake valve timing event, which shown to be compatible with the pressure limit of our spectrometer and the ionization laser repetition rate, both able to work at 10 Hz. The ionization laser beam was shaped by a cylindrical lens to create a sheet of light in the extraction region of the MS to maximize overlap with the gas burst. The coupling of the desorption step is ongoing. In this configuration, the opening of short capillary overhangs the desorption region and is aiming at driving the analytes to the first valve. First spectra have been obtained for a pure pyrene pellet using single valve system. Optimization of the system requires the best synchronization of four steps: laser desorption, the opening time of two valves, and laser ionization. Currently, two valves and laser ionizations are synchronized and finding of best delay is going on, then we can synchronize laser desorption to be able to record the best spectra.

PhD student name / Nom de l'étudiant : Stefano Negrini

PhD year (1/2/3/…) / Année du doctorat : 2

Thesis title / Titre de la thèse : Gain Though Loss in passive fiber cavities.

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Pr. Arnaud Mussot Université de Lille, Doc. Matteo Conforti CNRS .

Keywords (max. 5) / Mots-clés : Modulation Instability, Fiber Cavities, Gain Through Loss/Filtering, Bragg Gratings

<u>Abstract / Résumé</u>

The main focus of my thesis is the study of a phenomenon known as Gain through Loss or, in our particular application, Gain Though Filtering in passive fiber ring cavities.
Fiber cavities are a family of optical resonators which can take different forms. In our case consists in a fiber optics ring, obtained by closing a piece of fiber into itself by means of an optical coupler.
This setup is particularly suited for study of nonlinear effects thanks to its interferometric nature: when light is injected into the device, at each roundtrip interfere with itself, enhancing the onset of different nonlinear phenomena. One of the most famous and studied is Modulation Instability (MI), which consists in the parametric amplification of specific frequencies of light, which satisfy a phase-matching condition, ruled by the parameters of the cavity.
Recently, a series of studies showed how, by inserting a localized loss inside the cavity, is possible to add a new degree of freedom in the control of the phase-matching condition. In other words, the frequency position of the loss, influence the position of the frequencies that satisfy the phase-matching relation. Thus is a very straight forward way to control which frequency amplify, and this explain the origin of the name Gain through Loss, or Gain though Filtering when the loss is induced by an optical filter.
Since the phenomenon is new, the first part of the thesis is focused on its characterization, and will include the theoretical and experimental study of the dependency of different cavity and filter parameters (intracavity power, linear phase detuning, and filter's width and spectral position). The entire first part of the thesis will be conducted on a "Non-Polarization-Maintaining" setup, which means that both the cavity and the filter are made of simple single mode fiber.
With the aim of studying the field of "double frequency combs", the second part of the thesis will shift over a complete Polarization Maintaining setup. The idea behind this choice is to stimulate a spectrum on each polarization axis of the cavity, by means of the same GTF phenomenon developed before.

PhD student name: Cecilia Ouarkoub

PhD year (1/2/3/…): 2nd

Thesis title: Ultrafast measurement of topological excitations in a polariton gas

Cotutelle (Y/N): N

Supervisors & affiliations: Pierre Suret / Alberto Amo (Université de Lille/ CNRS)

Keywords (max. 5): Nonlinear optics, Polaritons, Fluids of light, Turbulence

Abstract

Turbulence has been a subject of vivid interest for a few decades. It manifests in a variety of phenomena such as the creation of vortices in hydrodynamic experiments, or the redistribution of energy to smaller-scale structures as in the Kolmogorov cascades. Light can act as a fluid and can exhibit turbulent behaviour, which has been observed in experiments using cold atoms or polariton microcavities.

Polariton microcavities have become a popular platform for the study of quantum fluids of light. Polaritons are light-matter quasi-particles that decay into photons after a lifetime of a few picoseconds giving access to all the polariton fluid's properties inside the microcavity.

Under specific conditions, the polariton fluid gives rise to hydrodynamic like turbulent phenomena among them: the stochastic ejection of vortices at a time scale of a few picoseconds. Our motivation is to image this turbulent fluid and obtain single-shot images of the dynamic of these vortices. With that in mind, we have built a set-up to create and image the polariton fluid. A semiconductor microcavity sample composed of a quantum well sandwiched between two Bragg mirrors has been designed and fabricated by our collaborators at C2N (Centre de nanosciences et de nanotechnologies) in Palaiseau. This sample is kept inside a cryostat and cooled to a temperature of a few kelvins. We excite this sample with a laser beam and then image the emitted light using a set-up. This consequently gives us access to both the real and the Fourier space emissions and allows us to rapidly switch between them.

The images obtained on the CCD camera are averaged images because the timescale for the turbulent behaviour is of the picosecond magnitude. To image at this time scale, we created a set-up that is based on the principle of optical sampling at two dimensions; we used a high-intensity pulsed picosecond pump source to sample and amplify a low-intensity continuous signal via a nonlinear optical interaction occurring inside a nonlinear crystal. We imaged the signal resulting from the non-linear interaction on a CMOS camera whose shutter is triggered on the pump laser repetition rate.

Firstly, we built the optical sampling set-up using the Difference Frequency Generation (DFG). This nonlinear interaction was utilized to sample a signal that simulates the polariton signal. Secondly, we studied the semiconductor sample and created the polariton signal. Thirdly, using these two experimental set-ups we obtained single-shot images of the polariton fluid. Presently, we are working on the experiment to find the set of parameters that allows the fluid to exhibit a turbulent behaviour.

PhLAM Doctoral Days
March - April 2022

PhD student name / Nom de l'étudiant : Shivang SRIVASTAVA

PhD year (1/2/3/…) / Année du doctorat : 2

Thesis title / Titre de la thèse : Characterization and manipulation of quantum states of the light with high-dimensional encoding

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Mikhail KOLOBOV, Université de Lille

Keywords (max. 5) / Mots-clés : Photon indistinguishability, HOM interferometry, Time Lens, Galilean telescope

Abstract / Résumé

Making photons indistinguishable by a time lens

Indistinguishability of the photons plays an important role in quantum information theories and communication tasks. Having no classical paradigm gives two-photon interference a higher ground in the entanglement studies and further opportunities to manipulate the quantum states of the light for high dimensional encoding. Here, we present a theory of quantum temporal imaging, and demonstrate a possibility of noiseless compression and stretching of temporal waveform carrying quantum information. Moreover, we provide a protocol to observe maximum visibility in Hong-Ou-Mandel interferometer, even if the input photons are non-identical in shape and structure hence, proving that the photon indistinguishability could be absolutely possible using the means of a time lens.

PhD student name : Sadain Zafar

PhD year (1/2/3/…) : 2nd Year

Thesis title : CO_2 hydrates as an alternative solution to water desalination and greenhouse gas mitigation

Cotutelle (Y/N): N

Supervisors & affiliations : Claire Pirim and Bertrand Chazallon, PhLAM

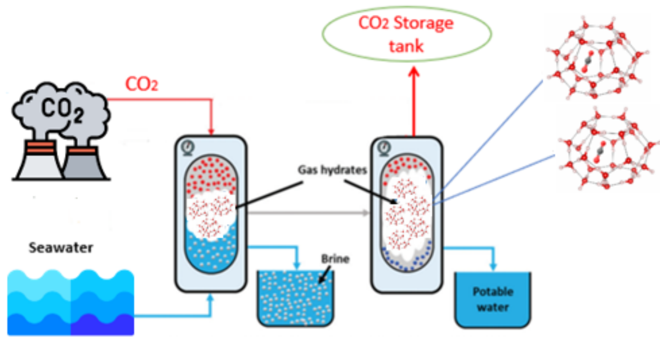
Keywords (max. 5) / Mots-clés : Hydrates, water desalination, CO_2 Capture, Raman Spectroscopy

Abstract / Résumé

Currently, releasing high levels of CO_2 into the atmosphere – as in flue-gas emissions – is not sustainable and must be reduced due to the significant impact on global warming. Indeed, the Intergovernmental Panel on Climate Change (IPCC, 2018) predicts an increase in temperature of around 1.5 degrees Celsius between 2030 and 2052 if present CO_2 emissions continue. In the meantime, water shortage is a major problem all around the world which could be alleviated by the desalination of seawater[1]. Gas hydrate technology is one of the promising approaches to mitigate both ongoing challenges when performing simultaneous CO_2 capture and water desalination[2]. The process is depicted in a modified scheme below[3].

A unique in-situ Raman-coupled high-pressure cell was utilized to demonstrate the influence of salt (NaCl) concentration on water recovery with CO_2 hydrates. Raman spectroscopy is shown to be a sensitive tool to measure any disruption in the hydrogen bonded water network of the solution by probing water stretching vibrations. It is used as a stand-alone approach for the first time to determine water recovery utilizing the signature of water and corresponding calibration curves. CO_2 clathrates are synthesized in the presence of 15 and 3.5 wt.% salt solutions at low temperature and high pressure.

The salt is primarily rejected from the forming CO_2 clathrate structure, as evidenced by the analysis of the Raman molecular spectra of water. This contributes to rise the salty water concentration around hydrate crystals. Inversely, the salinity decreases by increasing temperature due to the progressive dissociation of CO_2 clathrates as well as the release of the water molecules in the salt solution. The influence of the initial salt concentration is further investigated by in-situ Raman spectroscopy to determine the relevant parameters that can improve the water recovery process.



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PhLAM Doctoral Days / Journées des doctorants du PhLAM
25 & 30 Mars 2022

Abstracts des 3^{èmes} années

PhD student name: Kawssar Mujtaba HAIDER

PhD year (1/2/3/…): 3

Thesis title: Role of the organic waste products reactivity on secondary organic aerosol formation

Cotutelle (Y/N): N

Supervisors & affiliations: Cristian FOCSA (PhLAM, CNRS, UMR 8523, Univ. Lille), Raluca CIURARU (INRAE, UMR ECOSYS, AgroParisTech, Université Paris-Saclay, 78850 Thiveral-Grignon), Denis PETITPREZ (PC2A, CNRS, UMR 8522, Univ. Lille)

Keywords (max. 5): volatile organic compounds, mass spectrometry, sewage sludge, anaerobic digestion and dewatering, secondary organic aerosols

Abstract

The recycling of different types of organic waste products (e.g. sewage sludge) is currently being promoted as a substitute for mineral fertilizers for agricultural lands. The spreading of sewage sludge (SS) allows the recycling of the nutrients and organic matter they contain. SS contains various pollutants such as Volatile Organic Compounds (VOCs) that adversely affect the ecosystem and human health through ozone production and serve as critical precursors of secondary organic aerosols in the atmosphere. There are very few studies quantifying the gaseous compounds emitted from sewage sludge, and those studies primarily address their odorant properties for identifying suitable odour abatement techniques. There is an urgent need for more comprehensive quantitative information on VOCs emitted from SS as aerosol precursors and their comparability at different treatment stages. In this context, an experimental study was performed on SS samples taken from a wastewater treatment plant located in France. Undigested (UDSS), digested (DSS), SS with 30% and 60% of dryness were collected from different stages of treatment sequence and analyzed using atmospheric simulation chambers coupled to a proton-transfer-reaction quadrupole ion-guide time-of-flight mass spectrometry. Our study revealed that SS samples emitted a large spectrum of VOCs. 380 compounds were detected, quantified and classified into different chemical groups of compounds. The VOC emissions increased with the increase in the dryness of the sample; the highest were in SS 60%, followed by SS 30%, UDSS and DSS. The statistical analysis revealed that the anaerobic digestion and the dewatering to 60% of dryness decreased the emissions of odorous sulphuric compounds. Aromatic compounds and indoles (e.g. skatole) were significantly emitted from the UDSS. Such compounds can serve as precursor gases for atmospheric aerosol formation [(1)]. The experimental dataset obtained in this study would provide an accurate inventory reference for the VOC emissions from SS samples and show the positive impacts of the treatment in reducing the VOC emissions.

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25 & 30 Mars 2022

PhD student name / Nom de l'étudiant : Julien HURBAIN

PhD year (1/2/3/…) / Année du doctorat : 3

Thesis title / Titre de la thèse : Modelling investigation of metabolic adaptation to oxidative stress

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Benjamin PFEUTY, Quentin THOMMEN, François ANQUEZ & EDSMRE

Keywords (max. 5) / Mots-clés : Cancer, Oxidative Stress, Mathematical modelling

Abstract / Résumé :

Living cells are continually exposed to multiple and varied sources of stress. To cope with stress-induced damages, cells are endowed with biochemical adaptation mechanisms that maintain metabolic homeostasis and promote survival. In my thesis project, we investigate the cellular adaptation response to oxidative stress produced by Reactive Oxygen Species (ROS) such as hydrogen peroxide H2O2. One important mechanisms to detoxify ROS and restore redox homeostasis is the increased production of the NADPH reducing agent, which is supported by the rerouting of metabolic flux from glycolysis to the oxidative pentose phosphate pathway (PPP) (Figure 1-A). Although numerous mechanistic models of oxidative stress response have been developed (Antunes and Brito, 2017; Benfeitas et al., 2014; Grimbs et al., 2007; Marín-Hernández et al., 2011; Salvador and Savageau, 2003), a comprehensive and quantitative description of metabolic adaptation and remodelling during oxidative stress is lacking.

Starting from a metabolomic data sets (Kuehne et al., 2015) and an ODE model of the metabolic network shown in Figure 1-A, we perform a systematic parameter estimation procedure combining genetic algorithm and MCMC techniques to obtain a plausible class of models which can be thoroughly analyzed (Figure 1-B). First, dynamical response analysis highlights a biphasic time-course where metabolic imbalance is followed the adaptation response in less than a minute. Second, dose response analysis reveals that adaptation mechanism and efficiency depends on the level of stress, due to saturation of some key enzymatic reactions (ie., GPx, 6PGDH). Third, perturbation analysis emphasizes a cooperative regulation pattern where allosteric inhibition of PGI by 6PG and of GAPDH by H2O2 coordinates metabolic flux rerouting and cycling toward oxidative PPP over a broad range of stress level. These results support that autonomous, rapid and efficient adaptation to oxidative stress response can be mediated by passive and allosteric control of metabolic pathways without necessarily requiring transcriptional and post-translational signalling pathways

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Grimbs, S. et al. (2007). The stability and robustness of metabolic states: Identifying stabilizing sites in metabolic networks. Molecular Systems Biology, 3.

Kuehne, A. et al. (2015). Acute Activation of Oxidative Pentose Phosphate Pathway as First-Line Response to Oxidative Stress in Human Skin Cells. Molecular Cell , 59(3), 359–371.

Marín-Hernández, A. et al. (2011). Modeling cancer glycolysis. Biochimica et Biophysica Acta – Bioenergetics, 1807(6), 755–767.

Salvador, A. and Savageau, M. A. (2003). Quantitative evolutionary design of glucose 6-phosphate dehydrogenase expression in human erythrocytes.

PhD student name / Nom de l'étudiant : Infuso Maxime

PhD year (1/2/3/…) / Année du doctorat : 3

Thesis title / Titre de la thèse : Unravelling the atmospheric iodine chemistry using molecular simulations

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : F. Louis (PC2A), C. Toubin (PhLAM), D. Duflot (PhLAM)

Keywords (max. 5) / Mots-clés : iodomethane, adsorption, sea-salt aerosols, molecular frequencies, computational chemistry.

Abstract / Résumé

A severe nuclear accident can release Iodine-131, which is carcinogenic for humans [1]. There is missing knowledge about interactions between iodinated compounds and aerosols in the troposphere. In this context, this work investigates the adsorption of gaseous iodomethane (CH_3I) on sea salt aerosols. We parametrized a force field and used it in classical molecular dynamics calculations. We can sample large systems and a wide range of configurations. They serve as starting geometries in a QM/QM' ONIOM [2, 3] approach to compute the IR frequencies. In addition, periodic ab initio calculations have been carried out [4, 5]. Adsorption energies and vibrational frequency shifts upon adsorption are thus quantified. There is no strong coupling between the adsorbates and the surfaces, leading to small vibrational frequency shifts. Moreover, the adsorption energy is higher in the presence of water.

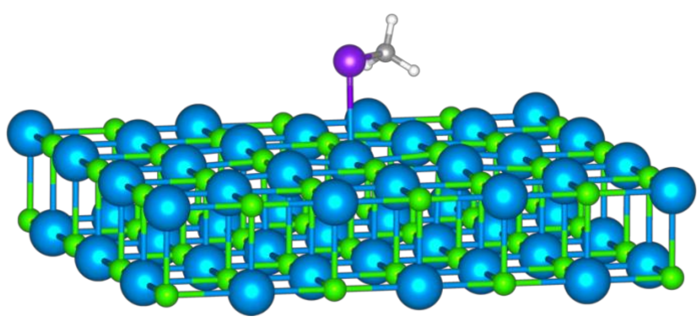

Figure 1: *Optimized geometry of CH_3I adsorbed on a dry NaCl(100) surface from a QM/QM' ONIOM (DFT/PM7) calculation.*

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PhD student name / Nom de l'étudiant : Lechevalier Corentin

PhD year (1/2/3/...) / Année du doctorat : 3

Thesis title / Titre de la thèse : Measurement of the band dispersions of a Floquet-Bloch lattice realised with coupled fiber rings

Cotutelle (Y/N):

Supervisors & affiliations / Encadrement et affiliations : Randoux Stephane PhLAM

Keywords (max. 5) / Mots-clés : Photonic network, optical fiber ring, Dispersion Relation

Abstract / Résumé

Photonic systems have recently emerged as very powerful emulators of lattice physics. A number of works have used coupled waveguides and photonic resonators to study fundamental phenomena like Bloch oscillations, gap solitons and one-way topological edge states. Of particular interest are systems that implement lattice systems subject to periodic time modulation: they open the possibility of studying phenomena hardly accessible in solid state or ultracold atoms systems, such as anomalous quantum Hall edge transport, or Thouless pumps. Here, we use a system of two coupled fibre rings that implements a time-multiplexed Floquet-Bloch lattice. The use of an elegant heterodyne interference open the acces of the full description of the Floquet-Bloch eigenvectors over the entire Brillouin zone. Our results open promising perspectives for the observation of topological effects.

PhD student name / Nom de l'étudiant : Dylan Septier

PhD year (1/2/3/…) / Année du doctorat : 3

Thesis title / Titre de la thèse : Double clad hollow core fibers for nonlinear microendoscopy

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Alexandre Kudlinski (Université Lille), Géraud Bouwmans (Université Lille)

Keywords (max. 5) / Mots-clés : photonics, fiber-optics, micro-endoscopy, nonlinear imaging

Abstract / Résumé

In the early cancer diagnostic, there is a need to develop intra-operative *in vivo* imaging tools to replace biopsy and histology processes which are time consuming and therefore delay decision making, surgery and post treatment. To provide a real-time identification of potential tumors and monitoring of surgical acts, a flexible multimodal nonlinear microendoscope is under development. It combines the advantages of nonlinear imaging (selectivity, high resolution, label-free) with the compactness and deep tissue penetration of fiber-based endoscopes. A key point in developing such a tool concerns the endoscopic fiber. It must be able to deliver high power ultrashort pulses in order to excite the nonlinear response of the tissue, but also to efficiently collect the nonlinear signal generated in the biological sample and deliver it to the detection channel.

Our goal is to develop a system performing simultaneously two (2PEF, at 920 nm) and three (3PEF, at 1300 and 1700 nm) photon excited fluorescence. Although 2PEF endoscopes have been demonstrated, 3PEF endoscopy remains a blank field. 3PEF has the advantages of being performed at wavelengths where water absorption and tissue scattering drop down, allowing for increased imaging depth, as well as providing dramatic reduction of out-of-focus background. It is therefore highly adapted to medical needs.

The high power pulse delivery is provided by a tubular hollow core fiber, combining low nonlinearity and group velocity dispersion over a wide spectral range. It allows ultrashort pulse delivery with almost no temporal nor spectral distortion. The transmission band is determined by the fiber geometry and especially the thickness of the capillaries, working as an antiresonant layer. The fiber must therefore be designed to transmit light at 920, 1300 and 1700 nm. We have designed, fabricated and characterized such a fiber. We have also functionalized it in order to obtain an almost diffraction limited spot at the output, by splicing then polishing a graded index (GRIN) fiber at the distal tip of the fiber. We have also optimized the collection efficiency by a using a double clad in which light is confined using a low index polymer layer. 2 and 3PEF imaging, as well as second (SHG) and third (THG) harmonic generation imaging was demonstrated on various biological samples, highlighting the improvements in imaging quality of 3PEF over 2PEF, as well as the multimodality of the endoscope.

PhD student name: Tomboza Wendy

PhD year (1/2/3/…): 3

Thesis title:

Development of high temperature fiber optic pressure sensor for aircraft engines instrumentation

Cotutelle (Y/N): N

Supervisors & affiliations: Géraud Bouwmans (thesis supervisor) - PhLAM, Minh Chau Phan Huy (co-supervisor) - Safran Tech, Guillaume Laffont (co-supervisor) - CEA List

Keywords (max. 5): Sensor, pressure, optical fiber, Fabry-Pérot, high temperature

Abstract

Aeronautic components such as aircraft engines are subject to harsh environment, where temperature can reach 1000 °C. The most widespread solutions for pressure monitoring in aeronautic field are based on piezoresistive sensor. However, the maximum operational temperature is often limited to 300 °C. Optical fiber sensor are excellent candidate for structure monitoring in harsh environment for industrial applications. It has the advantage of compact and robust structure and therefore can be located closest to aircraft components. Optical fiber sensor based on Fabry-Pérot interferometer are one of the most widespread solution for pressure measurement.

In the context of the thesis which aims at developing high temperature Fabry-Pérot interferometer fiber pressure sensor for aircraft engines monitoring, the goal is to design a sensor which consist in an in-fiber transductor (without external diaphragm). The sensor will be able to measure static pressure and temperature above 500 °C.

A part of the work is focused on the Fabry-Pérot interferometric sensor modeling by using finite element modeling software (COMSOL), in order to study the pressure response of the sensor. Besides, the objective is to realize different pressure sensors prototypes by using femtosecond laser micromachining. Temperature characterizations of the sensors are performed in order to assess its high temperature response (up to 900 °C). It demonstrates the need to apply thermal annealing in order to stabilize the temperature response of the sensor. Then, pressure measurements are also performed in order to study the pressure response of the sensor and evaluate the parameters we need to optimize to enhance its pressure sensitivity. Moreover, the realization of a hybrid sensor (Fiber Bragg Grating in serie with the Fabry-Pérot cavity) will allow decoupling the effect of temperature and pressure.

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PhD student name / Nom de l'étudiant : Alan Vandenberghe

PhD year (1/2/3/…) / Année du doctorat :3

Thesis title / Titre de la thèse : Deciphering circadian clock coupling with cell metabolism by fluorescence and bioluminescence.

Cotutelle (Y/N):N

Supervisors & affiliations / Encadrement et affiliations : Professor Marc Lefranc, CNRS PhLAM / Assitant professor, Alessandro Furlan Univ Lille IRCL.

Keywords (max. 5) / Mots-clés : Circadian clock, Oscillation, Biology, Bioluminescence, Microscopy

Abstract / Résumé

Life on Earth is subject to periodic changes in its environment as influenced by Earth's rotation. Most organisms developped circadian clock to prevent environmental changes. This circadian clock is composed by transcription translation feedback loop generating circadian oscillation with a period of 24H. Entrainment of master circadian clock is due to inputs from the environment like day/night cycle. Indeed, the primary signal to synchronize the master circadian clock, located in suprachiasmatic nucleus, is light. There are also peripherals clock located in the others organs and the primary signal to synchronize them is fasting/feeding cycle. The mechanisms concerning synchronization by F/F are poorly understood. In 2016 a mathematical model developp in PhLAM laboratory integrate metabolic factors to explain synchronization by fasting/feeding cycle. The model predicts action of AMPK and SIRT1 enzymes acting on the regulation of PGC1α, a master regulator of transcription of *bmal1.* BMAL1 is a critical protein acting for generation of circadian oscillation. The goal of the thesis is to understand the synchronization of circadian clock by studying the action of AMPK and other factor like SIRT1 and NAMPT with inhibitors or activators thanks to bioluminescence and fluorescence techniques.

PhD student name: Vanderhaegen Guillaume

PhD year (1/2/3/…): 3

Thesis title: Multiple Fermi Pasta Ulam Tsingou recurrences in uniform and dispersion oscillating fibers

Cotutelle (Y/N): N

Supervisors & affiliations: Arnaud Mussot, Pascal Szriftgiser

Keywords (max. 5): Modulation instability, Akhmediev breather, nonlinear fiber optics

Abstract

Modulation instability (MI) is an ubiquitous phenomenon in nonlinear physics, at the origin of supercontinuum generation and rogue wave formation. When such a process is seeded i.e. coherently driven with a sinusoidal modulation wave, the modulation wave is amplified and higher order harmonics are generated during the propagation. It is all made at the expense of the pump wave, the energy supply of the system. However, this power flow can't continue indefinitely and the pump saturates. Then the power transfers are reversed and the energy flows back to the pump wave, the system returning to its initial state. Such repetition of back and forth energy transfer are called Fermi Pasta Ulam Tsingou (FPUT) recurrences. They have especially been observed in hydrodynamics and fiber optics. However due to the fiber attenuation, the long distance studies and the multiple recurrences recordings (which was limited to 2 recurrences) have always been a challenge. Going beyond has a key role to play in the overall understanding of the Fermi Pasta Ulam Tsingou recurrences and breathers and rogue waves formation. The aim of this thesis was to investigate the richness of coherently driven MI in long length uniform fibers firstly, but also in dispersion oscillating fibers, developed in FiberTech then. To this end, we used an experimental setup allowing to map all along the fiber the amplitude and phase evolution of all waves involved in the mixing process.

This presentation will first introduce the modulation instability in optical fibers, and especially the Fermi Pasta Ulam Tsingou phenomenon. It will then focus on the experimental results in long uniform fibers (4 FPUT recurrences recording, demonstration of doubly periodic solutions of the nonlinear Schrödinger equation, demonstration of gain outside the conventional MI band, effect of loss and gain on FPUT dynamic). Finally, it will end by opening on the study of MI in dispersion oscillating fibers.

PhD student name: Xiang Yuan

PhD year (1/2/3/…): 3

Thesis title: Molecular properties in the linear response regime and beyond with relativistic equation of motion coupled cluster

Cotutelle (Y/N): Y

Supervisors & affiliations: Andre Severo Pereira Gomes PhLAM (Uni. Lille);

Lucas Visscher Section Theoretical Chemistry (VU University Amsterdam)

Keywords (max. 5):MP2; frozen natural orbital; molecular property

Abstract

The O(N^6) high computational cost is a bottleneck preventing performing Coupled-Cluster (CC) on large systems, particularly when employing 4-component based relativistic Hamiltonians, for which in practice one often uses uncontracted basis set generating large virtual molecular orbital (VMO) spaces.

The canonical Hartree-Fock (HF) orbitals are not the most compact representation for post HF method. Alternative, using natural orbitals is an efficient way to reduce the orbital space while retaining accuracy. We therefore implemented the MP2 frozen natural orbital (FNO) method [1] in the Exacorr code [2], with the particularity that our implementation can generate both complex and quaternion FNOs, and also express these in AO basis. It also allows us to obtain CCSD natural orbitals on AO basis, which can be subsequently used in analysis.

We have investigated the orbital truncation errors for both correlation energy (at CCSD(T) level) and molecular properties (at CCSD level) such as the electric field gradients at the nuclei (EFGs), dipole and quadrupole moments for hydrogen halides HX (X=F, Cl, Br, I, At, Ts), and parity violation energy shift for the H_2X_2 systems (X= O, S, Se). We find that using FNOs accelerates the convergence of the correlation energy in a roughly uniform manner across the periodic table and that, with VMO spaces truncated to around half of the complete ones, we obtain reliable estimates for both energies and molecular properties in the complete VMO spaces.

[1] T. L. Barr, E. R. Davidson, *Phys. Rev. A* 1970, **1**, 644; A. G. Taube, R. J. Bartlett, *J. Chem. Phys.* 2008, **128**, 164101

[2] J. V. Pototschnig, A. Papadopoulos, D. I. Lyakh, M. Repisky, L. Halbert, A. S. P. Gomes, H- J Aa. Jensen, L. Visscher, *J. Chem. Theory. Comput.* 2021, **17**, 5509

Posters

PhD student name,year : Marouane AYYAD, 3 ème année. **Cotutelle (Y/N)**: N.

Thesis title: Caractérisation et contrôle des états chimères dans des réseaux optiques.

Supervisors & affiliation: Saliya COULIBALY/ DYSCO.

Keywords : Cellular automata – Chimera states – Spatiotemporal chaos – Computational abilities – reservoir computing.

Abstract

Dans la mythologie grecque, une **chimère** est une créature fantastique dont certaines parties du corps appartiennent à des animaux différents. Par analogie à cette mythologie, en physique et plus particulièrement dans l'étude des systèmes complexes discrets spatialement étendus, ces états chimères correspondent à la coexistence de deux comportements dynamiques spatio-temporels opposés. La coexistence de deux domaines l'un cohérent et l'autre incohérent dans une chaîne d'oscillateurs non-linéaires couplés en est l'exemple historique, à l'image des différentes parties du corps d'une chimère.

Ces auto-organisations spatio-temporelles ont été largement étudiées théoriquement et expérimentalement. Cependant, rares sont les études menées pour explorer les liens entre ce type de dynamique et les **automates cellulaires**. Ces automates, malgré leur simplicité, possèdent des propriétés dynamiques remarquables et, par conséquent, représentent un des socles de la théorie d'information.

Pour répondre à cette problématique, nous avons considéré des états chimères obtenus dans une chaîne de résonateurs optiques identiques couplés. Ces structures ont alors fait l'objet d'analyses quantitatives et qualitatives par les mêmes outils que ceux utilisés pour caractériser les automates cellulaires. Cela nous a permis de mettre en évidence une dynamique de type automate cellulaire élémentaire cachée dans l'évolution de nos états chimères. Nous avons alors été en mesure de déduire, un ensemble de propriétés en terme de calculabilité, ouvrant des perspectives vers des potentielles applications pour le traitement de l'information.

Par la suite, nous avons utilisé les automates obtenus dans le cadre des réseaux de neurones récurrents (**RNN à état écho**). Il s'agit d'un nouveau paradigme, qui se distingue par sa grande simplicité, sa rapidité ainsi que son efficacité incontournable dans le traitement de l'information. Cependant, les performances de cette technique d'apprentissage automatique, dépendent notamment du design du réservoir. Nos résultats montrent que l'implémentation de nos états chimères optiques au lieu des réservoirs 'classiques', peut fournir une alternative prometteuse permettant d'améliorer davantage la vitesse du traitement d'information.

PhD student name: Maroun BSAIBES

PhD year (1/2/3/…): 3

Thesis title: Towards a better understanding of light scattering and mode coupling mechanisms in few mode optical fibers

Cotutelle (Y/N): N

Supervisors & affiliations: Laurent BIGOT and Yves QUIQUEMPOIS, PhLAM

Keywords (max. 5): optical fibers, telecommunication, light scattering, few-mode fibers, mode coupling

Abstract

Today, 99.8% of the worldwide Internet traffic transits via submarine fiber optic cables that can deliver several hundreds of Terabits/second of data[1]. However, every year, the demand for data transmission continues to grow while the maximum capacity transportable by currently installed optical fiber cables saturates: the moment for which the limits of the global bandwidth will be reached is known as "capacity crunch" and could occur in the coming decade. A new step forward in capacity is then needed and one of the solutions is to use Few-Mode Fibers (FMF) instead of Single-Mode Fibers (SMF), allowing to exploit a new technology named "Space Division Multiplexing" (SDM). This new approach consists in opening spatially distinguishable paths in the optical fiber via the use of different spatial modes as data carriers. Although it is accessible to produce a fiber guiding several modes, the problem here is to find and manufacture FMF designs that will minimize deleterious effects like the modal coupling or the differential modal losses. Research is hence needed to further improve the performances of the already-proposed FMF and make them compatible with end-user's requirements. To do so, this thesis aims at analyzing and modelling the guiding and loss properties of several types of FMF, in collaboration with Draka-Prysmian, the world's largest producer of telecom cables and a long-time partner of the PhLAM laboratory through the joint laboratory LIFT. The main goals are: (i) to quantify the causes of the degradation of the quality of the data transmission in an FMF, with a focus on the contribution to the optical losses and cross-talk of Rayleigh scattering and SALS (Small Angle Light Scattering, a light scattering mechanism linked to the non-perfect quality of the core/cladding interface), (ii) to set up a theoretical model seeking to a better characterization of mode coupling caused by light scattering effects in FMF, (iii) to investigate new designs of FMF that minimize Rayleigh scattering, SALS and mode coupling.

[1] Fiber Atlantic 2017, submarine cable map, <http://www.fiberatlantic.com/submarinecablemap/>

PhD student name: Alex CHEDID

PhD year (1/2/3/…): 3

Thesis title: Multimodal photonics - Dynamic characterization of the transmission channel of a few mode optical fiber

Cotutelle (Y/N): N

Supervisors & affiliations: Yves Quiquempois, Esben Ravn Andresen

Keywords (max. 5): data rate, Optical fiber, few mode fiber, eigen modes, Transmission Matrix

Abstract

Recently, there has been an increasing demand on data rate transmission (television, cloud computing, data center backup, video…). Current networks based on the use of single-mode optical fibers will no longer be able to support such rates in the coming years. We're talking about "Capacity Crunch". Solutions based on the use of new multi-mode optical fibers are therefore being studied, in which each mode will be able to transfer as much information as a single-mode fiber. For example, for a multi-mode optical fiber that can guide N modes, the capacity is multiplied by N. Despite their advantages, the modes of the multi-mode optical fiber tend to couple and exchange information, thus reducing the distances that can be reached or limiting the bandwidth of the transmission - a process known as cross-talk. The measured or calculated cross-talk between all combinations of modes can be arranged in a matrix – the cross-talk matrix. However, the cross-talk matrix describes an average behavior. In order to go further in understanding and developing fast data transmission solutions, the instantaneous behavior of the fiber need to be described more precisely, by what is called a transmission matrix. This matrix characterizes the phase and amplitude of the exchanges between modes in real time or at least on time scales smaller than those governing environmental changes such as traffic induced vibrations, gusts of wind, temperature changes. Optical communications rely on DSP (Digital Signal Processing) which estimates the channel matrix in order to be able to reproduce the data, so knowledge about the typical behavior of the transmission matrix would make it possible to design faster algorithms necessary for the codes used at the end of the line to reconstruct the data sent: these codes are known as MIMO (multiple-input multiple-output) codes. In addition, a method that identifies and quantifies the modal content of a probed fiber under different conditions is needed since the transmission matrix describes only the coupling between modes considering that the modal content is known previously.

In this thesis, the analysis technique that quantifies and identifies the modal content of a few mode fiber FMF is based on the use of data obtained with the well-known spatially and spectrally resolved imaging (S^2) technique. A new correlation-based method has been developed in our work to surpass the measurement limitations of the standard method using the same dataset. On the other hand, to measure the transmission matrix that characterizes the phase and amplitude of the exchange between modes, we used the original measurement tool developed by our team based on a spatial light modulator (SLM). The measurement setup and the numerical treatment developed in parallel have been designed to identify the eigen modes of the FMF and then express the transmission matrix in the basis of these eigen modes. Furthermore, a new and fast tool compared to the former ones (52 times faster) has been developed to measure the transmission matrix. Finally, two different FMF fibers subjected to external perturbations (micro-bending) have been tested and compared.

PhD student name / Nom de l'étudiant : DENIS Maxime

PhD year (1/2/3/…) / Année du doctorat :3

Thesis title / Titre de la thèse : Disordered quantum systems simulation with Potassium Bose-Einstein condensate

Cotutelle (Y/N):N

Supervisors & affiliations / Encadrement et affiliations : R. Chicireanu, P. Szriftgiser and J. F. Clément

Keywords (max. 5) / Mots-clés : Quantum Chaos, Bose Einstein Condensate, Periodically pulsed laser, Fano-Feshbach resonance, Kicked Bose gas

Abstract / Résumé :

The kicked rotor is a paradigmatic model for classical and quantum chaos. This model displays a classical diffusive motion, where quantum interference may lead to dynamical localization. This phenomenon has been shown to equivalent to Anderson localization, a ubiquitous quantum phenomenon which governs the properties of a large class of insulator materials in condensed matter physics. Since its introduction in 1979, the kicked rotor model aroused wide interest theoretically and experimentally. Recently, theoretical studies have reported new results on periodically kicked Bose gas in the presence of interatomic interactions. A new experimental apparatus creating quantum degenerate gases has been recently built in the Cold Atom Group to investigate this new and exciting physics.

Experimentally, a Bose Einstein Condensate (BEC) submitted to a periodically pulsed standing wave of light reproduces the kicked rotor model. In a BEC, interaction strength between atoms can be controlled by applying a uniform magnetic field, this phenomenon is known as Fano-Feshbach resonance. That is why we have built a ^{41}K BEC experiment which is able to generate nearly pure ^{41}K BECs of 400k atoms with high repetition rate (~16s). We have recently observed a resonance of 39mG wide at 409,17G in the $^{2}S_{1/2}$ (F=1,m_F=1) state. This resonance allows us to reach several interatomic interaction regimes: repulsive, attractive and non-interacting. The last ingredient needed for the study of our system is the periodically-pulsed optical potential, which I built and characterized during my thesis. The originality of the system lies in the generation of powerful infrared pulses,converted to the near infrared domain using second harmonic generation. We are able to produce pulses at a repetition frequency between 100 kHz to 500 kHz with peak optical power up to 350W. This new laser system will allow us to explore physics of the periodically kicked Bose Einstein Condensate in the presence of tunable interatomic interactions.

Fatima El Moussawi

3rd year PhD student

Thesis title: Specialty optical fibers for ultraminiaturized biomedical endoscopes.

Supervisors: Esben Ravn Andresen (HDR) & Olivier Vanvincq (HDR)

Keywords: Endoscope; Multicore fiber; Miniaturization; In-vivo cellular level imaging

Abstract

Lensless endoscope is a promising ultra-miniaturized imaging tool with the potential to enable minimally invasive and cellular-level resolution in-vivo imaging deep inside biological tissue. The main idea of the lensless endoscope is a head-mountable device containing only an optical waveguide capable of collecting light, retaining its information content, and transporting it fiber-optically to remote optics and opto-electronics. Thus, it is capable of imaging objects close to the tip of an optical fiber without any elements between object and fiber. This has the dual benefits of a flexible optical fiber that could be fixed onto mouse's head, allowing free movement and a smaller head-mountable device which could reduce space constraints, thus allow fixing several probes simultaneously. Lensless endoscopes can be based on multi-mode fiber (MMF) as well as multi-core fiber (MCF). In my thesis project, we focus on MCF because it is more readily compatible with nonlinear imaging modalities.

The lensless endoscope is most commonly implemented with image acquisition by point-scanning, and its generic concept (Figure 1) is: (i) the transmission matrix (TM) in the basis of localized modes of the fiber is measured in a preliminary step; (ii) the columns of the TM are identified as the input fields that give rise to focused output fields; (iii) the phase masks that convert the laser beam into said input fields are calculated; (iv) said phase masks are displayed sequentially on a spatial light modulator (SLM) resulting in a two-dimensional scan of the output focus, all the while back-scattered fluorescence signal is recorded, as in a point-scanning microscope.

The challenge in our work is combining minimally invasive, flexible operation, high resolution, and advanced imaging in one single piece of optical fiber. Therefore, we aim to conceive a novel fiber-optic component, a "tapered multi-core fiber (MCF)", that carries certain specification requirements for in-vivo imaging application. The work is devoted to modeling, fabrication, characterization, and application of the tapered MCF. MCF is numerically modeled using a perturbative model based on coupled-mode theory (CMT) to calculate the TM, derive its principal properties, and identify an optimal design of the MCF. The optimized MCF is fabricated by stack and draw method and a short length at its tip is tapered using a CO_2 laser-based glass processing and splicing system. The fabricated tapered MCF is then characterized by measuring its transmission matrix (TM) using spatial light modulator (SLM), and finally implemented in a lensless endoscope system for the application of two-photon fluorescence imaging.

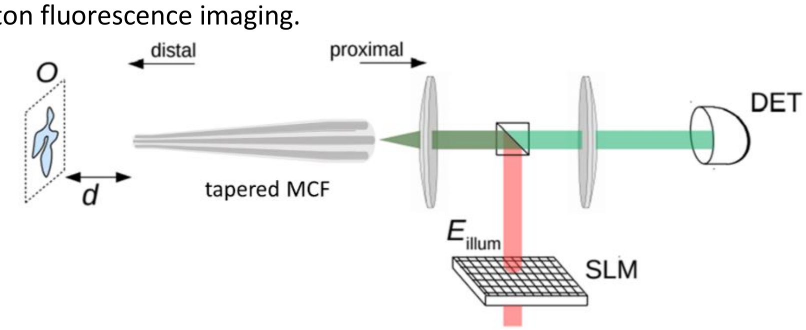

Fig. 1: Sketch of an experimental realization of a point-scanning lensless endoscope using tapered MCF.

PhD student name: Richard Asamoah OPOKU

PhD year (1/2/3/…): 3

Thesis title: Theoretical core spectroscopy of molecules interacting with ice surfaces

Cotutelle (Y/N): N

Supervisors & affiliations: Céline Toubin et André S. P. Gomes, Université de Lille, Cite Scientifique, 59655 Villeneuve d'Ascq Cedex, France

Keywords (max. 5): Core spectroscopy, ice, trace gases, frozen density embedding, coupled cluster

Abstract

Ice is everywhere in the environment and plays an essential role as a catalyst for reactions between atmospheric trace gases. The uptake of trace gases to ice has been proposed to have a major impact on geo-chemical cycles, human health and ozone depletion in the stratosphere [1]. X-ray photoelectron spectroscopy (XPS) [2], serves as a powerful technique to delineate the elemental composition of such interacting species due its surface sensitivity. Given the existence of complex physico-chemical processes such as adsorption, desorption and migration within the ice matrix, it is important to establish a theoretical framework to determine the structural and electronic properties of these molecules or species under different conditions such as temperature and concentration. The focus of this work is to construct an embedding framework employing DFT and WFT to model and interpret the photoelectron spectra of adsorbed halogenated species on ice surfaces at the core level with the highest accuracy possible.

We make use of relativistic quantum embedding method to determine core electron binding energies and chemical shift of the adsorbed halogenated species such HCl, Cl^- and I^-, which has been suggested to cause perturbation in the hydrogen bonding network of the liquid-like layer on ice [3]. We construct model systems consisting of the halide/halide ion adsorbed on different (H_2O)-cluster systems. For the interpretation of XPS spectra, core energy shift is of relevance and the interaction of molecules needs to be modeled in a relativistic manner [4].

We show that the use of fully quantum mechanical embedded method to treat solute-solvent systems is computationally efficient, yet accurate enough to determine the electronic properties of the solute system (halides/halide ions).

This project has been supported by the French Ministry of Higher Education, Research and Innovation.

[1] Abbatt, J. P. Interactions of atmospheric trace gases with ice surfaces: Adsorption and reaction. Chemical reviews 2003, 103, 4783–4800.
[2] A. Křepelová, T. Bartels-Rausch, M. A. Brown, H. Bluhm, M. Ammann J. Phys. Chem. A 2013, 117, 401−409.
[3] X. Kong, A. Waldner, F. Orlando, L. Artiglia, T. Huthwelker, M. Ammann, T. Bartels-Rausch, J. Phys. Chem. Lett. 2017, 8, 4757−4762.
[4] T. Fleig, Chem. Phys., 2, 395 (2012); T. Saue, ChemPhysChem, 12, 3077 (2011)

PhD student name / Nom de l'étudiant : SAWADOGO Bewindin Alfred

PhD year (1/2/3/…) / Année du doctorat : 3

Thesis title / Titre de la thèse : Manipulation de faisceaux RF MIMO à des fréquences THz pour des applications point à point très haut débit

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Davy GAILLOT (IEMN) et Laurent BIGOT (PhLAM)

Keywords (max. 5) / Mots-clés : Communications THz, Photonique THz, UTC-PD, fibres multi-cœurs, multiplexage spatial

Abstract / Résumé

Les ondes THz occupent la partie du spectre électromagnétique qui s'étend de 100 GHz à 10 THz. Elles sont utilisées dans divers champ d'applications, notamment en spectroscopie, en radioastronomie, en télécommunications. En télécommunications, les ondes THz sont aujourd'hui envisagées comme des porteuses dans les transmissions dans des contextes tels que les WLAN, les réseaux mobiles, la maison intelligente, les communications dans les datacenters… L'un des atouts majeurs des ondes THz est la large bande passante qu'elles offrent, ce qui permet d'envisager des transmissions à très haut débit. A titre d'exemple, ces systèmes peuvent autoriser des débits de 100 Gbit/s, soit plus de 30 fois les débits actuels (la 4G avancée – bande de fréquence 0,8, 1,8 et 2,6 GHz – offre au mieux 3 Gbits/s). Par contre, il est à noter que les ondes THz sont soumises à d'importantes pertes de puissance lors de leur propagation en espace libre. L'état de l'art fait ressortir que différents laboratoires ont déjà réalisé des transmissions THz. Elles consistaient pour la plupart en des transmissions monocanal.

L'objectif de ma thèse est de démontrer une transmission multicanaux via un réseau de photomélangeurs excité par une fibre optique multicoeurs. Comparativement à la transmission monocanal, cette approche permettra d'augmenter la puissance d'émission et donc la portée de la transmission. En outre, l'ajout d'un système permettant un contrôle de la phase sur chacun des canaux est envisagé pour donner la possibilité de contrôler la directionnalité du faisceau THz. Dans un premier temps, nous reproduisons une démonstration de transmission THz monocanal. Le transmetteur THz sera composé de deux lasers (une porteuse, comportant les données à transmettre, et un oscillateur local) dont le battement génère le signal THz par photomélange sur une photodiode à transport unipolaire (UTC-PD). Le signal rayonné, après propagation en espace libre, sera capté à l'aide d'une antenne. Pour aller au-delà de l'état de l'art, nous réaliserons ensuite une transmission multicanaux basée sur une matrice d'UTC-PD couplée à une fibre à 7 cœurs.

L'utilisation d'une approche multi-antennes nécessitera cependant une bonne connaissance du canal THz ainsi que l'adoption d'algorithmes de type MIMO (multiple-input multiple-output) pour reconstruire l'information.

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PhD student name / Nom de l'étudiant : Vuatelet Vincent

PhD year (1/2/3/…) / Année du doctorat : 3

Thesis title / Titre de la thèse : Many-body dynamical localization of a Tonks gas

Cotutelle (Y/N): N

Supervisors & affiliations / Encadrement et affiliations : Adam Rançon, PhLAM

Keywords (max. 5) / Mots-clés : Cold atoms, quantum chaos, interaction, quantum kicked rotor

Abstract / Résumé

In the quantum kicked-rotor, the alternation of kicks and free propagation gives rise to exponentially localized single-particle wave-functions in momentum space [1], known as dynamical localization, which is the quantum chaos analog of the well-known Anderson localization predicted in disordered system [2].

The consequences of adding interactions in such periodically driven system remains unclear, especially for one dimensional system where mean-field theory breaks down. We study the many-body dynamical localization of a kicked Bose gas in the Tonks regime (strong interactions). We will show that the steady-state of such system at long time can be described by a thermal density matrix, with an effective temperature depending on the kicking parameters and the number of particles, while a loss of coherence is enlightened by the one-body reduced density matrix.

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[2] P. W. Anderson. "Absence of Diffusion in Certain Random Lattices". In : Phys. Rev. 109 (5 Mar. 1958), pp. 1492–1505

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