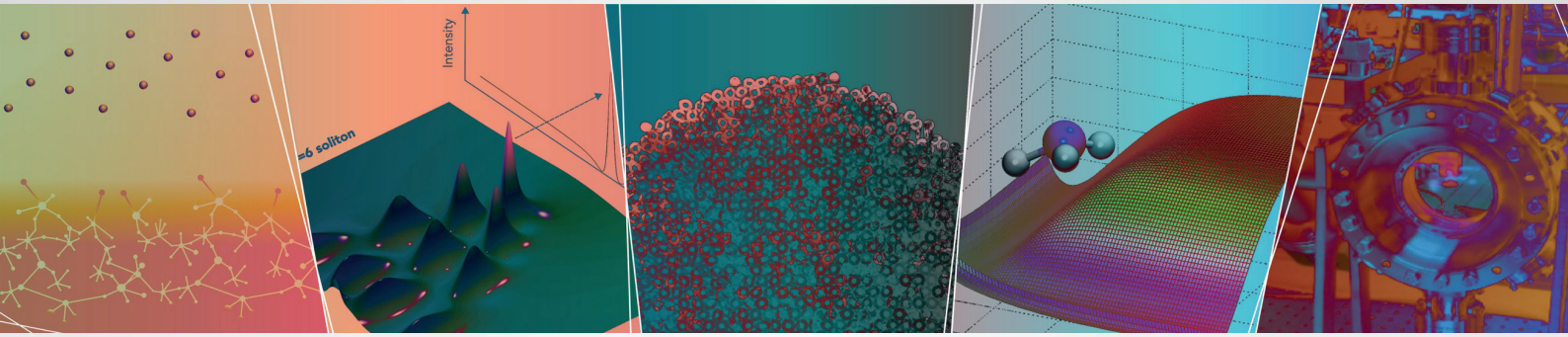
Les journées des doctorants du PhLAM 2023

Le **10 mai** à l'**IRCICA**

PhLAM
Physique des Lasers
Atomes et Molécules



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Programme

PHLAM DOCTORAL DAYS / JOURNÉES DES DOCTORANTS DU PHLAM MERCREDI 10 MAI 2023	
IRCICA	
9:15	***Introduction by the PhLAM director***
9:30	**DEL FRE Samuel:** Ab initio molecular dynamics study of vibrational energy redistribution in CO aggregates: towards a new understanding of the (photo) desorption mechanism.
9:50	**MADANI Farid:** Experimental study of disordered quantum systems in the presence of interactions with a Bose-Einstein condensate.
10:10	**BADIN Sylvain:** Theoretical study of ion-ion collision in iodine plasma for spacecraft propulsion.
10:30	**DIOUM Bakhao:** Manipulation of Quantum Pulses.
10:50	***Coffee Break & Posters by the 3rd year PhDs @ IRCICA***
11:15	**SRIVASTAVA Shivang:** Temporal imaging to make photons indistinguishable.
11:35	**HASEEB Eden:** Rewiring Necroptosis and Inflammation via Modulation of ERK Signaling Dynamics.
11:55	**EL SOKHEN Rabih:** Observation of the bulk-edge correspondence in anomalous Floquet-Chern insulators in a synthetic photonic lattice.
12:15	**ABOUHAIDAR Rawan:** Theoretical characterization of the kinetics of the multiphase reaction of ozone with an aqueous maleic acid droplet.
12:35	***Lunch break & posters by the 1st year and 3rd year PhDs @ IRCICA***
14:15	**BUNEL Thomas:** Generation of multiple frequency combs in few mode passive fiber resonators.
14:35	**MURR Georges:** Optimisation de l'horizon de prédictibilité des évènements extrêmes par « deep learning ».
14:55	**BON Mathilde:** Molecular characterization of Gloeocapsomorpha prisca microfossils by mass spectrometry to the celluar scale.
15:15	**ZGHARI Ismail:** Silice dopée et fibre optique pour la dosimétrie en radiothérapie pulsée.
15:35	**MUCCI Alexandre:** Manipulation of solitons in optical fiber experiments.
15:55	***Closing remarks***

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Sommaire

Abstracts des 2èmes années

DEL FRE Samuel: *Ab initio* molecular dynamics study of vibrational energy redistribution in CO aggregates: towards a new understanding of the (photo) desorption mechanism. 7

MADANI Farid: Experimental study of disordered quantum systems in the presence of interactions with a Bose-Einstein condensate. 8

BADIN Sylvain: Theoretical study of ion-ion collision in iodine plasma for spacecraft propulsion. 9

DIOUM Bakhao: Manipulation of Quantum Pulses. 10

SRIVASTAVA Shivang: Temporal imaging to make photons indistinguishable. 11

HASEEB Eden: Rewiring Necroptosis and Inflammation via Modulation of ERK Signaling Dynamics. 12

EL SOKHEN Rabih: Observation of the bulk-edge correspondence in anomalous Floquet-Chern insulators in a synthetic photonic lattice. 13

ABOUHAIDAR Rawan: Theoretical characterization of the kinetics of the multiphase reaction of ozone with an aqueous maleic acid droplet. 14

BUNEL Thomas: Generation of multiple frequency combs in few mode passive fiber resonators. 15

MURR Georges: Optimisation de l'horizon de prédictibilité des évènements extrêmes par « deep learning ». 16

BON Mathilde: Molecular characterization of Gloeocapsomorpha prisca microfossils by mass spectrometry to the celluar scale. 17

ZGHARI Ismail: Silice dopée et fibre optique pour la dosimétrie en radiothérapie pulsée. 18

MUCCI Alexandre: Manipulation of solitons in optical fiber experiments. 19

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Sommaire

Posters des 1ères années

ALOU ANGULO Gilberto: Ab Initio Molecular Dynamics calculation on NO oxidation over graphite oxides: A preliminary study. 21

BLESSAN Tony: Topological study of the dynamics of light in polariton networks. 22

BRACQUART Colwyn: Secondary organic aerosols: micro-solvation, hygroscopicity and atmospheric reactivity of precursors. 23

DAOUMA Zouhair 24

DEDUYTSCHAEVER Martin: Conception, réalisation et caractérisation de fibres multicœurs pour les télécommunication à très haut débit. 25

DEMAZEUX Quentin: Ultrafast measurements in accelerator-based sources. 26

FACHE Loïc: Génération contrôlée et propagation d'un gaz de solitons dans une chaîne électrique d'oscillateurs non-linéaires modélisée par l'équation de Korteweg-de-Vries. 27

GOUSPILLOU Noémie: Dynamiques de glycosylation d'oncoprotéines en cellule vivante. 28

HAIDAR Rima: Infrared Spectroscopic study of CO2 capture and separation by gas hydrates crystallization. 29

LEFEBVRE Eloise: Miniaturized endoscopic probe dedicated to real-time histopathology. 30

SHAABAN Tamara: Effect of inorganic ligands on Pa^{5+} and PaO^{3+} relative stabilities: A computational study 31

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

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Sommaire

Posters des 3èmes années

AL ASEEL Joelle: Laser-Induced Thermal Desorption for Probing Adsorption on Carbon Surfaces: A Combined Experimental and Theoretical Study. 33

BAYDI Brahim: 34

CLAUS Jordan: 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. 35

DELPIERRE Pauline: Identifying the metabolic input pathways of the liver clock using minimal mathematical models. 36

HANOUN Christelle: PhD Doctoral Students Day 2023 Ultrafast measurements in storage rings and free electron lasers. 37

LERNER Alexandre: Intégration de réseaux de Bragg haute température au sein de structures métalliques 4 obtenues par fabrication additive. 38

MADHUR Vikas: Development of a new instrument coupling mass spectroscopy and optical diagnostics for the analysis of environmental samples at atmospheric pressure. 39

NEGRINI Stefano: Gain Though Loss in passive fiber cavities. 40

OUARKOUB Cecilia: Ultrafast imaging of Turbulence in a Polariton fluid. 41

PRAKASH Gyawali: The spectroscopic study of molecules with C3V internal rotation and two large amplitude motions. 42

ZAFAR Sadain: Impact of dissolved CO2 concentration on hydrate formation and resulting water recovery in salt solutions 43

Abstracts des 2èmes années

DEL FRE Samuel

Ab initio molecular dynamics study of vibrational energy redistribution in CO aggregates: towards a new understanding of the (photo) desorption mechanism.

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In the coldest regions (~ 10 K) of the interstellar medium (ISM), most molecular species apart from H_2 accrete on dust grains to form ice mantles, acting as particularly rich molecular reservoirs. Nevertheless, large amounts of gas phase species are also detected in these regions and their existence can be explained by desorption processes at the ice surface.
Among these processes, the desorption induced by UV radiations, known as UV photodesorption, has been the subject of several experimental and theoretical studies on different compounds, such as CO[1-3], the second most abundant species in the interstellar medium. It has been shown that the UV photodesorption in pure CO ices may follow an indirect «Desorption Induced by Electronic Transition» (DIET) mechanism.[4]
In this astrochemical context, the theoretical work presented here aims to understand at the molecular level, the vibrational energy redistribution mechanism in pure CO ices that could lead to the desorption of molecular CO. The chosen approach is the *ab initio* molecular dynamics one (AIMD) based on Density Functional Theory (DFT) as implemented in the VASP package. In particular, the focus is on the end of the DIET mechanism where the electronic energy of the excited molecule, redistributed on a high vibrational state of its electronic ground state, is transferred to neighbouring molecules inducing or not a desorption. To do this, an aggregate approach is used to model the amorphous structure of the simulated ice. These aggregates, initially created, optimised, and then thermalised at 10K, are then used in molecular dynamics simulations in which a single CO molecule is excited at the vibrational level v = 40. The vibrational energy redistribution in translational, rotational, and vibrational modes in the aggregate after this excitation as well as the desorption mechanism are analysed.
The results show efficient energy transfers between the excited molecule and neighbouring ones leading to the desorption of CO molecules in almost all the trajectories, which is in very good agreement with the experimental results and in disagreement with previous theoretical studies.[3]

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MADANI Farid

Experimental study of disordered quantum systems in the presence of interactions with a Bose-Einstein condensate.

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

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, we built a new experimental setup, which produces potassium (41K isotope) Bose-Einstein condensates (BEC) with typically 4.105 atoms, and fast repetition rates of ~16 s, for which low-field Feshbach resonances are available, and can be used to tune inter-atomic interactions.

The Anderson model describes the behavior of an electron going through a lattice of random potentials. In 1D we observe a localization of the wave function of the electron in position space due to interference effects, we call this the Anderson localization and the medium is an insulator. In our group we use the kick rotor, a paradigm of quantum chaos, which consists on putting atoms in a periodically pulsed potential, to simulate the Anderson model. Since the beginning of my PhD we realized experimentally the kick rotor in 1D and observed the dynamical localization which is the analog of Anderson localization in momentum space.

It is also possible to simulate Anderson model in higher dimensions with the kick rotor model by modulating the pulsed potential with incommensurable frequencies. This allows to create additional synthetic dimensions, which opens the way towards studying quantum disorder in higher dimensions. The group succeeded in the past to simulate the 2D and the 3D Anderson models, where they observed a dynamical localization in the 2D case, and a phase transition in the 3D case from a localized regime to a delocalized regime, and measured the critical exponent of this transition. We are currently interested in observing the 4D Anderson transition and measure the critical exponent. This would be the first observation of this phase transition, and the first observation of a 4D quantum phase transition in general. To do this we are working for now on reproducing the 3D Anderson transition experiment, which would be a verification of the precision of the data of our experiment.

For the perspectives of the experiment, we are planning to study quasi-1D gases in the strongly-correlated (Tonks-Girardeau) quantum-gas regime that we can create experimentally by implementing 2D optical lattices. We plan to use a Feshbach resonance of width 361mG that we observed to tune inter- atomic interactions.
This resonance is not much broad and we will need to work on controlling precisely the magnetic field to tune finely the interactions.
1D gases in Tonks-Girardeau régime 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.

BADIN Sylvain

Theoretical study of ion-ion collision in iodine plasma for spacecraft propulsion.

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Spacecraft electric propulsion provides a low thrust for a long period of time, which is particularly useful for interplanetary missions or for satellites trajectory correction maneuvers [1]. Recently, a new type of electric thruster was developed using iodine as a propellant. An iodine plasma is formed and an electric field expels ions from the reactor thus creating a thrust. The iodine has the advantages over other types of propellant (like Xenon) of being easy to store in a solid form and to be cheaper. The first launch of a satellite using iodine plasma took place recently (on November 6, 2020) with a thruster developed by the French start-up ThrustMe on a satellite of the Chinese aerospace company SpaceTy [2].

The development of more efficient iodine thruster is impeded by the lack of knowledge about the chemical properties of the iodine plasma [3]. In this work, our objective is to compute the cross-sections of the most important chemical reactions occurring in the plasma, in order to use them in a global kinetic model describing the plasma.

In order to compute these cross-sections, we are using advanced relativistic electronic structure calculation [4] to obtain the relevant potential energy surfaces, and then a semi-classical dynamic method (i.e. Landau-Zener surface hoping [5]).

I will present our first results concerning the neutralization reaction $I^+ + I^- \rightarrow 2I$ [6]. This is a particularly important reaction since it reduces the amount of ions in the plasma and thus lowers the number of species that could be used for propulsion. These results are in accordance with experimental measurements that were carried out in the ion ring DESIREE in Stockholm.
I will also give details about our current work concerning the $I_2^+ + I^- \rightarrow 3I$ reaction [7].

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DIOUM Bakhao

Manipulation of Quantum Pulses.

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

Quantum information science provides new ways to encode, transmit, and manipulate 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 using an orthogonal set of broadband optical pulses: Photonic Temporal Modes (PTM). PTMs offer a promising approach to quantum information processing and quantum metrology due to their flexibility, quality, and reliability.

However, manipulating PTMs without destroying the encoded quantum information poses a significant challenge. Although techniques such as the quantum pulse gate (QPG) have been developed to address this challenge, a genuine temporal mode filter is currently missing. Such a tool would enable sorting temporal modes while preserving their carrier frequency and original time-frequency shape, therefore preserving the orthogonality.

To address this, we propose the original idea of “temporal cavity” as the temporal equivalent of spatial mode-cleaner cavities. Our method leverages mode-dependent resonances for effective demultiplexing of the modal content of multimode pulse in terms of temporal Hermite Gaussian modes.

SRIVASTAVA Shivang

Temporal imaging to make photons indistinguishable.

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Indistinguishability of photons plays an important role in quantum information and communication theory. Having no classical counterpart, it opens up further opportunities to manipulate the quantum states of light for linear optical quantum computation, boson sampling, and quantum information processing with high-dimensional encoding. However, single photons produced by modern sources are not always perfectly indistinguishable. Here, we present a method for making one photon indistinguishable from another by means of quantum temporal imaging [1], providing noiseless compression and stretching of temporal waveforms carrying quantum information. This method allows one to reach a unit visibility in Hong-Ou-Mandel (HOM) interference picture, which is a signature of photons indistinguishability [2].

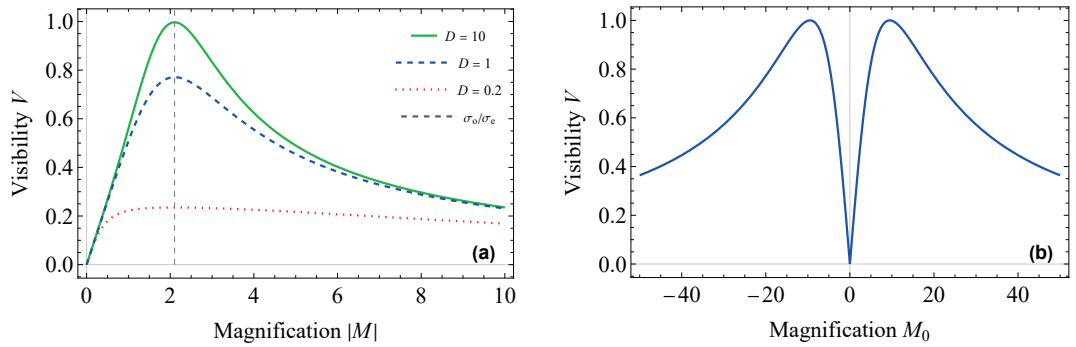

Fig. 1 (a) In case of a single-lens temporal imaging system, the visibility of HOM as a function of the magnification |M| for different values of dimensionless focal GDD of the time lens, D = 2Ω2 pDf, where Ωp is the standard deviation of the pump spectrum (in circular frequency). For any D, the maximal visibility is reached at the optimal magnification, corresponding to the ratio Δte/Δto = σo/σe. However, a higher D provides higher visibility. (b) In case of a two-lens temporal imaging system, the visibility of HOM as a function of the magnification M0 for any arbitrary focal GDD. A time telescope even with a low focal GDD is able to restore the visibility to 100%.

We conclude that a time lens with a sufficiently high focal GDD is necessary for reaching full indistinguishability of the photons. We argue that this condition might be difficult to reach for time lenses realized with an electro-optical modulator, but is more feasible for a parametric time lens.
We also present a way of eliminating the residual chirp by installing another time lens in addition to the existing one. We show that removing the residual chirp at arbitrary focal GDD is possible for a two-time-lens system satisfying the telescopic condition. We exploit the phenomenon of the existence of negative dispersion in the temporal domain, which (negative diffraction) is not possible in the spatial systems. We show a possibility of making two photons indistinguishable by a time telescope with arbitrary focal GDD of its objective time lens.

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HASEEB Eden

Rewiring Necroptosis and Inflammation via Modulation of ERK Signaling Dynamics.

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Cellular stress can promote responses via the activation of signaling pathways ranging from survival to eliciting the initiation of regulated cell deaths (RCDs) 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 a less immunogenic cell death modality. To date, there are no inhibitors of necroptosis available in the clinic. Thus, one strategy is to identify inhibitors of necroptosis from already FDA-approved drugs or at least to identify modulators that can dampen the immunogenic signature associated with RCDs, especially in necroptosis conditions. In this context, we have shown that ERK1/2 functions as a pro death modulator in TNF induced necroptosis, while displaying a pro survival role in apoptosi s in L929sAhFas cells. Our findings and that of others show that ERK1/2 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, we 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 show that inhibition of the characteristic (AM/FM) ERK signaling dynamics in TNF-induced necroptosis inhibits the gene expression increase of the proinflammatory cytokines TNF and IL-6 during TNF-induced necroptosis in the L929sAhFas cell line. The objectives of the project are 3-fold: 1- To identify inhibitors or modulators of necroptosis in FDA-approved drugs to fill the existing gap in the clinical management of necroptosis. 2- To determine the mechanism of action including the ERK pulse generator governing the characteristic of ERK signaling dynamics during necroptosis. 3- To establish the causality link by investigating the correlation between ERK signaling dynamics and pro-inflammatory gene expression patterns at the single-cell level during necroptosis.
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) around a fully functional biosensing pipeline that will be transversally coupled to modeling approaches and multiplex screening assay context with planned secondments with Coll. D. Audernaert C-BioS at VIB Ghent Belgium & H. Fearnhead ARC NUI Galway.

EL SOKHEN Rabih

Observation of the bulk-edge correspondence in anomalous Floquet-Chern insulators in a synthetic photonic lattice.

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Periodically driven lattices present fascinating properties such as the existence of anomalous topological phases with no counterpart in static systems. The periodic driving in time of the lattice gives rise to a spectrum of modes that is not only periodic in space but also in quasienergy. This feature opens the possibility of having bands with topological chiral edge states traversing the gap while showing trivial Chern indices [1].

Since their discovery, anomalous topological phases have been experimentally identified via the presence of edge states in one- and two-dimensional lattices of couple waveguides and in split step walks subject to a periodic modulation of the hoppings. However the absence of spectral information in these systems has prevented both the identification of the gap in which the anomalous edge modes are present, and access to the bulk topological invariants.

In this work we provide the first simultaneous measurement of the bulk topological invariants and of the anomalous edge states of a two-dimensional synthetic lattice. To do so, we use a system of two coupled rings (see figure). The time evolution of light pulses in the rings can be mapped into a one-dimensional lattice subject to a coherent step walk. The time step corresponds to each round trip of light in the rings and the split walk can be designed to have a time periodicity of two or four round trips. A second (parametric) dimension appears in the system when one of the rings includes a phase modulator that adds a phase f to the light pulses [2].

The two-dimensional synthetic lattice has two bands and two gaps. By modifying the splitting ratio at the beamsplitter connecting the two rings we can control the topological phase of the lattice and access trivial phases, anomalous phases with zero Chern number and anomalous-Chern phases. Using a heterodyne detection technique [3] we measure both the intensity and the phase of the eigenvectors, and we extract the Berry curvature and the Chern number of the bands (see figure). By inspecting the local changes of the Berry curvature at a topological phase transition we also measure the winding number characterising the anomalous phases. The measured topological indices match perfectly the observed number of edge states in each gap when an interface with vacuum is engineered in the experiment. These experimental observations are well described by an extension of the Rudner invariant [4] and provide the first experimental verification of the Bulk edge correspondance in Floquet-Chern insulators.

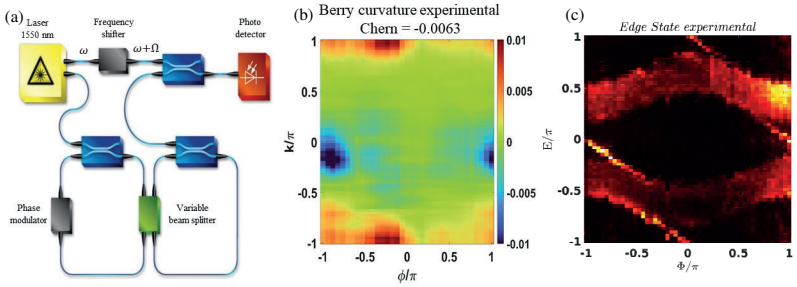

Fig. 1 (a) Experimental steup. (b) Measured band structure and edge states. (c) Measured Berry curvature in the upper band.

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ABOUHAIDAR Rawan

Theoretical characterization of the kinetics of the multiphase reaction of ozone with an aqueous maleic acid droplet.

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Univ. Lille, CNRS, UMR 8523 – PhLAM – Physique des Lasers Atomes et Molécules, F-59000 Lille, France

Dicarboxylic acids are an essential component of tropospheric aerosols emitted directly or formed in chemical processes. Multiphase reactions of these organic molecules in atmospheric aqueous phases are governed by coupled kinetic processes between the gas-phase, the particle interface and its bulk. However, models of atmospheric aerosol reactivity often do not account for the coupled nature of multiphase processes. The goal of the present study is to investigate hysiochemical properties and heterogeneous ozone oxidation of aerosol particles containing maleic acid (MA). Rate constants have been evaluated in different environments, in the gas phase, at the particle interface, and in the bulk, using a mixed quantum and classical approach. The presence of interfacial water molecules enhances the initial reaction step of MA + O3, with a larger rate constant at the air-water interface than in the gas phase. By assuming a Langmuir-Hinshelwood behavior and comparing it with the bulk, the ozonolysis of maleic acid mainly occurs in the bulk, O3 diffusion in the bulk being the limiting process. The calculated rates are compared with reported values. The original method presented here quantifies the influence of the heterogeneous environment on the reaction rates taking into account explicitly the heterogeneous environment.

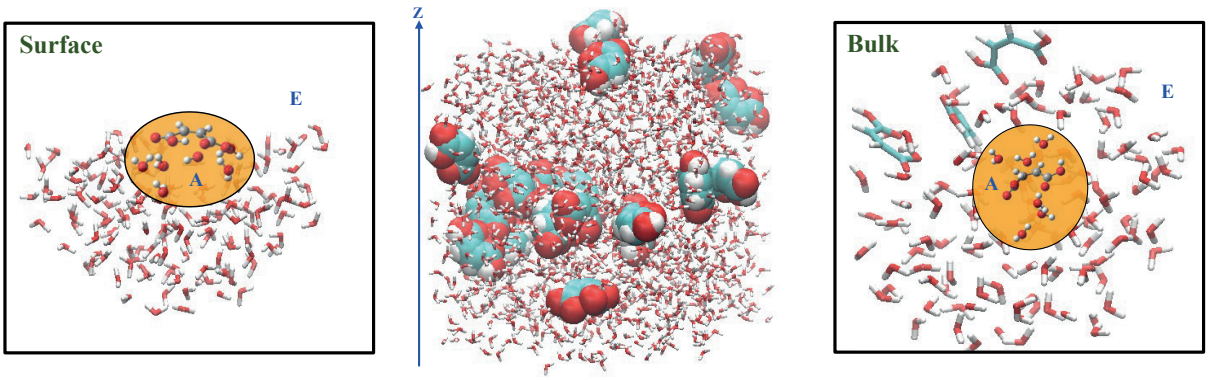

Figure: Snapshot of 20 maleic acid droplet and a schematic representations of the QM/QM' description of maleic acid at the surface and in the bulk.

Acknowledgment:
The presented work benefits from the support the CaPPA project (Chemical and Physical Properties of the Atmosphere) funded by the French National Research Agency (ANR) through the PIA (Programme d'Investissement d'Avenir) under Contract No. ANR-10-LABX-005; the Région Hauts de France and the Ministère de l'Enseignement Supérieur et de la Recherche (CPER Climibio) and the European Fund for Regional Economic Development for their financial support. This work was performed using HPC resources from GENCI-TGCC (Grant No. 2022–A0110801859) and the Centre de Ressources Informatiques (CRI) of the Université de Lille.

BUNEL Thomas

Generation of multiple frequency combs in few mode passive fiber resonators.

Supervisors & affiliations: Arnaud Mussot and Matteo Conforti
(Ulille/PhLAM/Photonics team)

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 or cores. 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.

The used resonators are fiber Fabry-Perot cavities made from optical fibers with a fiber length of around 6 to 10 cm. Both fiber ends are mounted in ceramic ferrules and Bragg mirrors are deposited at each extremity. An experimental setup was made to pump the cavity with a tens of picosecond pulse train and stabilize the pump laser on a cavity resonance. That way, nonlinear effects occur in the cavity making possible frequency comb generations. Several studies could be conducted. First, the modulation instability process was investigated in a cavity with an anomalous dispersion and characterized in intensity and phase with a high resolution. It was shown that the cross-phase modulation effect occurring in Fabry-Pérot cavities, due to the temporal overlap between the forward and the backward waves, have a significant impact on the modulation instability process which therefore depends on the input pulse duration. Second, frequency comb generation triggered by Brillouin effect was studied in a cavity with a normal dispersion. Frequency combs with line spacing equals to the Brillouin shift and 9 times greater than the cavity free spectral range, corresponding to a 10 GHz low noise and stable pulse train, could be generated.

For the future, we plan to study the dark soliton generation in normal dispersion cavities and then, transfer our knowledge in frequency comb generation in a single mode cavity to multimode or multicore cavities allowing to develop a multiple frequency comb light source.

MURR Georges

Optimisation de l'horizon de prédictibilité des évènements extrêmes par « deep learning ».

Supervisors & affiliations: COULIBALY Saliya

Long-term forecasting of extreme events such as oceanic freak waves, heat waves, floods, earthquakes, has always been a challenge due to their highly complex dynamics. Recently, machine learning methods have been used for model-free forecasting of physical systems. In this work, we investigated the ability of these methods to forecast the emergence of extreme events in a spatiotemporal chaotic passive ring cavity by detecting the precursors of high intensity pulses. To this end, we have implemented supervised sequence (precursors) to sequence (pulses) machine learning algorithms, corresponding to a local forecasting of when and where extreme events will appear.

To take this local forecasting process a step further, we also used the same strategy to predict the full dynamics. We observed a decrease in accuracy as the size of the system to be predicted increases, proving the extensive property of chaos in the ring cavity.

To test the robustness of our method, in collaboration with a Sydney meteorologist, we studied wind speed data at different locations during different months and calculated the energy exchange flow (transfer entropy) between different stations to understand the directionality of information from one station to another and to shed light on causalities. These results will help us develop accurate predictions of wind gusts, which are large fluctuations in wind speed on a relatively fast time scale. This study could help in the installation of future wind farms and in predicting wind speed for better precautions.

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BON Mathilde

Molecular characterization of Gloeocapsomorpha prisca microfossils by mass spectrometry to the celluar scale.

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Gloeocapsomorpha prisca is a microfossil (~10µm) with an organic wall of uncertain biological affinity, probably a cyanobacterium. This fossil microorganism constitutes the vast majority of the organic matter in «kukersite» rocks. Here we perform a pilot study in order to investigate the potential of laser-assisted mass spectrometry to analyze the molecular fingerprint of single microfossils. Bitumen and kerogen of a kukersite sample from a 460-million-year-old deposit of northwestern Russia, were analyzed after organic solvent extractions and demineralization. We analyze kerogen by secondary ion time-of-flight mass spectrometry (ToF-SIMS), by two-step laser desorption-ionization mass spectrometry (HR-µL2-MS) with a spatial resolution of 140 µm and by very-high mass resolution Fourier transform ion cyclotron resonance mass spectrometry coupled with laser desorption/ionization (LDI-FT-ICR-MS) on G. prisca aggregates. The spectra obtained show aromatic hydrocarbons, oxygenated and nitrogenous compounds, with a major contribution of oxygenated compounds for kerogen LDI-FT-ICR-MS spectra. The apparent aromaticity observed could be related to the mass spectrometry techniques used. Nevertheless, the predominance of oxygenated compounds (O2, O3, O4) seen in LDI-FT-ICR-MS, including some high H/C ions (e.g., C12H17O2+), is consistent with fragmentation, possibly associated with rearrangements and/or pyrolysis, of the n-alkylresorcinol based biopolymer proposed for the composition of G. Prisca.

ZGHARI Ismail

Silice dopée et fibre optique pour la dosimétrie en radiothérapie pulsée.

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

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 (la radiothérapie conformationnelle par modulation de l'intensité, la flash-thérapie, la protonthérapie). Ces techniques exigent des mesures in vivo et en temps réel de la dose absorbée avec une grande précision spatiale et temporelle. Dans ce contexte qui est le cadre du projet ANR FIDELIO (Fiber-based In-vivo realtime Dosimetry for Pulsed Radiotherapy), nous proposons l'étude de dosimètres à fibre scintillante, basés sur la radioluminescence (RL) de verres de silice dopée. Ainsi, nous nous intéressons à la dynamique temporelle du signal de radioluminescence (RL) de verre de silice dopés avec des ions de terre rares et aux effets de la température de mesure sur ce signal. De nouvelles mesures dosimétriques déportées ont été réalisés à différentes températures sur des barreaux de silice dopés par des ions Ce^{3+} ou Gd^{3+}, les barreaux ayant été soudés à une fibre de transport radio-durcie. Pour toutes les températures de mesure, le comportement de la RL est linéaire en fonction du débit de dose. De plus, la réponse RL augmente avec la température de mesure. Pour expliquer cette augmentation, une étude théorique est en cours. Un modèle reproduisant la réponse RL à température ambiante a été élaboré dans le cas des verres dopés par des ions Ce^{3+}. Ce modèle a permis de mettre évidence les mécanismes et les dynamiques impliqués dans ce matériau radio-sensible. Cependant, ce modèle reste à améliorer afin de reproduire la réponse RL à différentes températures de mesure. Par ailleurs, d'autres caractérisations dosimétriques de ces fibres sont prévues avec des rayonnements ionisants dans un régime pulsé. Afin d'évaluer le bénéfice d'un codopage par les deux terres rares, des études similaires, tant expérimentales que théoriques, utilisant des verres co-dopés Ce^{3+}/Gd^{3+}, sont aussi envisagées.

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MUCCI Alexandre

Manipulation of solitons in optical fiber experiments.

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In nonlinear physics, more precisely in integrable system like Sine-Gordon (SG), Korteweg–de Vries (KDV) and the one dimensional nonlinear Schr¨odinger equation (1D-NLSE), the concept of fundamental soliton plays a key role in understanding the dynamics due to its main property : the preservation of its shape during the evolution and of its parameters when interacting with other solitons. In 1D-NLSE, a spatially localized wavefield contain a high-order soliton solution known as a bound state of solitons, they form when two or more fundamental solitons coexist spatially with no relative velocity [1]. In this work, we use optical fibers to study the spatio-temporal dynamics associated with a localised phase odulation of a bound state of solitons in order to manipulate the velocity of a selected soliton. Finally we compare the results with a perturbed Inverse Scattering Transform spectrum theory (IST) in which the signal is decomposed into solitons characterized by their amplitudes and velocities.
Experimentally, we generate a square-shaped light pulse composed of several solitons that is launched into a Recirculating Optical Fiber Loop. Each loop, a portion of the light is collected allowing us to record the spatio-temporal dynamic in single shot [2]. Figure 1 shows the propagation of a square-shaped light pulses composed initially of 5 solitons over 2400 km. In the first panel (a) no phase modulation is applied exhibiting the spatio-temporal dynamic of a bound state of solitons. In the second panel (b) a phase modulation is applied initially, changing the velocity of one of the soliton. [2].

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Posters des 1ères années

ALOU ANGULO Gilberto

Ab Initio Molecular Dynamics calculation on NO oxidation over graphite oxides: A preliminary study.

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Oxygen functionalized graphite surfaces (HOPG-O) are common in the atmosphere due to the presence of oxidising pollutants such as ozone (O3) and hydrogen peroxide (H2O2). These oxygen functional groups can have a significant impact on atmospheric chemistry, as they can react with a wide variety of pollutants such as hydrocarbons and NOX. Among these pollutants, NOX are key components of smog and acid rain, with nitric oxide being the precursor of NO2, which is also a contributor to the formation of secondary organic aerosols, which can have negative effects on human health and the environment. In this chemical-atmospheric context, the aim of the present work is to obtain an initial characterization of the reaction system HOPG-O + NO(g) -> HOPG + NO2(g).

To this end, spin-polarized calculations using the DFT based Vienna Ab Initio Simulation Package (VASP) were performed. HOPG surfaces (3 layers, 54 atoms) with an oxygen atom in different positions were optimized and the one with the oxygen at the bridge position was found to be the most stable. The NO dissociation energy and the exothermicity of the reaction were also determined showing a good agreement with previous theoretical and experimental results. Also, adsorption energies of the NO and NO2 molecules over the O-HOPG and HOPG surfaces respectively were obtained. Finally, potential energy curves of the normal NO approximation to the O-HOPG surface were calculated showing that there exists a large repulsion barrier on the reaction coordinates at the studied conditions.

BLESSAN Tony Mathew

Topological study of the dynamics of light in polariton networks.

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The main objective of this thesis is to study experimentally novel topological phases in photonic lattices by employing coupled semiconductor micropillars in which photons can hop from site to site. Taking advantage of the extraordinary photon-photon interactions in this system, we aim at observing nonlinear topological effects [1]. By the design of these networks, the dynamics of light propagation can be manipulated in many ways: the light can be slowed down, trapped or, on the contrary, propagate in a ballistic way (without backscattering), furthermore even in the presence of an obstacle in his path. The thesis concentrates pre-dominantly on experiment, however it also includes the modeling of the propagation of light in these networks.

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BRACQUART Colwyn

Secondary organic aerosols: micro-solvation, hygroscopicity and atmospheric reactivity of precursors.

C. Bracquart, M. Goubet, A. Cuisset

Atmospheric aerosol particles strongly influence the Earth's atmosphere, and their contribution to climate change is versatile. Their hygroscopic properties (i.e. the ability to take up water) play a crucial role for their radiative forcing and the clouds formation. Especially, Secondary Organic Aerosols (SOA) play a major role on climate through atmospheric chemistry. Mass fluxes of 30–270 Tg yr−1 have been estimated to be emitted by tropospheric oxidation of biogenic and anthropogenic volatile organic compounds (VOCs). On a global scale, the emissions of natural VOCs are estimated to be several times higher than anthropogenic VOC emissions. However, in local area such as urban area, the emission of anthropogenic VOC is much higher. This leads to localized air quality problems and contribute to the formation of smog and other forms of air pollution. PhLAM and LPCA worked independently to characterize the physico-chemical properties of AOS precursors and their hydrated complexes, on the one hand by pure rotational spectroscopy in the context of micro-solvation studies at the molecular level and on the other hand to study their reactivity and their ability to form SOAs in the CHARME simulation chamber. To complement the work of Coeur et al. and Ahmad et al. concerning SAO formation from 2-methoxyphenols and their hygroscopicity, the pure rotational spectroscopy of two isomers of nitro-methoxyphenols has been studied using quantum calculations on the PhLAM cluster and using both jet-cooled CP-FTMW and FP-FTMW. The study of nitro-methoxyphenol hydrates and nitro-dimethoxyphenol are ongoing. Combined micro-solvation / SOA hygroscopicity studies are planed about xylenes emitted by the gas combustion and prenol which constitutes an alternative biofuel.

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DAOUMA Zouhair

Adam Rançon et Radu Chicireanu

La dynamique hors équilibre des systèmes quantiques drivés périodiquement a récemment suscité un intérêt croissant en raison de son importance fondamentale et de ses récentes réalisations expérimentales. Nous nous intéressons spécifiquement aux effets des interactions sur l'absorption d'énergie, la thermalisation et le comportement asymptotique du système. Notre étude se concentre sur le Quantum Kicked Rotor (QKR), un modèle emblématique du chaos quantique qui, en l'absence d'interaction, présente une localisation dynamique, c'est-à-dire une saturation de l'énergie cinétique sur de longues périodes.

L'impact des interactions sur la localisation dynamique demeure mal compris. Certaines approches champ-moyen prédisent une destruction de la localisation, tandis qu'à une dimension, celle-ci persiste en présence d'interactions très fortes, comme dans le régime de Tonks-Girardeau. Dans ce contexte, nous étudions un modèle permettant d'interpoler entre ces deux régimes pour mieux comprendre comment les interactions peuvent influencer la localisation dynamique à N-corps.

Notre recherche vise à élucider les mécanismes sous-jacents à la localisation dynamique dans différentes conditions d'interaction et à déterminer les régimes où cette localisation est préservée ou détruite. Nous analysons également l'effet des interactions sur la structure des états propres et la distribution des valeurs propres des opérateurs de Floquet. De plus, nous examinons les propriétés de transport et la diffusion dans le modèle étudié afin d'appréhender le rôle des interactions dans le comportement dynamique à long terme.

Pour mener à bien notre étude, nous utilisons diverses méthodes numériques et analytiques, telles que la méthode des perturbations, l'approche de champ moyen, les techniques de renormalisation et les simulations numériques, pour explorer les caractéristiques du modèle à différentes échelles d'interaction. En comparant les résultats obtenus, nous cherchons à identifier les tendances et les régimes universels qui pourraient aider à clarifier la relation entre les interactions et la localisation dynamique.

En outre, nous examinons l'influence des désordres et des fluctuations sur la localisation dynamique, en tenant compte de l'effet des interactions sur la robustesse du système face à ces perturbations. Cette analyse permettra de mieux comprendre la stabilité du modèle Quantum Kicked Rotor face aux imperfections réalistes.

Dans l'ensemble, notre étude vise à fournir une compréhension plus approfondie des mécanismes régissant la dynamique hors équilibre des systèmes quantiques périodiquement drivés, en particulier en ce qui concerne les effets des interactions sur la localisation dynamique. Cette compréhension pourrait avoir des implications importantes pour les applications potentielles dans les domaines de la simulation quantique, de l'information quantique et de la manipulation cohérente de systèmes quantiques complexes.

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DEDUYTSCHAEVER Martin

Conception, réalisation et caractérisation de fibres multicœurs pour les télécommunication à très haut débit.

Nous savons de nos jours que la capacité des réseaux fibrés arrive progressivement à saturation, dû au volume toujours croissant de données échangées sur les réseaux mondiaux. La fibre optique monomode atteint ses limites et les chercheurs tentent donc de trouver des alternatives pour pouvoir augmenter le débit maximal transportable par fibre optique. Une des alternatives, connue sous le nom de fibre multi-cœurs, a la particularité d'utiliser différents cœurs au sein d'une même fibre pour réaliser un multiplexage spatial de l'information. Le but de ma première année de thèse est de pouvoir implémenter un modèle numérique de couplage permettant de modéliser de la manière la plus réaliste possible le couplage de la lumière entre les différents cœurs de fibres réalisées par Draka-Prysmian, partenaire industriel du projet. Un des autres objectifs est la fabrication d'un composant dit FAN-IN/FAN-OUT ayant pour fonction d'adresser et d'extraire l'information de chaque cœur avec des pertes d'insertion raisonnables et une faible diaphonie. J'aimerais aussi dans cette première année de thèse, pouvoir mettre en place une expérience caractérisant la diffusion de la lumière dans les fibres multicœurs, ainsi que la modélisation de fibres avec une plus grande densité de cœurs.

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DEMAZEUX Quentin

Ultrafast measurements in accelerator-based sources.

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The main purpose of this thesis is to realize systems that are able to record in single shot the shapes of pico or femtosecond relativistic electron bunch shapes, as well as the terahertz light that is emitted by accelerator-based sources. To do so, we will use the single-shot electro-optic (EO) detection, where a THz electric field is encoding into the spectrum of a chirped probe laser pulse inside a Pockels crystal.
The project is the fruit of a collaboration between DESY (German national research center on accelerators science) and the PhLAM CNRS laboratory at Lille University which give us the opportunity to develop and test new measurements strategies at accelerator facilities (FLASH and EuXFEL).
Recently single shot measurements of THz electric field with simultaneously high temporal and spectral resolution at high repetition rate (1-2 MHz) become possible [1][2].
However the sensitivity of EO detection at this high repetition rate remains a strong limitation that may cause distortions of the THz field reconstruction [3]. In this poster we highlight the different strategies we are investigating to increase sensitivity and cures the distortions. PhLAM has a table-top prototype that is similar to DESY's setup, which enables us to explore these different strategies. A solution has been found to increase the sensitivity using Brewster plates [4].
For EO detection, the chirped probe laser needed to be 'clean' of higher order dispersion, which caused distortions. A possibility to compensate this higher order dispersion using a new algorithm is under investigation.
In addition we also introduce a foreseen setup that will be built and used at DESY.

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FACHE Loïc

Génération contrôlée et propagation d'un gaz de solitons dans une chaîne électrique d'oscillateurs non-linéaires modélisée par l'équation de Korteweg-de-Vries.

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Nous étudions expérimentalement la propagation d'ondes non-linéaires dans une ligne de transmission électrique. Il s'agit d'un système non-linéaire discret, composé d'oscillateurs électriques de type LC, o`u la capacité est fonction de la tension (voir Fig.1.b). Dans la limite continue et dans l'approximation des ondes de faibles amplitudes, la propagation d'ondes dans ce système est régie par l'équation de Kortewegde- Vries (KdV) [1], décrivant aussi la propagation d'ondes hydrodynamiques unidimensionnelles en eau peu profonde.

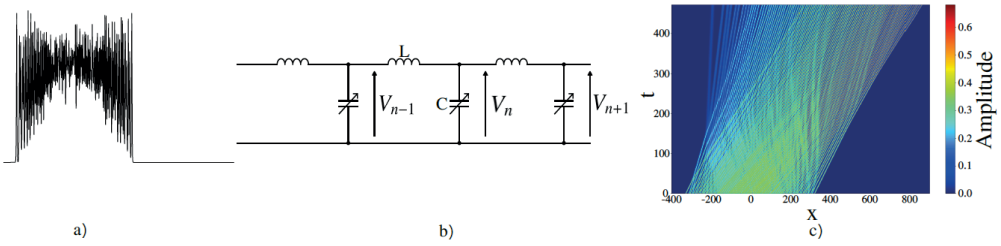

Figure 1. Représentation de la ligne électrique expérimentale et diagramme spatio-temporel issu d'une simulation de propagation d'un gaz de solitons KdV

Un générateur de fonction arbitraire produit au niveau du premier oscillateur une onde (distribution temporelle de tension) qui va se propager dans la ligne électrique composée de 160 oscillateurs LC identiques. Nous présentons ici une démonstration expérimentale de dynamique KdV dans cette ligne. L'équation KdV est dite intégrable et peut être résolue dans le formalisme de la méthode IST (Inverse Scattering Transform). Dans ce formalisme, un soliton est représenté par une valeur propre discrète, caractérisant à la fois son amplitude et sa vitesse. Plusieurs solitons distribués de manière aléatoire dans cet espace constituent ce que l'on appelle un gaz de solitons dont les propriétés statistiques sont caractérisées dans le cadre d'une théorie cinétique (analogue à la théorie cinétique des gaz) que nous cherchons à vérifier expérimentalement. Des méthodes numériques [2] nous permettent de générer ce gaz de solitons et de l'implémenter dans notre chaine. Nous observons ainsi sa dynamique spatio-temporelle et l'évolution de sa densité d'états, c'est-`a-dire la distribution de probabilité des valeurs propres caractérisant le gaz de solitons dans l'espace IST [3].

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GOUSPILLOU Noémie

Dynamiques de glycosylation d'oncoprotéines en cellule vivante.

Ce projet à l'interface de la biologie, de la chimie et de la physique vise à développer de nouveaux instruments et outils d'analyse des modifications post-traductionnelles impliquées dans la régulation d'oncoprotéines participant à l'émergence du médulloblastome, un cancer agressif du système nerveux central chez l'enfant. Pour les patients souffrant de médulloblastome, la glycosylation aberrante des oncoprotéines β-caténine et OTX2 en interaction avec un excès de nutriments est délétère. Les études viseront à étudier le rôle du niveau de O-GlcNAcylation sur ces oncoprotéines qui dépend étroitement de la disponibilité des nutriments.

Ces études s'appuieront sur les expertises et développements de l'UGSF et de PLBS dans le développement de nouvelles techniques de chimie bioorthogonales permettant la visualisation in vivo de modifications post traductionnelles comme la O-GlcNAcylation de la β-caténine (équipes T. Lefebvre, C. Biot et C. Spriet). Ces approches innovantes de biosenseur de la β-caténine sont disponibles pour le projet et seront transposées à l'étude de l'oncoprotéine OTX2 dans un contexte de maladie infantile (S. Olivier-van Stichelen lab, Medical College of Wisconsin).

Ce projet s'inscrit dans les expertises du laboratoire PhLAM en biophotonique quantitative et modélisation du stress cellulaire (groupe E. Courtade). En effet ce projet permettra de lever plusieurs verrous technologiques majeurs sur i) la transfection des oncoprotéines via une méthode de photoporation innovante développée dans le groupe d'accueil dans le cadre de l'ERC Nanobubulles ii) la dynamique des oncoprotéines en terme de mesures ratiométriques et de temps de vie iii) la modélisation du réseau de régulation pour établir un lien fonctionnel entre mesure et dynamique du senseur sur les niveaux de O-GlcNAcylation et d'effets tampon dans la cellule.

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HAIDAR Rima

Infrared Spectroscopic study of CO2 capture and separation by gas hydrates crystallization.

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Large quantities of greenhouse gases such as carbon dioxide (CO2) are released in the atmosphere and contribute to global warming. It therefore necessitates the development of efficient and environmentfriendly techniques such as Carbon Capture and Storage (CCS) technologies involving the Hydrate-Based Separation Process (HBSP) to capture CO2. Research works addressing the structure in which CO2-based hydrates could crystallize depending on the system's parameters have been carried out by vibrational spectroscopic techniques. The hydrate crystal structure is important because it directly relates to its capture and selectivity efficiency.

Three different hydrates systems (CO2-H2O, 20%CO2+80%N2-H2O, 10%CO2+80%N2-H2O) were synthesized in a high-pressure cell following a 2-step process whereby ice particles are placed in contact with the gas (CO2) or gas mixture (20%CO2+80%N2) at -3°C and a pressure of 25-100 bar (depending on the gas considered). Hydrate growth is monitored with the cell's dropping pressure and can last from a few days to several weeks. Once the pressure stops decreasing, the reaction of gas hydrates formation ended, and the hydrate crystals can be subsequently recovered from the cell now maintained at liquid nitrogen temperature to preserve their structure and composition. They are then transferred into another cryogenic reactor featuring an optical port for FTIR analysis.

Hydrates' structure is thus analyzed by FTIR spectroscopy to evidence which CO2 structure is the most stable and also how CO2 molecules are distributed when encapsulated within the large and small cages of the different hydrate structures.

LEFEBVRE Eloise

Miniaturized endoscopic probe dedicated to real-time histopathology.

Eloïse LEFEBVRE, Alexandre KUDLINSKI

In medicine and science of the living, the conventional analysis of samples is performed ex-vivo thanks to a massive optical microscope.
This imaging technique requires to prepare beforehand the sample by resection, sectioning and staining. This required marking is an irreversible process which degrades the molecular bonds to be analyzed. Besides the irreversibility of the technique, its many steps make it very time-consuming and impossible to realize in-vivo in real time.

An innovative solution and not marking consists to use a nonlinear micro-endoscope. This technology allows to image several molecular structures by using a variety of nonlinear techniques. Thus, a laser beam is injected in a hollow core fiber and shaped and focalized on the sample thanks to a micro lens and a micro-objective.

The project aims to develop a SRS (Stimulated Raman Scattering) micro-endoscope. The endoscopic head will be adapted to the characteristics of the non-linear process, in order to guarantee an imaging resolution sufficient to realize a real-time histopathological record. Its compacity will be to work on to allow its use in the medical field.

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SHAABAN Tamara

Effect of inorganic ligands on Pa^{5+} and PaO^{3+} relative stabilities: A computational study.

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A better understanding of the physical and chemical properties of actinide complexes in the solvated phase, i.e., their speciation, the nature of chemical bonds between actinides and their environment, their thermodynamic and spectroscopic properties, can have direct implications on societal and industrial applications. A key parameter is thus the coordination mechanism with ligands that acts strongly on many properties such as thermodynamics, optical or magnetism ones. The unique coordination and properties of felements with ligands [1] attracted the attention of many experimental and theoretical researchers. Among the actinides, protactinium (Z=91) keeps on being specific because, depending on its oxidation state it can behave as ‘’f element” (Pa(VI)) or “d element” (Pa(V)). In solution, Pa(V) is dominating because Pa(IV) is unstable and can be directly oxidized to Pa(V) unless a strong reducing agent is present [2]. Pa(V) can exist in solution as Pa^{5+} and in some specific solutions it will form PaO^{3+} [3], but apparently it does not form the actinyl moiety PaO^{2+} which is not the case of their heavier neighbours uranium, neptunium and plutonium. However, experimental characterization of Pa(V) and Pa(IV) is challenging because they have high tendency towards hydrolysis, polymerization and sorption on any solid.
In this work, with the use of the state-of-the-art quantum calculations, we investigate the two possible forms of Pa(V), namely PaO^{3+} and Pa^{5+} and the influence of coordinated ligands in order to determine the suitable experimental conditions to tune their relative stability. For that we consider two different stoichiometrically equivalent complexes $PaO(OH)_2(X)(H2O)$ and $Pa(OH)_4(X)$ where $X=HO^-$, F^-, Cl^-, Br^-, NO_3^-, SO_4^{2-}, $C2O_4^{2-}$ and SCN^- and compare their relative stabilities.

This work was supported by grants funded the French National Agency for Research (ANR-21-CE29-0027, LABEX CaPPA/ANR-11-LABX-0005-01 and I-SITE ULNE/ANR-16-IDEX-0004 ULNE).

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Posters des 3èmes années

AL ASEEL Joelle

Laser-Induced Thermal Desorption for Probing Adsorption on Carbon Surfaces: A Combined Experimental and Theoretical Study.

Joelle Al Aseel[1], Yvain Carpentier[1] , Eric Therssen[2] , Xavier Mercier[2] , Alejandro Rivero Santamaría[1] , Claire Pirim[1] , Celine Toubin[1] , Cristian Focsa[1]

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A few years ago, a new method for measuring the adsorption energy of molecules on carbonaceous surfaces was proposed by our team (1). This method involved using two-step laser mass spectrometry, where the first laser pulse was used to desorb labile molecules via laser-induced thermal desorption (LITD), and the second laser pulse was used to ionize the desorbed molecules. The ions were then separated and detected using a time-of-flight mass spectrometer. By recording the ion signal intensity corresponding to the adsorbate for successive nanosecond laser pulses applied to the same sample spot, it was possible to determine the adsorption energy by fitting the signal with a pseudo-exponential decay representing the number of molecules desorbing with the number of laser pulses.

However, the accuracy of this method depends on the way the surface temperature is described. Two approaches can be used: either a steady-state approximation, which assumes a quasi-thermal desorption of molecules, or a transient temperature approach, which takes into account the fast transient surface temperature observed upon laser irradiation. In the previous work, the temporal and spatial temperature profiles were computed using literature parameters for the same materials. However, this approach introduced significant uncertainty in the fitting procedure's parameters, which could be reduced using a time-consuming Bayesian statistics approach. To avoid relying on literature parameters, we now chose to measure the transient temporal and spatial temperature profiles. To do so, we designed a set of experiments that begin with heating a graphite sample to incandescence using a high-power nanosecond laser and then capture the emitted blackbody-like radiation using either fast photomultiplier tubes or an intensified CCD camera. Finally, using the theories of laser-induced incandescence and Planck's law while following the procedure described in S. Bejaoui et al. (2), we were able to ascertain the real temperature profiles.

In addition, we performed theoretical studies to complement and extend the experimental determinations of adsorption energies. One theoretical approach is based on classical molecular dynamics (MD) to retrieve the value of the adsorption energy of organic molecules on carbon surfaces using a simple Lennard-Jones model. This simulation gives a reliable value of the adsorption energy and can be used as a benchmark for experiments (3). In addition to well-known quantities of organic and inorganic molecules being adsorbed with a sub-monolayer coverage onto various substrates such as carbon nanoparticles, graphite sheets, and highly oriented pyrolytic graphite, several adsorbate-surfaces systems were studied by MD to increase the level of surface complexity. To further increase the complexity of the surface, a defective surface was created, and DFT calculations using the Vienna ab-initio simulation package (VASP) were performed to retrieve the adsorption energy of simple molecules. As expected, the increase in surface defects led to a slight increase in Eads; in these situations, the vacancies serve as adsorption sites and result in greater adsorption.

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BAYDI Brahim

Peignes de fréquences et nouvelles dynamiques paramétriques non linéaire en cavité optique.

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

Les structures temporelles dans les résonateurs optiques attirent de plus en plus d'attention, notamment celles permettant de générer des trains d'impulsions régulièrement espacées appellés peignes de fréquences. Ces impulsions dénommées soliton de cavité (CS) se propagent sans se déformer grâce à la compensation de la dispersion par la non-linéarité d'une part, et de l'autre de la dissipation par le pompage externe. Jusqu'ici, dans une grande majorité des études les CSs sont générés à la même fréquence que celle de la porteuse permettant de pomper la cavité. Récemment, il a été démontré expérimentalement que les CSs peuvent aussi être générer à une fréquence correspondant à 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. Cette configuration présente une dynamique avec des avantages importants par rapport à ceux d'un résonateur de type Kerr uniquement (non-linéarité cubique). Cependant, dans ces expériences seul le signal était résonnant dans la cavité.

Dans ce travail, nous étudions la dynamique des solitons dans des cavités optiques doublements résonantes en présence de non-linéarité du deuxième ordre (forçage paramétrique) et troisième ordre (fibre optique). L'objectif est de comprendre les conditions d'apparition et de stabilité des solitons paramétriques et leur interaction avec la pompe qui est désormais résonnante elle aussi dans ces résonateurs. L'influence de la dérive temporelle ou walk-off sur la dynamique et la stabilité de ces nouvelles structures solitoniques est aussi considérée.

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CLAUS Jordan

Caractérisation, microsolvatation et réactivité de précurseurs d'aérosols par spectroscopie microonde, infrarouge et calculs quantiques.

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

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 b-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 b-naphthaldehyde species could present two possible structures: cis, the most stable one for a, and trans for b.[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 a and two for b, corresponding to the most stable structures. All species are stabilized by intermolecular H-bonds between the water molecule and the aldehyde group of naphthaldehyde. [3]
Also, the development of a discharge injector is currently ongoing for studying open-shell species on our experimental devices. Open-shell species are suspected to be an alternative pathway to the formation of new molecules, which are not being detected yet in the interstellar medium. Their studies are important also for the atmospheric science since resonance-stabilized radicals for instance, are abundant in oil flames and leading to the formation of PAHs.

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DELPIERRE Pauline

Identifying the metabolic input pathways of the liver clock using minimal mathematical models.

Supervisor : Marc Lefranc

Living organisms orchestrate their physiology throughout the day thanks to a biological clock called circadian. 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 hyperlipidic 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 systemic 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 hyperlipidic diets can be reproduced very well by the minimal model by making only 1 or 2 parameters diet-dependent. These parameters can be traced back to putative inputs.

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HANOUN Christelle

Ultrafast measurements in storage rings and free electron lasers.

Supervisor: Serge BIELAWSKI
Member teams: Eléonore ROUSSEL, Christophe SZWAJ

Particle accelerators and free electron lasers (FEL) are large-scale facilities that produce coherent electromagnetic radiation for research in various scientific domains. This radiation exhibits ultrafast dynamics that makes its measurement and characterization challenging. Nevertheless, studying its properties is essential for understanding its formation and optimizing its emission. Despite numerous techniques available for detecting THz radiation, their performance are still limited when measuring long or broadband signals. THz detection relies on electro-optic sampling (EOS), a common measurement technique that involves imprinting the THz signal onto a chirped laser pulse and measuring it single-shot using a grating and a camera. The objective of this PhD project is to develop an innovative ultrafast detector that combines EOS with other photonic techniques, such as photonic time-stretch and phase diversity, to overcome limitations in temporal resolution and acquisition rate. In this context, we have developed a novel THz detector at 1030 nm wavelength that combines these techniques for the first time all together that enabled to measure coherent diffraction radiation (CDR) THz signals in single shot at the ELBE THz facility. This detector allowed as well to perform exceptional single-shot measurements of the complete FEL pulse in single shot at FELBE. In addition, we have designed another detector developed at the 1550 nm telecommunication wavelength, to push the limits of temporal stretching and provide scientists a low-cost measurement solution, affordable for table-top experiments and THz spectroscopy measurements.

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LERNER Alexandre

Intégration de réseaux de Bragg haute température au sein de structures métalliques 4 obtenues par fabrication additive.

Directeur de thèse : Géraud BOUWMANS (Université de Lille – PhLAM)
Encadrant CEA : Guillaume LAFFONT (CEA List, Laboratoire Systèmes et Photonique pour le Monitoring)

Les Capteurs à Fibre Optique (CFOs) basés sur des Réseaux de Bragg (RdBs) permettent la mesure de différents paramètres physiques (température, déformation, pression par exemple) en de multiples points suivant leur positionnement dans milieu sondé. Les RdBs photo-inscrits au coeur de la fibre optique à l'aide d'impulsion laser femtosecondes sont résistants à de hautes températures, permettant la réalisation de mesures jusqu'à environ 1000°C pour les fibres en silice.

L'intégration de ce type de capteur au sein de pièces réalisées par Fabrication Additive (FA) permet la réalisation de pièces complexes pré-instrumentées. Notamment, ce processus permet de s'affranchir d'une étape de fixation du CFO a posteriori de la fabrication de la pièce.

Dans ce contexte, les résultats présentés portent dans un premier temps sur l'étalonnage en température des capteurs à RdBs. Le suivi en ligne d'un procédé de FA métallique, la Fusion Sélective sur Lit de Poudre a été réalisée à l'aide de ces RdBs au sein de la pièce, mais également au niveau de l'enceinte de fabrication, permettant la détection des phénomènes thermiques caractéristiques de ce procédé.

Enfin, le poster présente l'intégration de ces capteurs au sein de structures céramiques réalisées par projection plasma, permettant la mesure de chargements mécaniques au sein de l'échantillon jusqu'à une température d'essai de 800°C.

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MADHUR Vikas

Development of a new instrument coupling mass spectroscopy and optical diagnostics for the analysis of environmental samples at atmospheric pressure.

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Two-step Laser Mass Spectrometry (L2MS) is widely used in the ANATRAC 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.

For the MS analysis of samples at atmospheric pressure, the main challenge is to transfer the analytes (laser-desorbed molecules) to the ionization region of the spectrometer which is under vacuum. This step is achieved using solenoid valves and a tubing system. Optimization of each stage of the injection has been achieved in two steps. In the first one we use a vapor (kerosene) to characterize the transfer line inside the spectrometer. The second step is aiming at optimizing the transfer of the analyte to the inlet valve after laser desorption. Results for different configurations studied will be presented.

NEGRINI Stefano

Gain Though Loss in passive fiber cavities.

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

The main focus of my thesis is the study of a phenomenon known as Gain Though Filtering (GTF) in fiber ring cavities.

Fiber cavities are a family of optical resonators which can take different forms. In our case it consists in a fiber optics ring, obtained by closing a piece of fiber into itself by means of an optical coupler.
One of the most famous phenomena studied is Modulation Instability (MI) which, when occurring inside a cavity, can be understood as an equilibrium between the effect of Kerr nonlinearity, group velocity dispersion and linear phase detuning of the laser respect to the cavity resonance.

By inserting a filter inside the cavity, it's possible to add a new degree of freedom in the balance that govern the MI process. This phenomenon becomes understandable by interpreting the MI as a phase matching problem: the phase of the filter modifies the phase of the signal which travel inside the cavity, allowing different frequencies to be phase-matched.

We organized the characterization of GTF-induced MI in fiber cavities as follow:
the first year has been dedicated to the theoretical study of GTF and the building of a working experimental setup. During the second year we focused on the characterization of the system, which included a complete study of competition between MI and GTF-stimulated MI inside the cavity in different dispersion regimes, and other control parameters such as synchronization mismatch in the cavity.

In the third and current year we have two main objective: to transition into an active cavity setup, where we can compensate for the linear losses (mainly due to couplers and splicing of different kind of fiber withing the cavity) by means of an fiber amplifier embedded directly inside the cavity. Secondly, within the context of "double frequency combs", we developed a numerical model of the GTF-induced MI in fiber maintaining fiber cavity, which can sustain MI spectra with slightly different free spectral range thanks to their birefringence nature. The main objective of this part is to characterize, at least numerically, this very interesting phenomenon with an experimental prospective for future activities.

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OUARKOUB Cecilia

Ultrafast imaging of Turbulence in a Polariton fluid.

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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 behavior, 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. This Turbulent behavior of the Polariton fluid has been observed using interferometry measurements by Alberto Amo et al in 2011 [1], they obtained averaged images and could not observe the stochasticity of this turbulent regime.

To observe that, we have built a single-shot high-resolution imaging experiment. The imaging set-up is based on the principle of optical sampling, developed by Pierre Suret's group [2]. The technique consists of the use of a high-intensity pulsed picosecond pump source to sample and amplify a low-intensity continuous signal via a nonlinear optical interaction: Difference Frequency Generation (DFG) occurring inside a nonlinear crystal. The sampled signal resulting from the DFG is imaged on a CMOS camera.

Using this Optical sampling set-up we have successfully imaged the Polariton signal in a stationary regime. We have recently observed signatures of a Turbulent regime and are presently working on a protocol to identify the vortices.

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PRAKASH Gyawali

The spectroscopic study of molecules with C3V internal rotation and two large amplitude motions.

PRAKASH GYAWALI, R. A. MOTIYENKO

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C3V internal rotation

Millimeter-wave spectra of acetyl chloride (CH3COCl) was measured in the frequency range 50–330 GHz. From a spectroscopic point of view, these molecules are interesting cases for studying methyl top internal rotation with relatively strong nuclear quadrupole coupling. Due to nonzero quadrupole moment of Cl, the quadrupole hyperfine splittings in CH3COCl are comparable with splittings due to internal rotation.
To fit the observed rotational transitions we used the so-called Rho-Axis-Method and RAM36hf codea that take nuclear quadrupole hyperfine structure into account. The analysis, which is in progress, includes the ground vibrational state as well as lowest excited torsional states.

Two large amplitude motions

The broadband rotational spectra of ammonia-water (NH3-H2O) complex were measured in the frequency range from 50 to 250 GHz using a supersonic-jet emission spectrometer. The NH3-H2O complex exhibits two large amplitude motions (LAMs): almost free internal rotation of ammonia owing to very low torsional barrier (≈10 cm^{-1}), and the inversion of water characterized by relatively high barrier (≈700 cm^{-1}). Because of the latter and taking Doppler-limited resolution of spectrometer into account, we could not observe inversion tunneling splittings of a-type rotational transitions. In total, about 150 rotational transitions of NH3-H2O were assigned in this study. They were fitted together with the data from previous studiesb using the “hybrid” Hamiltonian approachc. The analysis is in progress as we are currently trying to modify the characteristics of supersonic expansion in order to achieve higher rotational temperatures and consequently to measure higher Ka transitions. The latest results will be presented.

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ZAFAR Sadin

Impact of dissolved CO2 concentration on hydrate formation and resulting water recovery in salt solutions.

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Anthropogenic activity greatly contributes to the production and emission of greenhouse gases, and more specifically that of carbon dioxide (CO2). In the meantime, shortage of potable water is a significant challenge that will worsen in future years and needs immediate attention. While CO2 emissions substantially impact the Earth's climate, shortage of potable water poses a serious threat to the survival of most species. The hydrate-based desalination (HBD) technology (Fig. 1) is one of the potential approaches to address both current issues since it enables simultaneous CO2 extraction and water desalination in separating salt from water molecules forming the cages of CO2 hydrates.

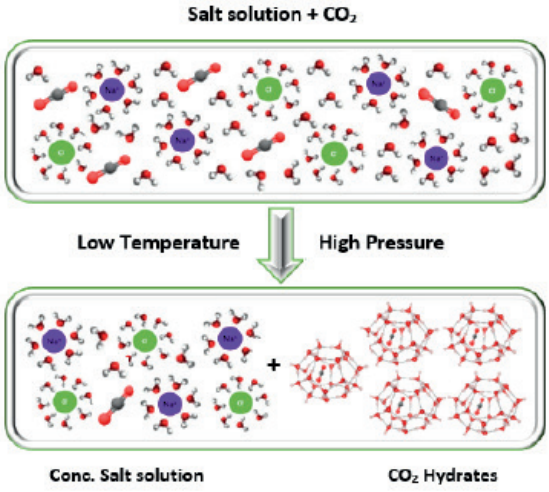

Figure 1. Artist representation of the HBD process for simultaneous CO2 capture and water desalination.

In this study, in-situ micro-Raman spectroscopy is applied to reveal the impact of initial dissolved CO2 concentration on hydrate formation as a function of salt (NaCl) concentration. A high-pressure temperature-controlled cell (capillary) is used to form CO2 hydrates in salt solutions of various concentrations. The cell is initially filled with a salt solution and then pressurized with CO2 gas. In doing so, CO2 molecules diffuse within the solution inside the capillary. The cell is then analyzed via micro-Raman to track CO2 diffusion kinetics in the solution at different locations throughout the capillary. Comparison between a system fully equilibrated (homogeneous CO2 concentration in the capillary) and non-equilibrated allows us to evaluate the impact of CO2 diffusion on hydrate structure and quantity (water recovery). We show that increasing the salt content reduces the diffusion coefficient of dissolved CO2. In the meantime, we notice that short initial CO2 diffusion periods (~30 minutes) are associated with fast hydrate formation kinetics at the gas-water interface that however rapidly ceases due to the limited diffusion of water molecules or CO2 gas through the bulky interfacial hydrate. Such a limited mass transfer results in an inhomogeneous hydrate distribution in the solution and a small water-to-hydrate conversion ratio, which in turn leads to a low water recovery. In contrast, we showed that longer CO2 diffusion periods (>1000 minutes) would significantly improve the water-to-hydrate conversion ratio. The subsequent analysis of the Raman molecular spectra of water demonstrates that the salt is primarily rejected from the forming CO2 clathrate structure and thereby contributes to rise saline water concentration around hydrate crystals. Our set of experiments allows us to refine specific experimental parameters in order to enhance water recovery in this dual CO2-capture-water recovery strategy.[1]

(1) Zafar et al., STET 2022, in preparation

DYSCO

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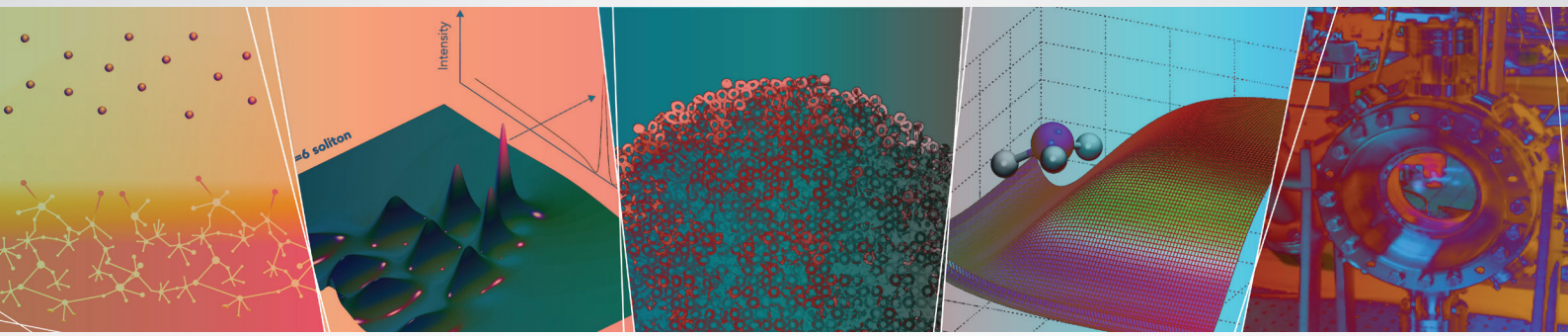
Physique des Lasers Atomes et Molécules



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