JOURNEE DES DOCTORANTS DU LABORATOIRE PhLAM

1er avril 2019, Amphithéâtre Pierre Glorieux, CERLA

PROGRAMME

8h45 – 9h00	**Introduction – C. Focsa, M. Douay**
9h00 – 9h30	**Hanna OHER** (2e année, encadrants: V. Vallet, F. Réal, *T. Vercouter – CEA Saclay*) **Development of innovative spectral modelling methods for the investigation of uranyl-ligand interactions using Time-Resolved Laser-Induced Fluorescence Spectroscopy**
9h30 – 10h00	**Abdelmounaim FAILALI** (2e année, encadrants: F. Réal, V. Vallet, *E. Acher, D. Guillaumont – CEA Marcoule*) **Molecular modelling of organic phases after plutonium extraction**
10h00 – 10h30	**Ramon Lorenzo PANADES-BARRUETA** (2e année, encadrant: D. Pelaez-Ruiz) **Simulations Quantiques de la Spectroscopie et de la Réactivité Photochimique de Molécules Atmosphériques sur de Particules de Suies**
10h30 – 11h00	Pause-café, Hall du CERLA
11h00 – 11h30	**Sandy MAKHLOUF** (2e année, encadrants: S. Magnier, *F. Taher - Université Libanaise,* cotutelle) **Modeling and Simulation of the electronic structure of small environmental molecules; An example: The halides and monoxides of Lanthanides (Ce & Lu)**
11h30 – 12h00	**Dumitru DUCA** (2e année, encadrants: C. Focsa, C. Pirim) **Physico-chemical characterization of combustion generated aerosols and surrogates**
12h00 – 12h30	**Morgane LEMAIRE** (3e année, encadrants: B. Chazallon, *A. Desmedt – ISM Bordeaux*) **Vapor deposition of nitrogen and water at low temperature and under 1 bar: the extreme condition of Enceladus environment**
12h30 – 14h30	Cocktail et session posters, salle P5/124
14h30 – 15h00	**Adrien KRAYCH** (2e année, encadrants: S. Randoux, P. Suret) **Télécommunications non-linéaires et turbulence intégrable dans les fibres optiques**
15h00 – 15h30	**Jessica BAHOUT** (2e année, encadrants: B. Capoen, H. El Hamzaoui) **Fibres optiques dédiées à la détection de rayonnements ionisantes : vers une dosimétrie aux extrêmes**
15h30 – 16h00	**Marie FOURNIER** (2e année, encadrant: L. Héliot) **Nouveaux outils de mesure de la dynamique moléculaire appliqués à l'étude de la régulation de la transcription en réponse au stress**
16h00 – 16h30	Pause-café, Hall du CERLA
16h30 – 17h00	**Brice NGOUA EDOU** (2e année, encadrants: P. Verkerk, D. Hennequin) **Study of spatio-temporal instabilities in a magneto-optical trap**
17h00 – 17h30	Echanges, conclusions, perspectives

PhLAM DOCTORAL DAY 2019

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JOURNEE DES DOCTORANTS DU LABORATOIRE PhLAM

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LISTE DES POSTERS

1. **Antoine BERTHIER** (1ère année, encadrants: C. Focsa, *D. Delhaye, I.K. Ortega – ONERA Palaiseau*)
   Impact des biocarburants sur les émissions des moteurs aéronautiques
2. **Charbel CHERFAN** (1ère année, encadrants: P. Szriftgiser, R. Chicireanu, J-F. Clément)
   Chaos Quantique avec un Condensat de Potassium: effets des interactions et de la topologie
3. **Alexandre LEBEL** (1ère année, encadrants: P. Suret, S. Randoux)
   Gaz de solitons optiques
4. **Noureddin OSSEIRAN** (1ère année, encadrants: T. Huet, P. Dréan, M. Goubet)
   Physico-chemical characterization of atmospheric pollutants - precursors of aerosols - by quantum chemistry calculations and microwave spectroscopy in a supersonic jet
5. **Etienne POEYDEBAT** (1ère année, encadrants: G. Bouwmans, *E. Hugonnot – CEA CESTA*)
   Conception et développement d'un oscillateur Mamyshev
6. **Bastián REAL ELGUEDA** (1ère année, encadrants: P. Suret, A. Amo)
   Dynamique de fluides de lumière dans des microcavités semiconductrices et fibres optiques
7. **Siveen THLAIJEH** (1ère année, encadrants: C. Focsa, Y. Carpentier, *K. Lepôt – LOG*)
   Characterization of organic matter using L2MS (Two-step Laser Mass Spectrometry): Application to early life and search of life on Mars
8. **Florent BESSIN** (3e année, encadrants: A. Mussot, M. Conforti)
   Etude de l'instabilité de modulation dans les cavités fibrées en régime de dispersion faible et dynamique temporelle
9. **Yassine BOUCHAFRA** (3e année, encadrants: A. Severo Pereira Gomes, V. Vallet)
   Approches de sous-systèmes pour la modélisation des molécules contenant des éléments lourds en phase liquide et adsorbés sur des surfaces
10. **Patrick BULOT** (4e année, encadrants: M. Douay, *G. Laffont – CEA LIST*)
    Study and realisation of optical fibre sensors with a draw tower for sensing in extreme conditions
11. **Hugo GEINDRE** (3e année, encadrant: D. Pelaez Ruiz)
    Analysis of the overestimation of the infrared intensity of the C-H stretching band in Polycyclic Aromatic Hydrocarbons
12. **Mohamed Tahar LADJIMI** (3e année, encadrants: E. Courtade, B. Pfeuty, Q. Thommen)
    Cellular stress response modelling
13. **Corentin NAVEAU** (3e année, encadrants: A. Mussot, P. Szriftgiser)
    Experimental study of modulation instability and Fermi-Pasta-Ulam-Tsingou recurrences in optical fibers
14. **Linh Dan NGO** (3e année, encadrants: Y. Carpentier, *E. Therssen – PC2A*)
    Investigation of polycyclic aromatic hydrocarbons and soot formation in swirled flames of n-butanol and conventional Diesel fuel
15. **Antoine ROOSE** (3e année, encadrants: D. Duflot, C. Toubin, *V. Riffault, S. Dusanter – SAGE IMT Douai*)
    Experimental and theoretical study of the uptake of peroxy radicals by organic aerosol surfaces
16. **Dana SIMIUC** (4e année, encadrants: E. Courtade, F. Anquez)
    Sensibilité de cellules cancéreuses au stress oxydatif : approche systémique pour étudier le couplage entre le métabolisme et le stress oxydatif
17. **Arsène TANDJE** (3e année, cotutelle, encadrants: L. Bigot, E. Andresen, *A. Vianou, M. Dossou - University of Abomey-Calavi*)
    Fibres optiques pour le guidage de modes à moment angulaire orbital : application aux Telecom et à la Photonique Non-Linéaire
18. **Jean YAMMINE** (3e année, cotutelle, encadrants: L. Bigot, E. Andresen)
    Study of the modal content and amplification properties of few-mode optical fibers

PhLAM DOCTORAL DAY 2019

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RESUMES

Présentations Orales

PhD student name, year: Hanna OHER, 2nd year

Thesis title: Development of innovative spectral modelling methods for the investigation of uranyl-ligand interactions using Time-Resolved Laser-Induced Fluorescence Spectroscopy (TRLFS)

Supervisors & affiliations: Valérie Vallet, University of Lille, PhLAM
Florent Réal, University of Lille, PhLAM
Thomas Vercouter, CEA-Saclay

Keywords: nuclear industry, uranium, photochemistry, TRLFS, ab initio quantum modelling

Abstract

Uranyl complexes have been the subject of many research works for fundamental chemistry of actinides, environmental issues, or nuclear fuel cycle processes. The formation of various uranyl complexes, with organic and inorganic ligands in solution, must be characterized for a better understanding of uranium speciation. Because uranyl-ligand interactions and symmetry of the complexes affect the electronic structure of U(VI) and thus its luminescence properties, time-resolved laser induced fluorescence spectroscopy (TRLFS) is one of the major techniques for analysis, with high sensitivity and selectivity to this element.

However, most of the relevant systems have a complex chemical composition in solution and the identification of each species from spectroscopic data remains a tricky issue. Nowadays, a combination of experimental and theoretical methods of the investigation became quite effective and progressive. In our study, the balance of highly sensitive and selective to heavy metals methods such as TRLFS and ab initio based interpretation allows a better description of the complexation data.

Luminescence spectra of uranyl complexes in solution show in general a narrow energetical range about 6000 cm^{-1} and we can identify a single electronic transition between the initial and target states with the vibrationally resolved band.

The main challenge consists in exploring a computationally cheap, fast and effective theoretical approach, in a relativistic context, to characterize the main spectral parameters and first excited state of symmetrical uranyl compounds which are very important in nuclear fuel cycle operation (i.e. UO2X42-, where X=Cl, Br; UO2(CO3)34-,UO2(NO3)n2-n) with different organic counterions (Aliquate 336, TBP, monoamides) after the photo-excitation and to compute with high accuracy vibronic progression observed in experiments. The most important steps are the ground and excited state geometry optimization followed by normal modes calculation and application of the Franck-Condon principle. The validation of results performs on each step by experimental data available in the literature.

PhD student name, year: Abdelmounaim FAILALI, 2nd Year

Thesis title: Molecular modelling of organic phases after plutonium extraction

Supervisors & affiliations: Florent RÉAL[1], Valérie VALLET[1], Éleonor ACHER[2], and Dominique GUILLAUMONT[2] ;
[1]PhLAM University of Lille France [2]DEN/DMRC/SPDS/LILA CEA Marcoule France

Keywords (max. 5): MD Simulations, Actinides, Extraction, ab initio-based Force fields, alkanes

Abstract

The nuclear fuel after its dwell time in reactor still bears a substantial amount of recoverable U and Pu. In France, in order to reduce the amount / radioactivity of nuclear waste, these elements are currently recovered by the PUREX process (Plutonium Uranium Refining by Extraction) in which U and Pu are first selectively extracted and separated thanks to liquid-liquid extraction technics using TBP (Tri-Butyl-Phosphate) as extractant molecule. As part of the studies carried out on 4th generation systems, separation processes are currently under development in CEA for the multi-recycling of these recoverable materials.

For the understanding and improvement of these separation process a microscopic description of the molecular organization of the actinides and separation ligands in the organic and aqueous phases is needed. To this end, molecular-level simulations can help gaining insights into the coordination, dynamics and mobility of these elements in the two phases and across the interface. Regarding the large size of those systems, the numerous species involved and since we are aiming at describing the temporal evolution of the system in a long-time scale, the classical mechanic simulation appears to be the most relevant tool. However, the reliability of the MD results depends on the force-field (FF) quality: the analytical description of the intermolecular energy potentials.

The first part of my Ph.D. consists in developing a FF model describing the interactions between Pu, HNO_3, counter-ion and solvent molecules. The parameters of the various analytical terms describing the solvent (alkanes and extractants), such as repulsion, polarization, were derived based on highly accurate quantum chemical data and these force fields were evaluated to reproduce experimental data; the density, the specific heat and the heat of vaporization.

The second part will be dedicated to the use of these force fields to explore the dynamical behavior of the Pu(IV) in organic solvent and extracts relevant quantities from the statistical analysis.

PhD student name, year: Ramon Lorenzo PANADES-BARRUETA, 2nd year

Thesis title: Simulations Quantiques de la Spectroscopie et de la Réactivité Photochimique de Molécules Atmosphériques sur de Particules de Suies

Supervisors & affiliations: Daniel PELAEZ-RUIZ, Maurice MONNERVILLE, PhLAM Laboratoire, Université de Lille, Région Hauts de France

Keywords (max. 5): Soot particles, Heterogeneous processes, Atmospheric Chemistry, Potential Energy Surface fitting, Nuclear Quantum Dynamics

Abstract

The goal of this Ph.D. Thesis is the full quantum mechanical simulation of the photophysical and photochemical processes of NO_2 adsorbed on soot (modelled as large Polycyclic Aromatic Hydrocarbons, PAHs) in atmospheric conditions. A detailed description of this process will help us to understand the differential day-nighttime behaviour of the production of HONO [1, 2], which is a precursor of the hydroxyl radical (OH) [3]. The specific mechanism of the soot-mediated interconversion between NO_2 and HONO is to date not fully understood. The first stage in this study consists in the determination of the stable configurations (stationary points, transition states and minima) of the NO_2-PAH system. To this end, we are using the van der Waals Transition State Search Using Chemical Dynamics (vdW-TSSCDS) method, developed in our laboratory [4], which permits in a fully automated fashion this characterisation. Once the relevant structures are known, a global description of the interaction potential is necessary for the elucidation of spectroscopic properties and reactivity of the adsorbed species. To achieve this, we have developed an algorithm Specific Reaction Parameter Multigrid POTFIT (SRP-MGPF) [5] and the corresponding software (SRPTucker) [6]. This method computes chemically accurate Potential Energy Surfaces (interaction potentials) by reparametrization of semiempirical methods using a set of stationary points. Furthermore, this software has been interfaced with the Multiconfiguration Time-Dependent Hartree (MCTDH) [7] quantum dynamics software package. In this talk we present and discuss in detail the SRP-MGPF method, its first applications to the atmospherically relevant cis-trans isomerization of the HONO molecule and our preliminary results on the Pyrene-NO_2 system.

References:

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PhD student name, year: MAKHLOUF Sandy, Second year

Thesis title: Modeling and Simulation of the electronic structure of small environmental molecules; An example: The halides and monoxides of Lanthanides (Ce & Lu)

Supervisors & affiliations : MAGNIER Sylvie and TAHER Fadia.

1- Lille University, Laboratoire de Physique des Lasers, Atomes et Molecules, UMR-CNRS 8523, F-559655 Villeneuve d'Ascq, France
2- Lebanese University, Faculty of Engineering III, Laboratory of Molecular Quantum Mechanics and Modeling (MQMM), Hadath Campus, Lebanon

Keywords: Electronic Structure, Ab-initio methods, Spin Orbit Coupling, spectroscopic constants.

Abstract

The Cerium Oxide is a rare earth monoxide formed at very high temperature (>1700ºK) [S. Wyckoff *et al.* (1977)]. It has presently significant interest in geochemistry as it is considered an environmental pollutant when interacting with CO_2 at high temperature [J. Dahle *et al.* (2015)], in the medical field [F. Caputo *et al.* (2017)] and in industry [L. Benameur *et al.* (2014)].
Up to now, the spectroscopy of this molecule is practically unknown. Experimental data are available for 16 low-lying states in the representation $^{2S+1}\Omega^{(-/+)}$ [C. Linton *et al.* (1983)]. Theoretically, the electronic structure of CeO is found to be very complicated because of the partially filled ***d*** and ***f*** orbitals present in the valence shell. In the last decades, several studies were elaborated for the low-lying states with energies below 25000 cm^{-1} but only 8 were identified in the $^{2S+1}\Lambda^{(-/+)}$ representation [M. Dolg *et al.* (1991)].

Using usual ab-initio methods (Multi-Configurational Self Consistent Field (MCSCF) and Multi Reference Configuration Interaction (MRCI)) including Davidson correction, the electronic structure of ^{140}CeO molecule has been determined in $^{2S+1}\Lambda^{(-/+)}$ and $^{2S+1}\Omega^{((-/+)}$ representations. Potential energy curves have been computed on a large range of internuclear distances and main spectroscopic constants have been deduced (equilibrium position (R_e), transition energy (T_e) and the vibrational constant (w_e)) for all states located below 30000 cm^{-1}, as well as relevant dipole moments. The ground state is found to be $(1)^3\Phi$ at an internuclear distance R_e=1,815Å in both calculations (with and without spin-orbit coupling). Our R_e value is so close to the experimental one: $R_{e(exp)}$=1,820Å [C. Linton *et al.* (1983)]. For the lower states, satisfying agreement with the available experimental data is obtained. This makes us confident of the accuracy of our present calculation for the unidentified states.
In parallel, calculations on CeF and LuO are performed in view to identify the main trends of these molecules' family.

PhD student name, year: **Dumitru DUCA, 2nd year**

Thesis title: **Physico-chemical characterization of combustion generated aerosols and surrogates**

Supervisors & affiliations: C. Focsa, C. Pirim - PhLAM

Keywords: Combustion generated aerosols, physico-chemical characterization, mass spectrometry, electron microscopy, advanced statistical analysis.

Abstract

Combustion generated aerosols (i.e.: soot) have an important influence on the atmospheric chemistry and physics. Besides having a significant impact on air quality and human health, these aerosols can also act as condensation nuclei for cloud droplets or atmospheric ice crystals. It is known that the reactivity and toxicity of aerosols is driven by the processes on their surface, where the nature and the strength of chemical bonds play an important role. Therefore, to fully understand and predict the impact of combustion related emissions, one should first attain deeper knowledge of the physical (structure, surface) and chemical (elemental and functional) composition of the particles in question. This information will also shed light on the formation mechanism of soot particles.

Since on-road motor vehicles are a major source of particulate matter, the first step in this study is to characterize the structure and chemical composition of soot particles emitted by automobile engines, as well as the variation of their characteristics with the size. The morphology of the emitted particles was probed with a Scanning Electron Microscope (SEM) and a Transmission Electron Microscope (TEM). The chemical characterization of collected particles is performed using a two-step laser mass spectrometer (L2MS) and Secondary Ion Mass Spectrometer (SIMS). Advanced statistical procedures such as principal component analysis (PCA) and hierarchical clustering analysis (HCA) were used to highlight subtle differences, as well as similarities, between different-sized soot particles. This allows not only to identify species accountable for the variation in the chemical composition but also to determine the influence of various experimental parameters (engine regime, fuel additives, lubricating oil, catalytic treatment etc.) onto the characteristics of soot particles. Additionally, the adsorption mechanism of organic molecules on carbonaceous surfaces was studied. Within this study, a new laser desorption method for measuring the adsorption energy was developed. The new method is utilizing a theoretical model based on either the assumption of quasi-thermal desorption at low laser fluences or the fast transient temperature profile upon laser irradiation. The first results are in good agreement with the values found in the literature.

The structure of soot particles will be later studied by Raman spectroscopy, also TERS and AFM (in collaboration with HORIBA), thus allowing us to better correlate physical and chemical characteristics of the analyzed particles with the combustion and sampling conditions.

PhD student name, year: Lemaire Morgane, 3rd year

Thesis title: Vapor deposition of nitrogen and water at low temperature and under 1 bar: the extreme condition of Enceladus environment

Supervisors & affiliations: Director: Bertrand Chazallon (Phlam, Univ. Lille, Lille, France); Co-director: Arnaud Desmedt (ISM- Univ. Bordeaux, Bordeaux, France)

Keywords (max. 5): Gas hydrate, Vapor-deposition, Astrophysical, Enceladus

Abstract

Because the water ice is ubiquitous in the solar system, gas hydrates are supposed to exist in astrophysical environment, since the thermodynamic conditions necessary for their formation and stability may exist on various comets and planets.1 Enceladus, a Saturnian moon, shows a South Plume whose activity implies a thin ice lithosphere with the plausible existence of a water ocean near the surface that could trapped guest molecule to form nitrogen hydrates.2,3 Most experimental investigations of gas hydrates are performed by using gas hydrates formed under high pressure and high temperature (with respect to astrophysical conditions), cooled down to 80 K, recovered and analysed at low temperature to suit the astrophysical conditions.4,5 Our team has recently performed water-gas deposition experiments at astrophysical conditions: low temperature and low pressure, in the Enceladus conditions according to previous calculated equilibrium curve6. In this work, in-situ microRaman spectroscopy, adapted to investigate gas hydrate7, are used to study three different protocols: (1) sequential multi-layer deposit, (2) sequential homogenous deposit and (3) co-deposit. In the first case, a porous amorphous multi-layered solid water ice (ALSW) is formed by several deposition of water vapor at 80 K, and then pressurized with 1.1 bar of gaseous nitrogen. The sample is then heated up until hydrate formation occurs: at 130 K, two distinct Raman contributions of N2 trapped into ALSW can be decomposed; at 160 K, the ALSW crystallises to cubic ice which is associated with a splitting of the two contributions of the N2 trapped attributed to N2 hydrate formation8. In the other two cases, all the N2 trapped is released upon heating and no hydrate formation is observed by Raman. The suitable condition for the hydrate formation appears to be the multi-layered deposit. Moreover, Enceladus is supposed to be composed of rocky core, coated with a liquid ocean, a ductile and a brittle ice. Thanks to this configuration, convection exists between the rocky core and the brittle ice that is heated and cooled, thus enabling the formation of a multi-layered ice in contact with nitrogen gas of the South Plume9,10.

Acknowledgements: This work is supported by ANR-15-CE29-0016 MI2C. Jennifer Noble (PhLAM – Univ. Lille) is thanked for fruitful and helpful discussions.

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PhD student name, year: Adrien Kraych, 2éme année

Thesis title: Télécommunications non-linéaires et turbulence intégrable dans les fibres optiques

Supervisors & affiliations: Stéphane Randoux et Pierre Suret. PHLAM

Keywords (max. 5): Optique non linéaire, Fibres optiques

Abstract

L'instabilité modulationnelle (aussi appelée instabilité de Benjamin-Feir en hydrodynamique) découverte en 1967, est un phénomène bien connu en physique non linéaire. L'instabilité modulationelle (modulation instability, MI) est un processus d'amplification de faibles perturbations en interaction avec une onde plane. En régime d'amplification dit linéaire, les perturbations croissent de façon exponentielle. Ce n'est plus le cas lorsque l'amplitude des perturbations devient comparable à celle de l'onde plane, on parle alors du stade non linéaire de l'instabilité modulationnelle.

Dans le régime non linéaire, on observe des dynamiques spatio-temporelles riches qui ont été, jusqu'à récemment, la source de vifs intérêts dans plusieurs domaines de la physique expérimentale et théorique. Nous rapportons ici, la première observation expérimentale de la dynamique spatio-temporelle d'une onde plane perturbée localement. Nous utilisons une boucle fibrée dans laquelle, l'onde plane perturbée se propage sur quelques centaines de kilomètres avec des pertes très faibles car compensées par amplification Raman. On observe notamment l'expansion de structures non linéaires oscillantes, conjointement à l'amplification du bruit optique de l'onde plane présent à l'état initial. Les comportements expérimentaux observés sont en accord avec les simulations numériques de l'équation de Schrödinger non linéaire (1D-NLSE) avec un terme d'amortissement. Ils démontrent la robustesse au bruit et à la dissipation du scénario théorique considéré.

Par ailleurs nous reportons également la première observation expérimentale de la dynamique spatio-temporelle d'une onde plane bruitée sujette au processus d'instabilité modulationelle dans les fibres optiques. Notre dispositif permet de mesurer le moment d'ordre deux des fluctuations d'intensité. Nous observons que celui-ci est caractérisé par une évolution quasi-périodique amortie en fonction de la longueur de propagation.

PhD student name, year: **Bahout** Jessica, 2éme année de these.

Thesis title: Fibres optiques dédiées à la détection de rayonnements ionisantes : vers une dosimétrie aux extrêmes.

Supervisors & affiliations: **CAPOEN** Bruno, **EL HAMZAOUI** Hicham.

Keywords (max. 5): Dosimétrie, Radioluminescence, Luminescence optiquement stimulée, les verres co-dopés Ce^{3+} et Cu^{+}.

Abstract

Cette thèse s'inscrit entièrement dans le projet SURFIN (Nouveaux matériaux pour la SURveillance par Fibre optique des Installations Nucléaires) labellisé par l'ANDRA, projet visant des applications en dosimétrie fibrée de radiations ionisantes. Le travail de thèse consiste à caractériser par spectroscopie et à montrer les potentialités dosimétriques de verres et de fibres optiques co-dopés Ce^{3+} et Cu^{+}. Notamment, les réponses de radioluminescence (RL) et de luminescence optiquement stimulée (OSL) de barreaux et de fibres ont été étudiées sous excitation X. L'objectif du codopage Cu/Ce est de profiter des avantages des deux ions dans la matrice silice : l'ion Cu^{+} présente en effet la meilleure efficacité quantique de photoluminescence et il est donc *a priori* plus adapté pour une dosimétrie à faible débit de dose. Par ailleurs, les verres dopés Ce^{3+} ont montré une meilleure résistance aux radiations ionisantes (X ou γ). Cela fait de ce dernier un matériau plus approprié pour des mesures dosimétriques à plus forte dose.

Le matériau codopé Cu^{+}/Ce^{3+} présente :

- Une réponse de RL linéaire dans la gamme de débits de dose comprise au moins jusqu'à 34 Gy/s.
- Un signal OSL indépendant du débit de dose.
- Un comportement non-linéaire du signal OSL, mais qui reste exploitable jusqu'à 10 kGy.

Ces résultats sont comparables à ceux obtenus sur des barreaux simplement dopés Cu^{+} ou Ce^{3+}.

Par ailleurs, une comparaison des spectres de RL et de photoluminescence sous excitation UV met en évidence des niveaux d'énergie identiques dans les deux processus.

Enfin, les premières mesures dosimétriques sur fibre optique dopée Cu/Ce seront également présentées.

PhD student name, year: Fournier Marie, 2nd year

Supervisors & affiliations: Laurent Héliot, Université de Lille

Thesis title: Nouveaux outils de mesure de la dynamique moléculaire appliqués à l'étude de la régulation de la transcription en réponse au stress / Molecular Dynamics: tools and study applied to transcription factor

Keywords (max. 5): molecular dynamics, FCS, FRET, FLIM, SPT, single molecule, subdiffusion, anomaly coefficient, P-TEFb.

Abstract

The study of transcription factors (TFs) is important to understand how genetic expression is regulated in the cell nucleus. Moreover, information on TF dynamics leads to a better understanding how it can affect transcriptional activity. We are focusing on P-TEFb complex (positive transcription elongation factor) which plays an essential role in the regulation of transcription by interacting with RNA polymerase II (RNA Pol II) in eukaryote cells. We developed different microscopy strategies to measure dynamics and molecular interactions in live cells (based in FLIM/FRET and FCS). FRET (Förster resonance energy transfer) measurements enable us to characterize molecular interactions with a great efficiency, but their acquisitions are limited in time (requiring up to few minutes). FCS (Fluorescence Correlation Spectroscopy) techniques have a smaller temporal scale (microsecond to few seconds) but measurements are limited spatially by the focal volume of the laser beam. SPT (single particule tracking) seems to be a good compromise to analyse spatio-temporal dynamics of TFs up to 10um²/s, but this technique is blind for faster molecules. We propose to combine these several technics in order to take the advantage of their complementarity. We will present our recent results on P-TEFb and RNA Pol II complexes, and how we construe dynamics information coming from different measurements techniques. Also, we present our new microscopy module 'StellarScan' specially design to perform CLSM (confocal laser scanning microscopy), TIRFM/HiLo (Total Internal Reflection Fluorescence Microscopy / Highly inclined and laminated optical sheet), LSFM (light sheet fluorescence microscopy). 'StellarScan' module is ready to plug to any fluorescence microscope and provides multimodal settings for such as FCS/SPT PALM or FLIM-FRET measurements for example, making it a perfect tool for our molecular dynamics studies.

PhD student name, year: **Brice NGOUA EDOU, 2nd year.**

Thesis title: **Study of spatio-temporal instabilities in a magneto-optical trap**

Supervisors & affiliations: **Philppe VERKERK** (DR) **and Daniel HENNEQUIN** (CR).

Keywords (max. 5): **Laser, cooling, atoms, instabilities, trap.**

Abstract :

The realization of the Magneto-Optical Trap (MOT) has been one of the most remarkable results of the physics of laser cooling, leading to many applications in the field of cold atoms.

Quickly becoming a common tool, it allows to quickly and repeatedly obtain a sample of cold atoms whose characteristics such as the number of atoms, density and temperature can be controlled. Although the MOT is used universally, under certain conditions, the shape of the cloud of atoms fluctuates with time. Two types of instabilities have been observed in the multiple scattering regime: stochastic and deterministic instabilities. The field of the instabilities of the MOT is now gaining renewed interest, particularly because of its analogies with plasma physics or astrophysics. The first part of my thesis consisted of the realization of the MOT which requires the optimization of the laser beams at the right frequency, intensity, power in order to be able to obtain our cloud of cold atoms and to observe the instabilities which depend on the value of these parameters. From the theoretical point of view, basic equations governing the evolution of the density in the phase space of cold atoms have been established by my team and are similar to the Vlasov-Fokker-Planck system encountered in several areas of physics. The current idea in my work is to find a method of analytical and numerical resolution of these really complex equations, nonlinear and coupled, while taking into account the time scales intervening in the MOT.

The next part of my thesis would be to apply the results obtained in other areas of physics using the Vlasov-Fokker-Planck system.

RESUMES

Posters

PhD student name, year: Berthier Antoine, 1ère année

Thesis title: Impact des biocarburants sur les émissions des moteurs aéronautiques

Supervisors & affiliations: Cristian FOCSA (PhLAM/Université de Lille)

David Delhaye et Ismaël K. Ortega (DMPE/ONERA)

Keywords (max. 5): Biofuel, aircraft engine emissions, soot, secondary organic aerosol

Abstract

The growth of air transport and the potential impact of aircraft emissions on climate and air quality have motivated the development of a new generation of biofuels to reduce these emissions. Indeed, the implementation of these alternative fuels appears as a technological innovation to contribute to the reduction of pollutant emissions. However, the reality of the potential gains should be studied.

This thesis aims to improve our understanding of turbojet emissions, mainly non-volatile and volatile particulate matter emissions, depending on the chemical nature of the fuel. Particular attention will be paid to the formation of volatile particles as they represent an important unknown whether in terms of chemical nature and/or quantity.

In order to determine the main fuel compounds that play a role in emissions, we will study a standard Jet A-1 reference fuel and various alternative fuels such as Synthetic Paraffinic Kerosene (SPK), an Alcohol to Jet (AtJ) and various blends of these fuels with standard kerosene. The Jet A-1 and the other fuels of interest differ not only in their content of sulfur but also in their amount of aromatic compounds or even in their molecular distribution.

The combustion of the various fuels will be carried out using a CAST particle generator designed to burn aviation fuels. The characterization of emissions will involve real-time measurements and sampling for laboratory analysis. We will be able to access, for example, to the particle size distribution, but also to the masse and particle number concentrations. Samples will be used to carry out fine chemical characterization, particularly through the use of mass spectrometry (L2MS and ToF-SIMS).

The most interesting fuels will be studied at actual scales on test bench. A comparison between the emissions of fuels burned on the CAST and engine test bench will be used to identify the representability of laboratory studies.

PhD student name, year: Charbel CHERFAN, Première année.

Thesis title: Chaos Quantique avec un Condensat de Potassium: effets des interactions et de la topologie.

Supervisors & affiliations: Pascal SZRIFTGISER, Radu CHICIREANU et Jean-François CLEMENT.

Laboratoire de Physique des Lasers, Atomes et Molécules (UMR 8523), UDL, CNRS.

Keywords (max. 5): Condensat de potassium, Chaos quantique, Localization d'Anderson, Interactions, Kicked Rotor.

Abstract :

Le premier objectif de cette thèse est de construire une expérience qui produira des gaz quantiques dégénérés d'atomes ultrafroids pour étudier les propriétés de transport dans des systèmes quantiques désordonnés en présence d'interactions.

Notre équipe a fait le choix d'utiliser le potassium grâce à l'existence d'une résonance de Feshbach large et à relativement faible champ magnétique, qui permettra de contrôler convenablement sa longueur de diffusion, et donc les interactions. Nous avons construit un système expérimental pour le refroidissement composé de deux chambres à vide: une 'chambre de collection' (10^{-8} mbar) et la chambre de science (10^{-11} mbar) dans laquelle sera créé le condensat. Pour le potassium, le refroidissement sub-Doppler classique (refroidissement Sisyphe) est inefficace à cause de la structure hyperfine étroite de l'état excité de la transition D2 (767 nm). Cependant, il existe une version de refroidissement sub-Doppler, appelée 'mélasse grise', qui permet de refroidir plus efficacement le potassium en utilisant la transition D1 (770 nm). Une particularité du système laser que nous avons mis au point est la génération des faisceaux avec des diodes fibrées à 1540 nm et 1534 nm, qui sont ensuite amplifiées (grâce à la technologie télécom) et doublées en fréquence, pour générer les longueurs d'onde nécessaires au refroidissement. Ces lasers sont également stabilisés en fréquence en utilisant une transition moléculaire d'acétylène.

Une fois le condensat crée, il sera soumis à un potentiel optique sinusoïdal pulsé dans le temps, pour réaliser expérimentalement le modèle du Rotateur Pulsé Quantique (Quantum Kicked Rotor). Dans ce système, le transport classique des particules peut être inhibé par des effets d'interférences quantiques, en analogie étroite avec le modèle d'Anderson. Cette expérience nous permettra d'étudier la localisation à N corps (Many-Body Localisation) et des effets topologiques dans les systèmes modulés périodiquement (Systèmes de Floquet).

JOURNEE DES DOCTORANTS DU LABORATOIRE PhLAM

1er avril 2019, Amphithéâtre Pierre Glorieux, CERLA

PhD student name, year: Lebel Alexandre, 1er année

Thesis title: Gaz de solitons optiques

Supervisors & affiliations: Pierre Suret & Stéphane Randoux

Keywords (max. 5): Ultrafast optic. Non-linear optic. Opticals solitons.

Abstract

Le développement de techniques de mesures en temps réel pour des signaux optiques ultra-rapides a suscité une attention considérable ces dernières années, et a contribué à d'impressionnants progrès en recherche tant appliquée que fondamentale. Par exemple, le développement de systèmes appelés lentille temporelle (time-lens) a permis l'observation en intensité d'événements uniques, ultra-courts (ps) typiques de l'instabilité modulationnelle démarrant du bruit autour d'une onde monochromatique.

Dans nos travaux, une étape supplémentaire est franchie, grâce à l'enregistrement instantané du champ complexe résolu dans le temps à la sortie d'une fibre optique. Ceci est rendu possible grâce à notre dispositif de lentille temporelle amélioré donnant accès à la phase du champ électrique en plus de son intensité. Il nous est alors possible de réaliser des acquisitions sur une large fenêtre temporelle de 200 ps avec une résolution de l'ordre de la picoseconde, couvrant ainsi un nombre sans précédent de structures non-linéaires adjacentes. L'accès à la phase est rendu possible en créant un battement entre le signal à analyser et un signal de référence.

Nous étudions ici le cas d'une onde monochromatique déstabilisée par le bruit (un des scénarios les plus courant de l'instabilité modulationnelle), se propageant dans 500 m de fibre optique. Dans ce système, l'apparition d'une grande variété de solutions exactes de l'équation de Schrödinger non linéaire (1D-NLSE) a été théoriquement prédit, notamment les solitons de Peregrine, les solitons de Kuznetsov-Ma ou les breathers d'Akhmediev. Dans notre cas, nous avons mis à profit la grande fenêtre temporelle d'acquisition de notre système pour observer des structures similaires à ces derniers.

Pour ce faire, nous avons ajusté la puissance à l'entrée de la fibre afin que la probabilité d'apparition de structures proches des breathers d'Akhmediev soit maximale en sortie de fibre. Après traitement des données, nous observons effectivement que des trains quasi périodiques d'impulsions apparaissent et notamment que chaque impulsion s'accompagne d'un saut de phase de pi comme attendu par la théorie.

Ce dispositif expérimental peut s'appliquer à d'autres régimes d'instabilité et peut être utilisé pour étudier l'impact de différents paramètres, tel que le niveau de bruit qui est susceptible de jouer un rôle crucial pour la dynamique et les propriétés statistiques du système.

PhD student name, year: Noureddin OSSEIRAN 1st year

Thesis title: Physico-chemical characterization of atmospheric pollutants - precursors of aerosols - by quantum chemistry calculations and microwave spectroscopy in a supersonic jet

Supervisors & affiliations: Therese HUET, Pascal DREAN, Manuel GOUBET

Keywords (max. 5): chemical physics, spectroscopy, quantum calculations, VOCs

Abstract

Biogenic hydrocarbons, although present in low concentrations in the atmosphere, have an impact on climate and health. They are precursors of aerosols. Thus, it is interesting to study these molecules, their oxygenated products, and associated hydrates. The objective of this thesis is to understand, on a molecular level, the physio-chemical interactions that lead to aerosol formation, mainly hydrogen bonding. knowing the structure of the molecular system under study can give an idea about the possible site of interaction of this system with water and/or other molecules. Thus, it is possible to understand the hydrogen bonding pattern of the molecule of interest. The research will be conducted using high resolution Fourier-transform microwave spectroscopy. Two 2 Balle-Flygare type spectrometers are used for obtaining rotational spectra of samples in the gas phase, within the range 2-20 GHz. Quantum chemistry calculations, namely ab-initio and DFT calculations are performed to help in the prediction and assignment of the experimental spectra. Two complementary investigations will be considered. The first one is the development of new spectrometer based on the chirped pulsed technique. It will be operating in the range 6-18 GHz. The new spectrometer has two main advantages over the cavity technique. First, it permits the acquisition of spectra in much faster rate. Second, it allows to collect the full range spectrum in one shot of the spectrometer. The second investigation is dedicated to the study of molecular complexes with sulfur molecules, namely hydrogen sulfide, and comparing their structures to those with water molecules.

PhD student name, year: Etienne POEYDEBAT, 1ère année

Supervisors & affiliations: Géraud BOUWMANS (PhLAM) & Emmanuel HUGONNOT (CEA CESTA)

Thesis title: Conception et développement d'un oscillateur Mamyshev

Keywords (max. 5): Fibres optiques – Optique non linéaire – Mamyshev – Oscillateur – Laser de puissance

Abstract

Le Centre d'Études Scientifiques et Technologiques d'Aquitaine (CESTA) accueille depuis plusieurs années les installations Laser Mega Joule (LMJ) et Petawatt Aquitaine Laser (PETAL) dans le cadre du programme Simulation lancé par la Direction des Applications Militaires (DAM) du Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA). PETAL est un laser ultra haute intensité qui repose sur une technique d'amplification à dérive en fréquence : une impulsion ultra courte est étirée temporellement et amplifiée par la suite dans une section amplificatrice composée de verre dopé Néodyme avant d'être comprimée temporellement puis focalisée au centre d'une chambre d'expérience pour atteindre des intensités très élevée de l'ordre de 10^{21}W/cm².

Actuellement, l'oscillateur que l'on retrouve en tout début de chaîne sur l'installation PETAL et qui délivre cette impulsion ultra courte est une source Ti : Sa (saphir dopé titane) à blocage de modes par lentille de Kerr. Il s'agit d'une technologie espace libre difficile à utiliser, qui a besoin d'une maintenance régulière (assurée par une société extérieure au CEA) et qui date du milieu des années 80. Afin de s'affranchir de ces inconvénients, l'idéal est de concevoir une source laser entièrement fibrée car celle-ci présente l'avantage d'être robuste, compacte, fiable et par conséquent nécessite peu voir pas de maintenance.

Une nouvelle architecture d'oscillateur fibré présentée récemment : l'oscillateur Mamyshev, est capable de délivrer des impulsions dont les puissances crêtes surpassent celles atteintes avec une source Ti : Sa. Cet oscillateur conçu pour fonctionner en régime fortement non-linéaire est capable d'atteindre des énergies de l'ordre de la centaine de nanojoule avec des impulsions large spectre, sur une durée de l'ordre de la dizaine de femtoseconde.

L'objectif de ma thèse est donc de concevoir et de développer une source de type Mamyshev afin de répondre aux besoins spécifiques de PETAL. Ces travaux se déroulent en collaboration avec le laboratoire du PhLAM (Physique Laser, Atomes et Molécules) avec qui le DLP (Département Laser de Puissance) du CEA CESTA travaille depuis des années.

PhD student name, year: Bastián REAL ELGUEDA

Thesis title: Dynamique de fluides de lumière dans des microcavités semiconductrices et fibres optiques.

Supervisors & affiliations: Pierre Suret et Alberto Amo, Laboratoire PhLAM – Université de Lille - CNRS

Keywords (max. 5): Microcavities, Optical lattices, Photonics, Semiconductors

Abstract

Planar semiconductor microcavities have shown to be an ideal environment to study the strong light-matter coupling regime. Their eigenstates are exciton-polaritons, quasiparticles mixed of exci- tons and photons, and their manipulation has allowed for studying many-body physics, superfluid hydrodynamics and solid-state phenomena [1]. Recently, the development of micro-fabrication tech- niques in semiconductor materials has led to the enginnering of high-quality lattices of polariton microcavity. The main advantage of this system is that both the wave functions and the spectrum associated to the lattice hamiltonian can be directly measured in photoluminesce experiments [2]. Recently, several experimental works have studied different topological properties in honeycomb lattices, a quantum simulator of graphene [3]. In this work, taking advantage of the fine control in the engineering of polariton lattices, we experimentally investigate the topological transition that takes place when graphene is uniformly strained [4]. We consider honeycomb lattices of polariton microcavities in which the hopping parameters change inside the lattice's unit cell on the vertical direction only. This hopping control emulates the unidirectional strain in a real graphene and, consequently, modifies the band structure of the lattice leading to a topological transition; namely, the merging of Dirac cones and gap opening. By scanning the frequencies of the luminescence light emitted by the honeycomb polariton lattices, we observe the different dispersion features that this topological transition exhibits. The engineering of more elaborate strain patterns, or the application of strain to orbital bands appear as a very promising way to explore novel kinds of Dirac cones and band crossings [5].

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[3] M. Milí ceví c et al. Phys. Rev. Lett. 118, 107403 (2017)
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[5] M. Milí ceví c et al. arXiv: 1807.08650.

PhD student name, year: Siveen Thlaijeh, 1st year

Thesis title: Characterization of organic matter using L2MS (two-step Laser Mass Spectrometry): Application to early life and search of life on Mars.

Supervisors & affiliations : Cristian Focsa (Laboratoire de Physique des Lasers, Atomes et Molécules - PhLAM)

Co-Supervisors: Yvain Carpentier (Laboratoire de Physique des Lasers, Atomes et Molécules - PhLAM)

Kevin Lepot (Laboratoire d'Océanologie et Géosciences - LOG)

Keywords (max. 5): molecular early-life tracers, laser desorption/ionization, organic matter, MOMA

Abstract:

The Mars Organic Molecular Analyzer (MOMA) instrument onboard the ESA/Roscosmos ExoMars rover addresses the main goal of the ExoMars project which is to search for past or present life on Mars. It will target biomarkers in samples drilled at 2 meters below the Martian surface. Chemical characterization of organic matter in current and fossil biomasses is a key prerequisite for such investigation of early life on the Earth or the preparation of reference material databases to help interpreting data produced in situ on Mars. Such preparation studies necessitate very detailed chemical information and the use of ultra-sensitive techniques. In the scope of my PhD, an original High-Resolution (R > 10 000) two-step Laser Mass Spectrometry (HR-L2MS) instrument is used to determine the chemical composition of various samples with controlled fragmentation and high sensitivity. As a first step, we analyzed various pure molecular compounds (including cholestane and tryptophan) and a geological sample (Orbagnoux from French Jura Mountains, Kimmerdgian, Jurassic). Results of cholestane and tryptophan deposited on silicon wafer showed that L2MS can detect the parent molecule (reference material) along with the presence of specific fragmentation patterns. The analysis of the Orbagnoux sample or its dichloromethane/methanol extract (deposited on silicon wafer) showed that the polymer on the surface of the sample was dissolved. Benzene and alkylbenzene fragments were detected along with carbon clusters. More studies will take place for complementary reference materials and further analysis will be held for Orbagnoux sample at different desorption and ionization wavelengths and on different substrates. Such studies aim to facilitate the interpretation of data that will be produced by laser desorption mass spectrometry with the MOMA instrument.

PhD student name, year: Florent BESSIN, 3e année

Thesis title: Etude de l'instabilité de modulation dans les cavités fibrées en régime de dispersion faible et dynamique temporelle

Supervisors & affiliations: A. Mussot, M. Conforti - PhLAM

Keywords (max. 5):

Abstract

En optique, l'instabilité de modulation (IM) résulte de l'interaction de deux effets, la dispersion, et la non-linéarité Kerr (l'indice du milieu dépend de l'intensité du signal). Elle se caractérise par l'amplification exponentielle d'une faible perturbation et par la génération de bandes spectrales autour de la fréquence de pompe. Dans les cavités fibrées ce processus s'observe également, cependant la périodicité du système ajoute un degré de liberté supplémentaire : la phase accumulée au cours de la propagation, et complexifie le système. La plupart des études en cavité sur l'IM, à ce jour, ont été réalisées dans des régimes de fortes dispersions où le développement de Taylor de la constante de propagation limité aux premiers ordres suffit à décrire la dynamique du système. Dans des régimes de dispersions faibles les nouvelles fréquences générées par l'IM apparaissent loin de la fréquence de pompe, les termes de dispersion d'ordre supérieur doivent alors être pris en compte et modifient le processus d'IM. Ils sont en particulier responsables de l'apparition de nouvelles bandes spectrales prédites par la théorie et confirmées par nos résultats expérimentaux ainsi que les simulations numériques réalisées. Dans un second temps peu d'études expérimentales ayant été réalisées dans les cavités fibrées pour caractériser l'IM dans le domaine temporel, nous avons donc construit une cavité permettant d'observer les deux comportements principaux attendus. Ces deux comportements appelés mode P1 et P2 correspondent à des oscillations d'IM, respectivement en phase et en opposition de phase tour à tour. Nous avons pu observer ces deux modes expérimentalement présentant des oscillations de l'ordre de la picoseconde, par l'utilisation d'équipement de hautes performances (lentille temporelle) avec une résolution sub-picoseconde. Nos résultats concordent avec les prédictions théoriques et les simulations numériques.

PhD student name, year: Yassine BOUCHAFRA, 3rd year.

Thesis title: Approches de sous-systèmes pour la modélisation des molécules contenant des éléments lourds en phase liquide et adsobés sur des surfaces

Supervisors & affiliations: André Severo Pereira Gomes, Valérie Vallet, Équipe PCMT.

Keywords (max. 5): Structure électronique, propriétés moléculaires, 'Frozen Density Embedding' (FDE), solavation.

Abstract :

Dans les calculs de la structure électronique, l'étude des systèmes étendus représente un défi majeur. En effet, les méthodes les plus exactes ne sont pas applicables dans plusieurs modèles réels, qui peuvent contenir un grand nombre d'atomes, en vertu de la quantité de mémoire et de temps de calcul demandé. La situation devient plus compliquée si nous traitons des éléments lourds où les effets relativistes sont présents. Cependant dans plusieurs cas, comme la solvatation, l'intérêt principal réside dans le calcul des propriétés d'une petite partie du système total et le reste n'est important que par son effet. Dans ce cadre, l'idée de concentrer l'effort de calcul sur les parts du système où une description précise est requise présente une issue.

La méthode 'Frozen Density Embedding' (FDE), basée sur la division de la densité électronique totale du système en sous-systèmes (nommés ici système d'intérêt et environnement, respectivement) dont l'interaction mutuelle est assurée à l'échelle quantique, à travers du potentiel d'embedding, est un outil puissant pour traiter ce genre de systèmes.

Dans la première partie de ce travail, nous étudions l'impact de la solvatation aqueuse sur le potentiel d'ionisation des halogénures X^- (X= F, Cl, Br, I, At), en utilisant une stratégie multi-échelle qui combine des calculs de la dynamique moléculaire classique (où l'halogénure est au cœur de gouttelettes), avec des calculs de la fonctionnelle de la densité électronique et de la méthode du cluster couplé. Les résultats obtenus montrent un bon accord entre théorie et expériences, et proposent des données pour l'astate, un élément potentiellement intéressant pour la médecine nucléaire, mais que, compte tenu de son court temps de demi-vie (~7h), est difficile à manipuler expérimentalement.

Dans la suite, nous poursuivrons nos études sur des gouttelettes, notamment pour examiner les effets de solvant lorsque les halogénures s'approchent des interfaces air-liquide. En plus, nous nous pencherons sur la construction de modèles théoriques pour la description de spectres d'ionisation de cœur pour des espèces atomiques ou moléculaires adsorbées sur des surfaces de glace.

Sur l'autre partie, nous continuons avec la FDE mais pour investiguer l'effet de la solvatation sur deux caractéristiques indispensables pour l'obtention des données vitales sur la structure locale autour des noyaux d'intérêt. Il s'agit du couplage nucléaire spin-spin (J-Coupling) et le décalage chimique isotropique pour les complexes de types $[(NC)^5Pt\text{-}Tl(NC)^n]^{n-}$ (n=0-5) solvatés dans l'eau.

PhD student name, year: Patrick Bulot, 4th year

Thesis title: Study and realisation of optical fibre sensors with a draw tower for sensing in extreme conditions

Supervisors & affiliations: Marc Douay (PhLAM / University of Lille), Guillaume Laffont (LCFO / CEA LIST)

Keywords (max. 5): Optical fibre sensors, High temperature, Fibre Bragg grating, Optical fibre coating, Fibre draw tower

Abstract

Industry and research need non-invasive sensors for high-temperature applications: above 350 °C. Fibre Bragg gratings in optical fibres are a valuable solution, because they are compact and temperature resistant. These sensors are used to monitor temperature in processes or in devices (for example: plane reactor or nuclear reactor) on several meters.

The Ph.D. work is included in a collaborative project between PhLAM laboratory and the LCFO laboratory (CEA LIST). The project goal is to inscribe high-temperature resistant fibre Bragg gratings during the fabrication of the optical fibre with a draw tower. The continuous manufacture of these sensors protected by a high-temperature resistant coating will improve their reliability, and will also decrease the manufacturing cost.

For the first time, a silicone coating with fillers is studied like a mechanical protection coating for optical fibre. The coating application is realised on optical fibres by two different ways. The coating is applied on fibre Bragg gratings by dip-coating to study the behaviour of the coating on the fibre up to 470 °C. The coating shows a small deterioration after heat treatment at 470 °C. The second method is to apply the high-temperature coating during fibre drawing in necessary conditions for fibre Bragg gratings inscription during drawing. A 100 meter-length fibre is protected with a thickness of around 13 µm.

PhD student name, year: Hugo Geindre, 3rd year

Supervisors & affiliations: Daniel Pelaez Ruiz, PCMT

Thesis title: Analysis of the overestimation of the infrared intensity of the C-H stretching band in Polycyclic Aromatic Hydrocarbons

Keywords (max. 5): PAHs, IR spectra, DFT, Long-range Correction

The infrared spectra of Polycyclic Aromatic Hydrocarbons (PAH) and related systems, such as fullerenes, have been extensively studied both from an experimental and from a theoretical perspective. In particular in the astrophysical community, the interest in their IR signatures lies in the fact that PAH-like molecules (and/or clusters thereof) are most likely the carriers of the so-called Aromatic Infrared Bands (AIBs). In this sense, only recently the first unambiguous assignment of an AIB band has been achieved.

Typically, the determination of the vibrational structure of large systems (PAH included) relies on vibrational second-order perturbation theory (VPT2) calculations on a potential energy surface (PES) expanded in a Taylor series up to fourth order. The VPT2 method in conjunction with the Density Functional Theory (DFT) has been shown to be very efficient in the computation of anharmonic vibrational energy levels, with the exception of some types of resonances. In the specific case of PAHs, this approach has been shown to be able to predict to a very good agreement the frequencies and intensities of most of the IR bands of PAHs. However, the intensity of the C-H stretching band is constantly overestimated.

With this problem in mind, we have carried out a systematic investigation of the IR spectrum, more specifically, of its C-H stretching region, for two related molecules, benzene and the smallest PAH, naphthalene. To this end, we have computed and compared the harmonic and anharmonic IR spectra of these two systems with several DFT functionals, with the Complete Active Space Self Consistent.
Field (CASSCF) and with its Second-order Perturbation extension (CASPT2).

Journée des doctorants du laboratoire PhLAM 1er Avril 2019, Amphithéâtre Pierre Glorieux, CERLA

PhD student name, year: Mohamed Tahar Ladjimi, 3rd year

Thesis title: Cellular stress reponse modelling

Supervisors & affiliations: Emmanuel Courtade, Benjamin Pfeuty, Quentin Thommen
Univ. Lille, CNRS, UMR 8523 – PhLAM – Physique des Lasers Atomes et Mol´ecules

Keywords: heat shock response, cell death, thermotolerance, CEM43

Abstract
Hyperthermia causes proteins to misfold and hence to lose their functionality, leading to a weakening of the cell. A standardized tool, the « Cumulative equivalent minutes at 43°C » (CEM43) [1], determines the thermal doses from regression analysis in the specific case of hyperthermia rectangular time profiles and is now widely used even for time varying profiles. We aim to revisit the concept of thermal doses in a mechanistic framework of signaling and regulatory network dynamics. We first extend a previous model of the heatshock response network [2] to quantitatively account for the survival response of Hela cells to rectangular heat shocks of varying duration and temperature [3], consistently with the CEM43 model. Such network model featured with specific dynamical properties further allows us for systematic and quantitative study of the influence of the temporal profile of the thermal protocol on the survival response. The model predicts that the hyperthermia temporal profile shape has a strong effect on cell survival. Such an effect has been experimentally confirmed with Hela cells. A mathematical analysis of a reduced model reveals that the dynamics of HSPdependent repair of misfolded proteins plays a critical role in this process.

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PhD student name, year: Corentin Naveau, 3rd year

Thesis title: Experimental study of modulation instability and Fermi-Pasta-Ulam-Tsingou recurrences in optical fibers.

Supervisors & affiliations: Arnaud Mussot, PhLAM & Pascal Szrifgiser, PhLAM

Keywords (max. 5): Nonlinear optics, modulation instability, breathers

Abstract : Optical fibers are a good testbed to investigate nonlinear phenomena with complex dynamics. Among them is the Fermi-Pasta-Ulam-Tsingou (FPUT) recurrences process which describes the ability of a nonlinear system with several modes to come back to its initials state, exhibiting multiple recurrences cycles. In optics, this phenomenon has particularly been studied in the context of modulation instability (MI), which corresponds to the exponential growth of a weak perturbation at the expense of a strong pump wave in the linear stage. By propagating further, the process is characterized by the amplification of subsequent harmonics of the initial modulation sideband until the process reverses and come back to its initial state (FPUT recurrence). However, experimental investigation of FPUT recurrences in optical fibers have been limited, especially because of the difficulty to perform distributed phase measurement and because of the intrinsic losses of fibers, which usually limit usually the number of recurrences to one.

Recently, we developed an original experimental which allows us to perform non-invasive distributed measurements of the intensity and phase of the main frequency components of a pulse via heterodyne detection of the Rayleigh backscattered signal. Associated with a loss-compensation scheme (using Raman amplification), it allowed us to observe two FPUT recurrences and to characterize them. By changing the initial input conditions and recording the evolutions of the pump and signal/idler, we were able to report for the first time the symmetry breaking nature of the FPUT process through phase planes. Then we improved our detection scheme to be able to record another set of sidebands (harmonics of the signal and idler), which enables, via inverse Fourier transform to reconstruct temporal dynamics for which the typical timescale is the picosecond. It allowed us to observe once again the symmetry breaking of FPUT but in the time domain. We also used this setup to study precisely the impact of the input modulation sidebands power and relative-phase on the recurrences and to investigate second-order breather dynamics linked to higher-order modulation instability.

Investigation of polycyclic aromatic hydrocarbons and soot formation in swirled flames of n-butanol and conventional diesel fuel

PhD student: Linh Dan NGO, 3rd year

Supervisors: Eric THERSSEN (PC2A)

Yvain CARPENTIER (PhLAM)

Abstract of poster:

As a second generation biofuel, n-butanol is considered as a promising partial or total substitute to fossil fuels due to its high energy density, low vapour pressure and low hygroscopicity. However, changes in the fuel chemical composition can modify the exhaust emission characteristics (composition, soot propensity, etc.). Thus it is necessary to study the formation of pollutants produced from this alternative fuel, particularly the formation of soot particles and their precursors as they are widely known as harmful pollutants. In this study, two fuels have been investigated: conventional diesel, n-butanol in a swirled jet burner. In-situ laser induced incandescence/fluorescence (LII/LIF) is used at different excitations to detect soot particles and their precursors. These laser-based diagnostics also allow us to characterize optical properties of these pollutants. Ex-situ Two-step laser mass spectrometry (L2MS) and Secondary ion mass spectrometry (SIMS) are coupled with in-situ techniques to better understand the chemical composition of particulate exhausts. Different behaviours are obtained within two flames in the similar experimental configuration. N-butanol flame shows a negligible amount of soot according to LII signal captured by coupled charge device (CCD) camera. Furthermore, its maximum LIF signal – emitted with 532 nm excitation – located at higher HAB compared to diesel flame but at significantly lower of intensity. Time decays of LII signal obtained in n-butanol flame indicate that soot particles in this flame have the same size at different HABs. This behaviour corresponds to nascent soot particles as confirmed by fluence curves.

PhD student name, year: ROOSE Antoine, 3rd year

Supervisors & affiliations: DUFLOT Denis (PhLAM); RIFFAULT Véronique (SAGE); TOUBIN Céline (PhLAM); DUSANTER Sébastien (SAGE)

Thesis title: Experimental and theoretical study of the uptake of peroxy radicals by organic aerosol surfaces

Keywords (max. 5): Uptake, Aerosol Flow Tube, Molecular modelling, Organic aerosol, Peroxy radicals

Abstract

Significant uncertainties are still associated to chemical reaction mechanisms used in atmospheric models, in particular for RO_x radicals (OH, HO_2, RO_2). Recent measurements of radicals in forested areas characterized by low NO_x (NO_2, NO) concentrations indicate that models can significantly overestimate peroxy radical concentrations (Griffith et al. 2013; Mao et al. 2012). These results question the ability of models to correctly simulate the oxidative capacity of the troposphere since peroxy radicals are a main source of the hydroxyl radical (OH), one of the most important oxidative species in the atmosphere (Stone et al. 2012). One possible explanation for the model overestimation of peroxy radicals is the occurrence of heterogeneous processes (uptake of radicals) on the surface of aerosols that are either misrepresented or not included in models. While recent studies have reported uptake coefficients of HO_2 on different types of aerosols, uptakes of RO_2 radicals have yet to be investigated.

Both theoretical and experimental tools have been used to study HO_2 uptake on organic aerosols. A PERCA (Peroxy Radical Chemical Amplifier) instrument capable of measuring HO_2 and RO_2 radical concentrations has been coupled to an aerosol flow tube to quantify HO_2 uptakes on glutaric acid aerosols at different relative humidities. In complement to this experimental work, molecular dynamics simulations combined with ab-initio calculations (MD) have been carried out to model a nanometer size aerosol particle and the sticking process of HO_2 onto it. These theoretical calculations provide insight into the uptake process at the molecular scale. In this presentation, both theoretical results (aerosol structure and properties, HO_2 mass accommodation) (Roose et al. 2019) and experimental results will be discussed. We will emphasize the advantage of using a dual experimental/theoretical approach to investigate the uptake of radical species on atmospheric aerosols.

This work is supported by 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) and by the regional council "Hauts-de-France". The authors also thank CPER Climibio and FEDER for their financial support. Calculations were performed using HPC resources from GENCI-TGCC (Grant 2017-A0010806820).

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PhD student name, year: Dana SIMIUC, 4th year

Thesis title: Sensibilité de cellules cancéreuses au stress oxydatif : approche systémique pour étudier le couplage entre le métabolisme et le stress oxydatif / The sensitivity of cancer cells to oxidative stress: systemic approach to study the interplay between metabolic flux and oxidative stress

Supervisors & affiliations: Emmanuel COURTADE, François ANQUEZ, Laboratoire de Physique des Lasers Atomes et Molécules, Université de Lille, Bâtiment P5, 59655 Villeneuve d'Ascq, France

Keywords (max. 5): oxidative stress, adaptation, molecular dynamics, metabolism

Abstract

Being motivated by the fact that some anticancer therapies are using oxidative stress to remove the tumor (Trachootam, 2009), we are trying to understand how the cell can orchestrate in time and space their response to oxidative stress and how it can influence the cellular fate (adaptation or death) (Ferrell, 2016). For this purpose, we perform experiments on living cells, by modulating an external oxidative stimulus, in order to probe the molecular dynamics of reactive oxygen species and their biochemical scavengers at the cellular level.

We built a custom cell culture chamber that can be connected to the fluidic system to create controlled temporal stress stimuli patterns. To monitor the molecular dynamic response to oxidative stress at single cell level with statistic data, we used fluorescence microscopy. By performing single cell analysis we observed different adaptation patterns as cellular response to the same stimuli. The dynamics of adaptation were induced by negative feedback at different timescales ranging from few minutes (fast adaptation) to half hour (slow adaptation).

The metabolic modulation was made by removing the glucose source or by modulating some key molecules (G6P, G6PDH, GAPDH and catalase), some of them being involved in rerouting of metabolic flux, by suppressing or overexpressing them. Our results showed that in the absence of glucose the cells were more sensitive to oxidative stress, showed higher death response to the same dose. We identified that the glucose uptake is important for adaptation, highlighting that the intracellular antioxidants system regeneration is dependent by its presence.

PhD student name, year: TANDJE Arsène, 3 rd.

Thesis title: Fibres optiques pour le guidage de modes à moment angulaire orbital : application aux Telecom et à la Photonique Non-Linéaire

Supervisors & affiliations: Laurent Bigot, Esben Andresen (University of Lille) & Antoine Vianou, Michel Dossou (University of Abomey-Calavi)

Keywords (max. 5): OAM, few-mode fibers, MIMO-less, MDM

Abstract

Step index and graded-index optical fibers are widely used for long (intercontinental, backbone) and short-haul (datacenter, access network) transmissions.

The constant rise of Internet services combined to the growth of the number of Internet users makes it necessary to increase the capacity of fiber networks. The fibers used today for very high data rate transmissions use only the fundamental mode (denoted LP_{01}, in the weakly guiding approximation) to transmit the information: there are known as single mode fibers. One of the ideas for increasing the capacity of fiber networks is to simultaneously use different modes in a so-called few-mode fiber (fiber supporting typically dozens of modes). Since 2010, several studies have been developed in this direction, mainly on fibers supporting LP (Linearly Polarized) modes and more recently OAM (Orbital Angular Momentum) modes, i.e. modes with helical phase and circular polarization.

LP modes are those that appear in the fibers under weakly guiding conditions and are obtained by linear combination of nearly degenerate vector modes which are eigenmodes of the fiber. Another combination of the vector modes makes it possible to obtain OAM modes whose symmetry properties are supposed to limit the coupling between them. The existence and stability of such modes is favored in the case of a ring-core optical fibers geometry possessing a high index contrast between core and cladding.

Our PhD work deals with the issue of the design and the realization of OAM fibers presenting weak couplings between modes, for application to the transport of data but also for study in nonlinear photonics. The fibers studied are annular core fibers made by optical fiber manufacturing methods, having internal / external radii and optimized ring indices. However, we also designed and manufactured a micro-structured optical fiber suitable for OAM mode guidance. We experimentally show that the fabricated fibers support OAM modes, and their transmission matrices have been measured. Currently, we are setting up a test bench for solitonic shifting experimentations in OAM fibers.

PhD student name, year: Jean YAMMINE - Third year

Thesis title: Study of the modal content and amplification properties of few-mode optical fibers.

Supervisors & affiliations: Laurent BIGOT and Esben Ravn Andresen

Keywords (max. 5) : Few mode fiber, Mode content, Transmission matrix, Multimode amplification.

Abstract

Currently, the capacity of the world's singlemode fiber (SMF)-based communication networks is approaching its physical limits. Mode division multiplexing (MDM) based on few-mode fibers (FMFs) has the potential for increased capacity. This thesis addresses some of the challenges facing the use of this new technology.

In order to be able to evaluate the potential offered by this new type of fiber, it is necessary to study its modal content according to the conditions of use. The first part of the thesis focused on the implementation of a method for the characterization of the modal content of FMFs, by measuring their transmission matrix using a spatial light modulator (SLM). This method has been well implemented and we have validated its performances by characterizing an FMF supporting 12 spatial modes (7 groups of linearly polarized "LP" modes) and a ring core fiber used to guide 10 annular modes (3 groups of angular orbital moment "OAM" modes). This method was also used to study the time dependence of the transmission matrix over a 2 days span.

Another challenge to implement MDM in practice is to have repeaters that can amplify a specific number of modes in an equalized way along a transmission chain. In this context, the second part of the thesis consists in continuing the work already initiated within our team in order to propose new geometries of amplifying fibers and to manufacture them. This work focuses on active fibers guiding LP modes and also amplifier fiber structures for OAM modes.