Scientific report LabEx PALM 2018-2020

Laboratoire d'excellence

PAIM

Physique : Atomes Lumière Matière

Table of content

Introduction	5
 Topic 1 "Quantum Matter: from the elementary to the strongly correlated"	99 12 12 12 13 13 14 15 15
 Topic 2 "Complex systems: from out of equilibrium systems to biological matter"	17 17 20
 Topic 3 "Ultrafast Dynamics: from radiation sources to multiscale responses"	25 27 28 29
 Topic 4 "Emergence, Evolution, Rapid Reaction"	33 35 36 36 37
 Topic 5 "Higher Education" 1. Master programs 2. Hands-on experience for master students 3. Predoctoral and doctoral schools 4. Popularization of science 5. PhD fellowship 	39 40 40 41
Topic 6 Innovation and Technology Transfer 1. Funded projects 2. Leverage effect Publications	45 48

Introduction

CONTEXT

The last scientific council was held two years and a half ago, in January 2018, and acted as a highly valuable trigger for the preparation of the ANR evaluation on the continuation of our LabEx for 5 more years after the end of the initially planned duration in 2019. Our LabEx was one of the 9 successfully renewed out of the initial 11 on the Paris-Saclay plateau – 3 in physics PALM, NanoSaclay and P2IO (Physique des 2 Infinis et des Origines). The outcome of the evaluation was very positive, concerning in particular the scientific perimeter and programme presented at our 2018 session, the important and effective local structuring impact both at the scientific and the educational levels, its connection to national and international experimental facilities, and the collaborative aspects. This positive feedback encouraged us to continue along the same lines while addressing new challenges in a rapidly evolving scientific context which is typical of our "low energy" physics.

Since 2018 the ever-changing complex organization and landscape of Paris-Saclay has evolved substantially, leading to the official creation of Paris-Saclay University in 2020, aiming successfully at a gain of international visibility. Research departments and schools, which were initially created to cover its anticipated landscape, have been abandoned in favour of the concept of Graduate Schools. They still are under construction and introduce a synergy between the educational and the research worlds. A call for interdisciplinary initiatives has also been launched, two of them being already approved: "Quantum" and the "Light Sciences Institute" which strongly overlap with PALM scientific perimeter. All the LabEx coordinators have been involved in the discussions at the numerous meetings presiding to the creation of these structures during year 2019 and P. Mendels is now a member of both the Graduate School of Physics board and its "Physics of Waves and Matter" research axis.

At the end of 2022, PALM research is expected to become a part of one of the three axes of the Graduate School of Physics, namely the PhOM (Physics of Waves and Matter) axis which is the former research department. The separation into two independent educational structures, Paris Saclay University, absorbing Paris-Sud University and bringing together four "grandes écoles", and Institut Polytechnique de Paris, centered on Ecole Polytechnique and four others "grandes écoles", is now effective. Despite this separation, the perimeter of the LabEx will remain unchanged until the end of 2022, including research teams and projects from both entities and fostering interactions in our community transcending that cleavage. PALM definitely appears as a stable element in this complex landscape not yet in a steady operation, that keeps an effective scientific research synergy.

In this context, at the end of 2022 our LabEx will be re-evaluated by the research board of Paris-Saclay University to decide the evolution of the scientific orientations, possibly leading to a modification of the corresponding fund allocation that will be restricted to the laboratories belonging exclusively to Paris-Saclay. It is our goal and that of our community to maintain a strong visibility and assert ourselves as an undisputable scientific element of the science at Paris-Saclay. This is a key issue to keep the spirit of our community and its funding!

ORGANIZATION OF THE REPORT

As for the 2018 report, this report is divided into three sections: (i) an **activity report** focusing on scientific, innovation and higher education projects supported by our LabEx with subsections corresponding to the topics listed below. It is not our aim to encompass all the science developed by the 750 researchers of the LabEx and funded through multiple institutions or agencies, but to give a good snapshot of the major PALM-funded scientific projects with key publications extracted from the list available at the end of this report. A few highlights provide more detailed illustrations. Further information can be found on the PALM website https://www.LabEx-PALM.fr/; (ii) a shorter report about **future scientific prospects** for 2020-2025. For some topics the strategy was refined, whereas other reiterate the same directions as already presented in 2018; (iii) an **appendix** provides details about governance, the list of participating labs and workforce, statistics, extended lists of funded projects, tables, graphs, budgets, and a few other statistics...

CONTOUR AND SPIRIT

As explained in the preliminary section, PALM preserved its robust scientific boundary. It encompasses the physics of condensed matter, atomic and molecular physics, optics, lasers and "extreme" light, statistical physics, physical chemistry, and the interface with biological sciences. The scientific project is organized around three focus topics, carefully selected in 2011 with the aim of developing collaborations and interactions between researchers working in different subfields and/or in different institutions on the Paris-Saclay campus. They actually fit very well with the national research strategy of CNRS and CEA.

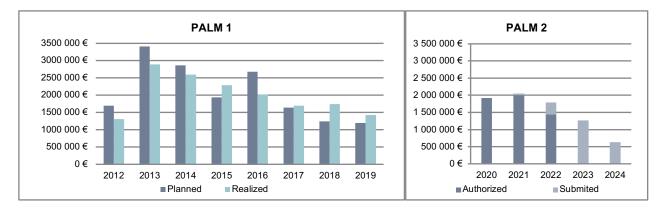
The focus topic short titles are "Quantum Matter", "Complex Systems" and "Ultrafast Dynamics". In addition, a fourth topic, named "Emergence, Evolution and Rapid Reaction" allows a rapid response to smaller scale projects and it can provide seed funding for

emergent subjects. Two other topics link our LabEx with the academic environment, the "Higher Education" projects, and the socio-economic ecosystem through the "Innovation and outreach" programmes.

These topics were evaluated and revisited at the mid-term 2015 stage. Part of the physics at the interface with biology then migrated from the 4th topic to the 2nd one. The innovation topic is run in collaboration with LabEx NanoSaclay. For the 2021 annual call, we have extended the possibility of such natural PALM - NanoSaclay collaborations to all topics then eliminating in some areas an artificial scientific separation but maintaining the bottom-up approach characteristic of PALM.

BUDGET

The comparison between budget figures from PALM 1 (2011 - 2019) and PALM 2 (2020 -2024) is given below with an annual timeline. It was decided to keep a smooth allocation strategy with a peak at the beginning of each phase (i.e.in 2013, 2016 and 2020) aimed at launching decisive actions while still keeping a sizeable part of the budget for the remaining time for fewer high level projects. This had the direct consequence that during the 2018 - 2020 period under review, only smaller scale projects or involving external ressources projects could be supported in 2018 and 2019. The 2020 budget increase made possible again the funding of financially ambitious projects.

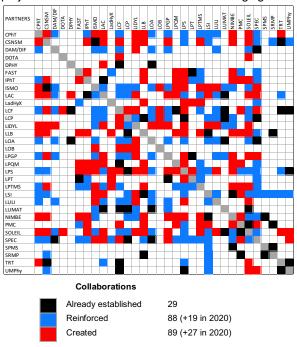


OPERATION

Below, we remind our operation mode, unchanged from the previous report and complying with the renewal proposal description for the current phase of the LabEx. The central operating tool of PALM is based on annual calls for proposals covering the six topics with a well-defined budget for each topic. This budget is approved upstream by the 11 institutions running the 31 partner labs. A **collaborative** action involving at least two labs is required for the projects. This acts as a virtuous filter encouraging local

collaborations, which has led in many cases to multi-partner intra-PALM publications and has resulted in structuring actions of the PALM community. The large-size of the LabEx - ~750 researchers are affiliated to PALM- is for sure a key-point for enabling this successful collaborating scheme while cultivating a diversity of scientific directions. This allows a real bottom-up spirit for defining innovative and ambitious projects. In 2020, we explored the opening to joint projects with LabExNanoSaclay in the specific area of "Quantum Technologies". There were a few projects benefitting of this action. In 2021 call, this possibility of common projects will be extended to the ensemble of PALM research topics, maintaining the principle that each LabEX funds their respective groups. Note that the budget model of LabEx Nanosaclay is different as it has a preemptive allocation of most of its budget to flagship actions thus limiting the scope of these common projects. The operating mode for selecting those projects is not detailed here but will be presented during the 2020 meeting with the international scientific council.

Scientific excellence, novelty, structuring and collaboration remain the keywords in the evaluation of the projects. The topic boards perform the evaluation of the proposals, which, depending on the amount requested, are reviewed by the researchers of the board or by external referees (generally two).



After the 2019 evaluation, we have renewed the topics boards (45% with a 43% women ratio) and the steering committee (56% change with a 19% women, a ratio close to that of the LabEx members) that enacts the final decision after the evaluation by the

topic boards. Nathalie Westbrook (LCF) for fhe Higher Education topic and Patrick Bouchon (DOTA) for the Innovation topic took over in place of Julien Bobroff (LPS) and Jérôme Primot (DOTA) respectively. Our way of working meets the expectations of the community, with a 4 months time typically between submission and the credits installation and a ~ 30% average success rate (ratio between the allocated and requested budgets).

The scientific actions of the annual call are listed and commented below, the project financial scale has extended for 2018-2020 from a few k€ to 153 k€:

- Equipment: multi-partner with leverage action for high budgets, exceptionally a single partner-project for a seed funding equipment on novel scientific directions.
- Junior chairs: aimed either at attracting promising young researchers with the idea of stabilizing them on the short term on a permanent position (external junior chair) or accelerating the initial carrier for recently hired young researchers and preparing them for obtaining further grants such as ANR-jeune or ERC (internal junior chair).
- Post doctoral grants: these grants cover a 2-years stay. They must complete within a 5 year time span after the PhD graduation (before the requirement was 4 years). Grant co-funding is possible.
- PhD fellowships: initially completely funded by the LabEx for a 3 years time, they can now be co-funded in view of the restricted budget of the 2018-2020 years of the LabEx and years to-come.
- Innnovation projects: they lie quite upstream, at the maturation level, in the chain leading from discoveries to patents. The focus is put on state-of-the-art instrumentation, innovative set-ups developed in the frame of the scientific activity, which are precious by-products which can fulfill academic or industrial requirements for other application fields. The PALM action, led together with the Labex NanoSaclay, is complementary to those led by Paris-Saclay University and the SATT dedicated to support technological innovation and the launching of start-ups. The innovation projets can fund personal costs, or small equipment.
- Senior chairs have not been in operation since 2015, when Paris-Saclay started a similar "d'Alembert" program, encompassing all the research spectrum of Paris-Saclay University. This program was not active any more in 2020 from Paris-Saclay University, we hope that it will be funded again in 2021. Note that in the same vein, the newly created Institut Pascal now welcomes long-term visitors and events. All these actions still need to be attuned in the near future.

It is important to note that these tools occur in a multiscale context of funding. First, PALM topics are also central in the research department PhOM (*Physics of Light and Matter*) of Paris-Saclay University which will transform into one of the three axis of the Physics Graduate School. Among the 8 different working groups structuring the scientific perimeters of that research department / axis, four of them, *Coherence and Quantum Correlations, Diluted or ionised matter: plasma atom and molecule, Complex Systems and Matter, Extreme Light* and the *Theory and Simulation* groups strongly resonate with our focus topics. This strong connection existing between PALM and PhOM has materialized in 3 large collaborative initiatives (IRS, *Initiatives de Recherche Stratégiques*) that have been funded or at least labelled and partly funded by Paris-Saclay with a significant implication of PALM researchers as mentioned in the previous report¹.

In a more transverse spirit and more recently, the research topics and researchers of PALM have been participating in preproposals for "Interdisciplinary Objects" launched by Paris-Saclay University mid-2019, as strategic scientific initiatives. Among them, two have been already approved: the Institute of Light Sciences (ISL) led by Institut d'Optique, IOGS; and "Quantum" gathering the topical fields of Quantum Sciences and Technologies, crossing the permeable borders between PALM and NanoSaclay. The latter aims at making the whole existing Paris-Saclay potential more visible. It already resulted in the selection of Paris-Saclay as one of the major centers in this field at the national scale, being promised then to get a substantial funding when "Quantum" will become a national scientific priority as in many countries worldwide. Again, there is a large commonality with "our" PALM topics: "our" Quantum Matter topic with Quantum and ISL, "our" Ultrafast Dynamics topic with ISL, "our" Complex systems" topic with the project "Systems Complexity and Artificial Intelligence", several initiatives at the interface with bipophysics and "our" Emergence topic with physical chemistry, materials projects, etc...Except the two already approved, all others are still under evaluation.

At the Ile-de-France regional scale, a network extending beyond the Paris-Saclay plateau, SIRTEQ, has been launched in 2017 for 4 years on Quantum Technologies with a 7.2 M€ budget. Our ANR national funding agency supports collaborative projects at the national level. The EquipEx Attolab, CilEx which are now in operation still require further financial support, in close relation

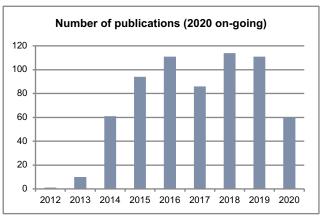
¹ IQUPS about quantum technologies (2017-2019, 300 k€); NAN'EAU a multimicroscopy approach to study the dynamical behaviour of nanoobjects in the liquid phase and in electrochemistry (2017-2018, 500 k€); PSI2, the Paris-Saclay *International Programs for Physical Sciences and their Interfaces* aimed at covering the gap of program for basic science before the proper functioning of the programs of the *Institut Pascal* (2017-2019, 300 k€).

with our topic 3 for Attolab and CilEx (see report) etc..A recent call for EquipEx+ was launched last May. Researchers of the PALM topic 3 community are involved in a proposal "AttoPLUS" by M. Marsi (Paris-Saclay University), and a proposal centered on Apollon laser (CNRS).

Some clear leverage effects can be identified among the ERC grants obtained by our researchers over the 2018-2020 period: François Parmentier (SPEC), Maurizio Fagotti (LPTMS), Hèlène Bouchiat (LPS) or CNRS awards such as silver medals: Claire Laulhé (SOLEIL), Satya Majumdar (LPTMS), Marie-Claire Schanne-Klein (LOB), to cite a few. Altogether with the chairs, PALM has kept its clear role of **research accelerator**.

A total of 64 research projects has been funded in the period 2018-2020 (total of 205 since 2011) with an average of 64 k€ per research project over the entire life of the LabEx. This document is dedicated to exclusively report on PALM-funded activity and the number ~110 of yearly publications –acknowledging PALM which is constantly repeated to project leaders but not completely integrated- seems to have come to a steady state, see graph.

Importantly, PALM strikes a balance between equipment and personnel expenditures at variance with most LabEx at the national level. In 2014, the national average was 55% for personal cost. For PALM it is 46% for 2018-2020, and has been 43% since the beginning.



Besides our pure research projects there are important channels which contribute to the **international visibility** at all levels **from confirmed researchers to undergraduate students**:

- an on-demand visitors program for stays up to 3 months (23 visitors in 2018-2020 from 13 countries);
- the funding of workshops and schools organized by members of PALM, 38 on the 2018-2020 period with a financial support up to 5k€);
- the full funding of a "PALM" school for each topic 2 and 3 (see Higher Education section in the report).
- the diffusion of PALM based science with outreach and financial support for the creation of innovative practical labs at the Master level and financial support for Master internships;
- a web-site in French and English not only for intra-LabEx use but now rather aimed at disseminating our action both at the researchers and general public level. We have pursued the efforts initiated in 2015 to enrich our website. Two or three short Newletters are published every year, giving concise information about the LabEx life.
- on the education side, there seems to be a move, as a first action of the Graduate School, to follow the virtuous PALM example.
- PhOM research seminars were active until last year we hope they will restart in the context of the Graduate School. The organizers of these one day events are often PALM members. These topical days were dedicated to Quantum Information, Complex Systems, UltraFast technical developments and Theory.

GENDER BALANCE

In the renewal phase of all topic boards and governance, we paid attention to keep some continuity and aimed at enrolling as many women as possible. We provide below some statistics about the gender distribution in the various decision committees and boards and among project PI's

It is worth noting that in our annual calls, it is clearly stated that "particular attention will be paid to the projects filed by a woman or to enable her to maintain the research activities of her team at the highest level within the framework of a maternity leave and/or after this leave.

	Μ	F
Directory board	67%	33%
Labex members	76%	24%
Steering committee	81%	19%
Topics boards	57%	43%
Filed research projects	78%	22%
Funded research projects	76%	24%
Success ratio	51%	57%
Post-doctoral fellows	74%	26%
PhD fellows	69%	31%

Topic 1 "Quantum Matter: from the elementary to the strongly correlated"

Since the beginning of the LabEx, a major goal of the Quantum Matter focus topic has been to narrow the gap between the atomic molecular and optical (AMO) physics community on the one hand, and the condensed matter physics community on the other by fostering collaborations between the two disciplines. In doing this we are participating in a trend which is visible in many countries. There has been notable progress, but the work of bringing together the two communities requires patience and long-term thinking. We emphasize that, as a structure with a planned lifetime longer than that of most research grants, the LabEx provides the community with one of the few funding sources in which one has any possibility of long term planning. Thus, Quantum information processing, pioneered using quantum optics techniques (trapped atoms and ions, single photons) have found analogs in condensed matter systems such as superconducting circuits, and quantum dots. On the other hand, questions concerning strong correlations, entanglement and coherence, which have long been of importance to the condensed matter community, are now also being addressed using ultracold atoms manipulated by laser beams. In addition, the field of quantum transport, in which matter waves (either electrons or atoms) propagate under the influence of various forces, either in a solid or an optical potential, also constitutes a new area of common ground between the two communities.

The Quantum Matter focus topic encourages researchers in the LabEx PALM to explore these subjects and we try especially hard to encourage collaborations and synergies between condensed matter and AMO physics. One of the most striking examples is the use of optical lattices to simulate topological many body effects. In PALM, at the Laboratoire Charles Fabry, there has been a successful effort to use programmable arrays of microscopic single atom traps to realize such simulations. Loading these traps with Rydberg atoms provides a system with strong, long range and anisotropic interactions. We expect much more progress on this topic in the near future. In a second topological project, researchers in PALM also studied topological insulators in bismuth nanowires. These two experimental results, realised in very different physical systems, illustrate the broad interest, which we hinted at in the last report, that topological effects are generating in both the condensed matter and AMO communities. They also show how PALM might able to inspire new synergies between the two communities, indeed we mention several recently funded projects in the last section.

See Highlight 1 (project XYLOS by Thierry Lahaye)

The LabEx PALM also financed several other projects addressing quantum information and more broadly, quantum technologies. A novel use of diamond NV centers to study very high pressure systems is an interesting example. Physics out of equilibrium has of course long been an important topic and it forms an important part of Focus Topics 2 and 3, but recent advances in our level of control over AMO systems has opened new possibilities and below we describe theoretical work on dissipative quantum dynamics in such systems. Out of equilibrium physics is clearly now an activity which is common to all three focus topics.

See Highlight 2 (project AIMHIP by Jean-François Roch)

There was also considerable work on electronic and structural states in quantum materials, spanning a large variety of questions. The traditional but still vigorous field of strongly 3d correlated systems has extensively studied exotic superconductivity, metalinsulator transitions, novel current loop excitations, Josephson and tunnel devices etc. This field has opened up to novel axes of research. For example, Dirac and Weyl matter offers a playground for new collective excitations, manipulation of Dirac points leads to topological transitions. Spin-orbit coupling is now visible in condensed matter physics and has opened up the traditional world of 3d correlated metals to a new class of Mott insulators whose metal-insulator transition has been is under study in PALM (see highlight below). Many frustrated quantum or rare earth magnetic materials have emerged quite recently leading to spin liquid ground states whose nature remains enigmatic, for example in Kagome antiferromagnets.

The sections below contain an overview of some of the larger projects which were funded by the LabEx.

1. Topological insulators in bismuth nanowires

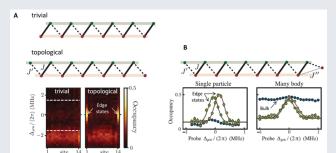
The current through two-dimensional topological insulators is predicted to run only through a few, perfectly conducting, narrow channels. In the JosephBismuth project, researchers at the LPS and the CEA/SPEC have used superconducting electrodes to reveal the ballistic nature of the current through bismuth nanowires, suggesting they are good topological insulator candidates.

One striking consequence of the macroscopic quantum nature of the superconducting state is the propensity of a supercurrent to flow through a thin insulating layer separating two superconductors. Brian Josephson even predicted how the supercurrent would flow across this

Highlight 1. Topological phases with Rydberg atoms Thierry Lahaye, Antoine Broaweys (LCF)

Topological matter has attracted a lot of interest over the last years, as it challenges conventional classifications of phases of matter and promises interesting applications in a variety of fields. Although topological effects at the single particle level are now well understood, the interplay of interactions and topology is a much more open field, for which quantum simulation could bring new insights. A major challenge for quantum simulation platforms is thus the realization of topological phases of matter where interactions play a crucial role.

Many quantum simulation platforms, as diverse as ultracold atoms, superconducting qubits, or exciton-polariton micro-cavities, have been used in recent years to explore synthetic topological matter. To date however, all these experiments can be described in the single-particle regime, and reaching the strongly interacting regime is a very active field of research. Using arrays of single atoms trapped in optical tweezers and excited to Rydberg levels, a group at the LCF realized a synthetic version of the Su-Schrieffer-Heeger model, a one-dimensional chain with alternating strong and week couplings between adjacent sites. Depending whether the chain ends with a strong or a weak link, it is referred to as "trivial" or "topological", and one can show that in the latter case, two degenerate, localized zero-energy states appear on the edges. We have observed these single-particle edge states by microwave spectroscopy (part A of the figure). In contrast with many other approaches, our platform easily allows injecting many excitations in the system and reaching the many-body ground state at half-filling. In the many-body regime, recent theoretical classifications of topological interacting systems have predicted that the phase thus realized would acquire new properties with respect to the single-particle level does *not* lift the degeneracy in the many-body regime (part B of the figure). This realization of a symmetry-protected topological phase for interacting bosons was supported in part by the LabEx through the **XYLOS 2017** project



A Site-resolved microwave spectroscopy reveals the existence of two zero-energy edge modes for a Su-Schrieffer-Heeger chain in the topological configuration (bottom), that do not exist in the trivial configuration (top). B Altering the position of a single atom at the end of the chain lifts the degeneracy of the two edge modes in the singleparticle regime (left), while, for a chain half-filled with interacting particles, the edge modes remain degenerate as predicted by the general classification of symmetry-protected topological phases for interacting bosons (right).

S. de Léséleuc, V. Lienhard, P. Scholl, D. Barredo, S. Weber, N. Lang, H. P. Büchler, T. Lahaye, KA. Browaeys, Observation of a symmetryprotected topological phase of interacting bosons with Rydberg atoms, Science **365**, 775 (2019)

Results achieved in the framework of the project XYLOS 2017 funded by topic 1 and carried out by Thierry Lahaye (LIDyL).

Superconductor/Insulator/Superconductor junction: the supercurrent should be proportional to the sine of the superconducting phase difference, i.e. the difference between the phases of the macroscopic order parameter of each superconductor. This phase difference is controlled by a magnetic field in a loop geometry and is proportional to the magnetic flux through the loop. The sine is related to the fact that the superconducting wave functions decay exponentially in the insulating layer, which should not be greater than a few angstroms in order for the supercurrent to flow through it. In contrast, it was later discovered that a supercurrent can propagate over several micrometers through non superconducting (also called "normal") materials, and the exact relation between the supercurrent and the phase difference (the so-called current-phase relation or CPR) can reveal how the propagation occurs through the normal metal. It turns out that a diffusive propagation through a disordered conductor should resemble a sine function, whereas a ballistic propagation (in a straight line) in a disorderless material should have a sawtooth-like dependence on the phase difference.

The researchers have exploited this sensitivity of the CPR to probe conduction through topological insulators. The current through such materials is predicted to run only through a few perfectly ballistic channels, called topological edge states. The topological insulator candidate is a monocrystalline bismuth nanowire whose crystalline orientation is chosen such that it contains two topological surfaces, each with onedimensional edge states. And indeed, we have found that the supercurrent through a 1.4 micrometer-long monocrystalline bismuth nanowire has just such a sawtoothshaped dependence on the phase difference between the superconductors at its ends. The signal is actually the sum of two sawtooths of slightly different periods, indicating that there are two such one-dimensional ballistic conduction paths in the wire, defining two slightly different loop areas. The fact that transport is ballistic over such a long distance hints at a possible topological protection against scattering in those wires.

High frequency measurements have been conducted on the same Bismuth SQUID coupled to a multimode superconducting cavity. Peaks of dissipation centered at odd multiple values of π could be detected at very low temperature for all eigen modes of the cavity. These dissipation peaks are related to strong current fluctuations taking place exclusively at the Andreev level crossings. These results constitute an experimental proof of the topological nature one these 1 dimensional ballistic states carrying the super current.

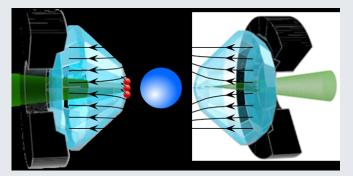
Highlight 2. Magnetism at very high-pressure

M. Lesik, L. Toraille, L. Rondin, J.-F. Roch, (ENS Paris-Saclay, LAC/LUMIN), F. Occelli, P. Loubeyre, T. Plisson (CEA), J. Renaud, O. Salord, A Delobbe (Orsay Physics), T. Debuisschert (Thales Research and Technology)

The study of matter subject to very high pressures makes it possible to understand conditions inside a planet, and also to highlight remarkable properties that we would like to stabilize at ambient pressure. For example, the solubility of hydrogen in metals increases sharply with pressure until it forms compounds that are very rich in hydrogen: super hydrides. These compounds lose their electrical resistivity and become superconducting at record critical temperatures. The compound LaH10, for example, becomes superconducting at -25°C at 1.8 million atmospheres. The synthesis of these new high pressure materials takes place in diamond anvils, whose pointed shape (see figure) enable such high pressures. In addition, the transparency of diamond provides a window for optical measurements for visualization and spectroscopy, as well as for X-ray measurements using synchrotron radiation. Numerous techniques have been developed to characterize samples inside these cells. However, until now, the measurement of magnetic properties has remained very difficult.

In the project partially funded by PALM, physicists from the Laboratoire Aimé Cotton (ENS Paris-Saclay/CNRS/University Paris-Saclay – now called LuMIn), in collaboration with CEA and Thales R&T, have overcome this difficulty by observing the response of point defects in the diamond crystal created on the head of one of the two anvils of the cell. These defects were realized by implanting nitrogen ions with a focused ion beam microscope designed with the company Orsay Physics. In the presence of a magnetic field, their luminescence varies, which can be observed by optical microscopy through the anvil. The technique has been validated by the observation of superconductivity in MgB2 by optically detecting the Meissner effect, which reflects the expulsion of the magnetic field from a superconducting material.

The results of this study provide a much better understanding of the relationship between electronic, magnetic and structural properties as a function of pressure. In particular, it will allow the thorough study of numerous metal hydride compounds. The experimental data will enable the identification of materials whose superconductivity would persist under conditions close to ambient pressure. Finally, this magnetic detection could reveal quantum effects in metallic hydrogen at high pressure, in particular its room temperature superconductivity. The scientific and industrial implications of such a discovery are obviously considerable.



Diamond anvil cell used to study the behaviour of matter under very high pressure. One of the anvils incorporates crystal defects (red) on the surface in the vicinity of the sample (blue). The magnetic field applied to the cell (arrows) is expelled from the sample when it becomes superconducting. The change in the magnetic field lines is then detected in situ by the light emitted by the defects when excited by a green laser © Margarita Lesik (ENS Paris-Saclay)

M. Lesik, T. Plisson, L. Toraille, J. Renaud, F. Occelli, M. Schmidt, O. Salord, A. Delobbe, T. Debuisschert, L. Rondin, P. Loubeyre, J.-F. Roch, Magnetic measurements on micron-size samples under high pressure using designed NV centers, Science (2019)

Results achieved in the framework of the project AIMHIP 2018 funded by topic 1 and carried out by Jean-Francois Roch (LAC/LuMIn)

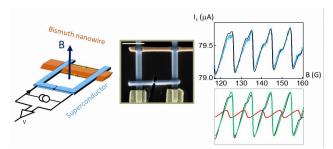


Figure 1. A SQUID configuration consisting of a superconducting tungsten loop (in blue) containing a reference junction. In parallel with the setond junction, whose current-phase relation is unknown (tungsten/bismuth nanowire/tungsten with the Bi shown in brown). The plot displays the current phase relation of the S/Bi/S junction (blue curve), which is the sum of two sawtooths with slightly different periods. (see the decomposition in the lower plot) This demonstrates that the supercurrent in the bismuth nanowire is carried ballistically along only two paths at two edges of the nanowire

Key publication (project JosephBismuth 2015)

A. Murani, et al., "Ballistic edge states in Bismuth nanowires revealed by SQUID interferometry", Nature Comm. 8, 15941 (2017).

A. Murani, B. Dassonneville, A. Kasumov, J. Basset, M. Ferrier, R. Deblock, S. Guéron, and H. Bouchiat, "Microwave signature of

Topological Andreev level crossing in abBismuth-based Josephson junction". Phys Rev. Lett, 122, 076802 (2019)

2. Rare earth q-bits for quantum information

PALM financed the postdoc of Lucile Veissier who worked at the Laboratoire Aimé Cotton on Erbium-yttrium symbiosis for quantum information processing. The project, called OptoRF-Er 2017 is an attempt to achieve a spin q-bit having both a long lifetime and optical addressability The LAC team has proposed a hybrid approach by coupling an optically active ion of erbium, and a long-lived nuclear spin of yttrium. These two compounds are naturally present when erbium is inserted into an yttrium orthosilicate matrix. The presence of multiple yttrium atoms around the Er is a complicated structure that makes the control particularly delicate (see figure). The researchers have shown that it is possible to selectively control an Er-Y pair without affecting other neighbors. Their experimental demonstration is based on a good understanding of the exceptional anisotropy of the magnetic field that erbium induces in its vicinity. This anisotropy is at the heart of the selective control of a specific

Er-Y pair which then forms a promising pair for the quantum processing of information.

Key publication (project Opto-rf 2017)

B. Car, L. Veissier, A. Louchet-Chauvet, J.-L. Le Gouët, and T. Chanelière, "Selective optical addressing of nuclear spins through superhyperfine interaction in rare-earth doped solids", Phys. Rev. Lett. 120, 197401 (2018)

3. Driven dissipative dynamics

In the DriDisMBS project, PALM financed the postdoc of Haggai Landa to work on the non-equilibrium dynamics of cold, trapped ions. Laser cooling can cool ions down to a milliKelvin. Despite this achievement, existing theories are mostly limited to the final stage of cooling where the timedependent drive and anharmonicity of the potential of real ion traps can be neglected. The DriDisMBS project has developed a semiclassical framework based on action-angle phase-space coordinates, that advances the understanding of ion dynamics far from thermal equilibrium. It captures the driven stochastic motion by using a Fokker-Planck equation for the probability distribution, adiabatically averaged over the angles in phase-space, with drift and diffusion expressed in terms of the action. Important open questions, like the optimal trapping potential and the most advantageous settings of the cooling laser, can now be quantitatively answered for realistically modeled traps and an arbitrary large-amplitude motion. Extending this theory, the researchers have predicted that due to the time-dependent trap drive, an ion subject to laser damping can nonetheless be captured in large-amplitude, nonequilibrium stationary states.

At the same time, trapped-ion experiments are well suited for experiments of nonequilibrium many-body dynamics. An extensive toolbox has been developed for coherent manipulation of electronic states forming, e.g., a two-level system in each ion, that is equivalent to a spin-1/2. Within one- and two-dimensional crystals of trapped ions, a coupling between the spins can be induced using light. When driven away from equilibrium and in the presence of dissipative processes, interacting spins form a fundamental model of nonequilibrium dynamics, which describes also solid-state systems such as superconducting circuits coupled to an array of light cavities. The possibility of studying emergent collective quantum phenomena in those systems raises a number of theoretical questions. The focus on three main questions; (i) What phases can be stabilized with nontrivial quantum correlations. (ii) What is the role of the correlations, and (iii) how does it depend on the dimension, the interaction range, and other system parameters?

The researchers have studied a model characterized by a frequency splitting Δ between the ground and excited state of the two-level systems, with XY interaction between nearest-neighbour spins of strength *J*, coherently driven at a Rabi frequency Ω , with damping at a fixed rate Γ introduced by a Lindblad superoperator. They identify regions where the system state is well described by its mean-field (MF) limit,

while beyond these regions, correlations build up in the lattice and must be included in the dynamics. In particular, the correlated regimes include parameters for which the MF manifests two coexisting stable steady states and the MF phase shows hysteresis. The role of quantum fluctuations is studied by using two approaches: by solving approximate MF-dynamics coupled to a leading order expansion of the quantum correlations, and by using advanced numerical approaches based on Matrix Product Operators (MPO). The results of these two approaches are compared in the figure. In regions of meanfield bistability and at nearby parameters, the system develops large correlations over a large spatial scale, accompanied by an increase in the time-scale of relaxation. These correlations are responsible for stabilizing the system state between its two MF-limit states.

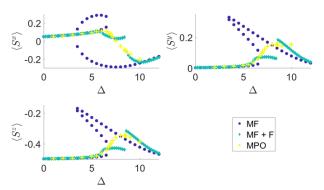


Figure 2. Mean values of the spin projection along the three directions, as a function of the spin up and down splitting Δ , at fixed values of the other paramaters, Γ =1, Ω =0.5, J=5, on a onedimensional lattice. The mean-field (MF) limit manifests bistability, seen as a region of parameters with three co-existing solutions, two of which are stable. When quantum fluctuations are included at leading order (MF+F), the bistability is replaced by a jump, while an essentially exact treatment using Matrix Product Operators (MPO) shows that the jump is smoothened. This behavior results from long- range spin-spin correlations forming in this region of parameters, as a separate analysis indicates.

Key publication (project DriDisMBS 2017)

H. Landa, *Tuning nonthermal to thermal distributions in timedependent Paul traps*, PRA 100, 013413 (2019)

H. Landa, M. Schiro, G. Misguich, *Correlation-induced steady states and limit cycles in driven dissipative quantum systems*, Physical Review B (2020)

H. Landa, M. Schiro, G. Misguich, *Multistability of Driven-Dissipative Quantum Spins*, Physical Review Letter (2020)

A. Maitra, D Leibfried, D. Ullmo, and H. Landa, *Far-from-equilibrium* noise heating and laser cooling dynamics in radio- frequency Paul traps, Phys. Rev. Letter (2020)

4. Spin-orbit coupling in Iridates

Strong electronic correlations and strong spin-orbit coupling are both able to create new electronic states. However, they are rarely encountered together in the same compound. Iridates like Sr_2IrO_4 present a rare situation where both are strong and interacting. The metallic phases emerging from the « spin-orbit Mott insulator » Sr_2IrO_4 are yet to ve characterized.

In the **SOC** project, which financed the thesis of Alex Louat, researchers at the LPS and the Synchrotron SOLEIL have studied Rh doping of Sr2IrO4 with angle-resolved photoemission. Unexpectedly, Rh localizes an electron, hence doping with holes the neighboring Ir sites. A bad metallic state is formed, characterized by a pseudogap (see Figure 3Erreur ! Source du renvoi introuvable.). Pseudogaps are often observed in correlated systems, but they may correspond to quite different situations and finding ways to characterize and classify them is necessary. In this case, we have shown that the pseudogap is actually better defined on incoherent states away from the Fermi Surface, which remains to be understood theoretically.

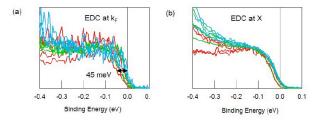


Figure 3. Energy distribution curves (EDC) observed in (Sr0.85Rh0.15)2IrO4 at the Fermi Surface (a) and away from

Fermi Surface on incoherent states (b). Instead of crossing the Fermi level (zero energy) with a sharp Fermi-Dirac edge, there is a loss of spectral weight (the edge is away from EF), generically called a pseudogap. Curiously, we find that the pseudogap is also present for incoherent states, with a well-defined value ~30meV, and actually depends very much at kF on the ratio between coherent and incoherent states, leading to a large distribution of values. This finding is important both for measuring the true pseudogap value and understanding its origin.

See Highllight 3 (project SOC by Fabrice Bert)

Key publication (project SOC 2017)

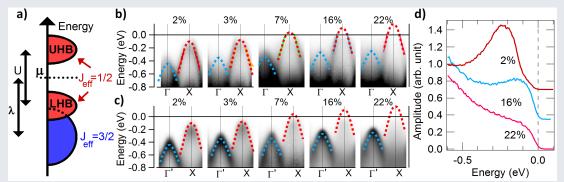
A. Louat, B. Lenz, S. Biermann, C. Martins, F. Bertran, P. Le Fevre, JE Rault, F. Bert, V. Brouet, *ARPES study of orbital character, symmetry breaking, and pseudogaps in doped and pure Sr2lrO4*, Physical Review B100, 205135 (2018)

5. Quantum spin liquids

Predicted long ago by P. W. Anderson, magnetic frustration is now a well-established route to stabilize a quantum spin liquid in dimension higher than one. The Heisenberg model on a corner-sharing kagome lattice populated with spin ½

Highlight 3. Formation of an incoherent metallic state in Rh-doped Sr₂IrO₄ F. Bertran, P. Le Fèvre, and J. Rault (Synchrotron SOLEIL)

Sr₂IrO₄ is considered as the archetype of a novel type of Mott insulator, the "Spin Orbit Mott Insulator". While it should be metallic, since Ir has 5 electrons in its 5d shell, it is an antiferromagnetic insulator. This canno't be understood in the standard Mott scenario because the electronic correlations, responsible for Mott insulating behavior, are relatively small for 5d transition metals. However, it was shown that the Spin-Orbit Coupling (SOC), which is very strong for heavy atoms like Ir, induces a reconstruction of the electronic structure (see figure 1a) with a narrow half-filled J_{eff}=1/2 band, where even small Coulomb repulsion may open a gap. This situation offers many similarities with cuprates and the evolution of this new type of insulator when doped is an active field of research.



{a) Sketch of the energy positions of the bands expected in Sr₂IrO₄. The J_{1/2} band is divided into a Lower Hubbard Band (LHB) and an Upper Hubbard Band (UHB). The chemical potential μ is represented by a dashed black line. U is the Columb repulsion and λ the SOC constant. b) Energy-momentum plot along IX for different Rh dopings. The J_{1/2} and J_{3/2} bands are emphasized by red and blue guides to the eye, respectively. c) Energy-momentum plots along IX. d) Energy Distribution Curve (EDC) at k_F in the IX direction for the indicated doping.

Researchers have synthesized and investigated with ARPES Sr2(Ir1-xRhx)O4, where Rh is a 4d element isovalent to Ir. With ARPES, we observe a rigid band shift toward the Fermi level until at least 22% of Rh doping (figure 1b et 1c). This corresponds to an effective hole doping, which was unexpected due to the isovalency of Ir and Rh. For a doping of about 7%, the J1/2 band just touches the Fermi level, which corresponds well to an Insulator-Metal transition also observed in transport. However, the metallic state does not present quasiparticle peaks, even at the optimal doping (around 15%), the bands are not renormalized compared to the band calculations, and a "pseudogap" of about 30meV (see figure 1d) is present on the entire Fermi surface. We attribute this to an incoherent behavior resulting from the interplay between correlation and disorder introduce by Rh. We suggest that the observed formation of charged defects around Rh holds clues to understand how doping proceeds in these compounds.

The effect of disorder in a strongly correlated compound is a rich theoretical and experimental subject. This study of the Insulator-metal transition in an exotic Mott insulator brings a novel point of view in this large field of research.

A. Louat, V. Brouet, F. Bert, L. Serrier-Brinon, F. Bertran, P. Le Fèvre and J. Rault, Formation of an incoherent metallic state in Rh-doped Sr2IrO4, Physical Review B 97, 161109 (2018)

Results obtained within project SOC 2017 funded by topic 1 and carried out by Fabrice Bert (LPS)

moments is the best-known example leading to such a spin liquid ground state. Its nature has been one of the most intriguing and still pending issues aver the last 20 years. In the project **SPINLIQ**, new Cu-based materials derived from the emblematic herbertsmithite $ZnCu_3(OH)_6Cl_2$ are investigated using local probes such as NMR and μ SR to study their ground state properties.

Doping a quantum spin liquid has also been a 'holy grail' since the seminal work of Anderson several decades ago. Many attempts over the years have struggled with various forms of localization. Recently it was found that the hyperkagome –the counterpart in 3D of the kagome lattice - iridate $Na_4Ir_3O_8$, which is a quantum spin liquid, can be doped by moving to the $Na_3Ir_3O_8$ stoichiometry. By a local nuclear magnetic resonance investigation, it was found that the susceptibility is governed by a semimetal electronic structure and that the antiferromagnetic fluctuations present in the parent spin liquid compound $Na_4Ir_3O_8$ persist in the doped regime, much alike the case of High Tc superconductors. The finding is highly relevant for future search of novel states of matter.

The diversity of exotic ground-states observed in the pyrochlore lattice stems from the competition and delicate balance between exchange, dipolar and spin-orbit interactions whose better understanding could lead to the stabilization of new quantum phases, including a spin liquid state.

One goal of the **QuantumPyroMan** chair project has been to investigate the phase diagram of the quantum pyrochlore magnet $Yb_2Ti_2O_7$ using inelastic neutron scattering. The nature of its ground state has been obscured by a strong sample-to-sample dependence, mainly due to oxygen vacancies defects and Yb/Ti site substitution, leading to experimental controversies oner the presence or absence of a quantum spin liquid phase. A new approach was developed, using chemically-controlled applied pressure by replacing Ti⁴⁺ by a larger non-magnetic ion Zr⁴⁺, thus avoiding the introduction of oxygen vacancies.

Over the course of this project, C. Decorse, our Paris-Saclay chemist collaborator, achieved a controlled substitution of Zr on the Ti with the synthesis of various compositions x of the solid-state solutions Yb₂(Ti_{1-x}Zr_x)₂O₇, and large single crystals of (1) the "ultra-pure" x=0 - with minimal oxygen vacancies as shown by its transparency (Fig.1e), and (2) compositions. Inelastic neutron scattering x=0.025 measurements have singled out a new phase for the peculiar composition x=0.025, which stands out with a highly suppressed diffuse scattering above $|Q| = 1 \text{ Å}^{-1}$ (Fig. 1b). Armed with the knowledge of the magnetic and nonmagnetic contribution to the diffuse scattering in the x=0 single crystal (Fig.1 g,h) and in the x=0.025, new theoretical simulations (started with a new collaboration with M. Gingras (Waterloo University)) will help to refine the change of the Hamiltonian through chemical pressure effect and to identify this exotic phase located near $x \sim 0.025$.

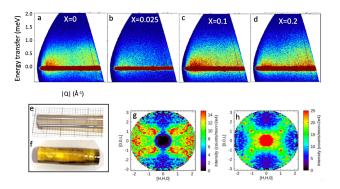


Figure 4. Inelastic neutron scattering of Yb2(Ti1-xZrx)2O7 pyrochlores (a-d) Evolution of the dynamical structure factor $S(q,\omega)$ as a function of x in polycrystalline samples measured at 2K on the LET spectrometer (ISIS). The x=0.025 stands out with a reduced scattering intensity. (e,f) Large single crystal of x=0 (e) and x=0.025 (f). The transparency of the x=0 confirms its stoichiometry. (g,h) Polarized inelastic neutron scattering data measured at 60mK for the x=0 single crystal at an energy transfer of 0.3meV, showing the spin-flip (g) and non-spin flip (h) channel.

6. Metal insulator transitions in transition metal oxides

Researchers at the Soleil Synchroton and Ecole Polytechnique collaborated in the **MITRIX** project to perform a study of the metal insulator transition in La1-xSrxVO3 thorough resonant inelastic X-ray scattering (RIXS) and nonresonant inelastic X-ray scattering (IXS), in order to both provide insight into the phase diagram of La1-xSrxVO3 and to provide a solid data set for theory development. Transition metal oxides exhibit partially filled narrow bands and electron correlation effects are significant. Thus advanced methods of many-body theory are required to understand their properties. The resonant scattering cross section is naturally more complicated than the non-resonant case, hence combining RIXS and non-resonant IXS is particularly interesting as the IXS cross section is theoretically well understood.

Several experiments were performed at Synchrotron Soleil and the European Synchrotron Radiation Facility to characterize the metal to insulator transition in La1-xSrxVO3. One particularly interesting finding concerns the temperature evolution of the low energy excitation attributed to orbital excitations and present in the insulating part of the phase diagram of La1-xSrxVO3 (near x=0) as well as in the closely related compound YVO3. High resolution RIXS measurements of the temperature dependence of the excitation together with the temperature and doping dependence of the excitation energy permitted an unambiguous connection to the the antiferromagnetic and orbital ordering phase transition occurring in the La1xSrxVO3 family of compounds at 140 K.

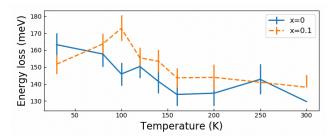


Figure 5. Temperature and doping dependence of the observed low energy excitation in La1-xSrxVO3 for x=0 and x=0.1. The critical temperature of the antiferromagnetic and orbital ordering transitions is approximately 140 K. The sudden change in the temperature dependence of the energy of the excitation near the critical temperature connects the excitation to this phase transition.

Key publication (project MITRIX 2017)

K. Ruotsalainen, M. Gatti, J. Ablett, J.-P. Rueff, D. Adrian, W. Prellier and A. Nicolaou, Low-energy electronic excitations and band-gap renormalization in CuO, Physical Review B, 95, 19, 195142 (2017)

7. Gate-tunable superconductivity in an oxide heterostructure

Two-dimensional electron gases (2DEGs) at oxide interfaces have emerged as a platform to study the phenomenon of superconductivity in low dimensions. An important property of these systems is that the carrier density is tunable with an electrostatic gate voltage. This allows exploration of the phase diagram by accessing a broad range of carrier densities. Researchers had previously demonstrated that a metallic 2DEG can be generated by evaporating a thin layer of Al under ultra-high vacuum on a SrTiO₃ crystal, whereby Al oxidizes into amorphous insulating alumina, doping the SrTiO₃ surface with oxygen vacancies. From transport experiments with this AIOx/SrTiO₃ interface, researchers at the CSNSM and the LPS determined the superconducting critical temperature of the 2DEG to be 360 mK (the 2DTROX project). The critical temperature was observed to vary with the gate voltage, leading to a 'superconducting dome' in the phase diagram (figure below). The system exhibits a magnetic-field-induced superconductor-to-insulator transition. They demonstrated a gate-induced switching between superconducting and resistive states. These results open up the possibility of designing novel devices using the 2DEG in AlOx/SrTiO₃ for studying complex many-body-phenomena in reduced dimensions..

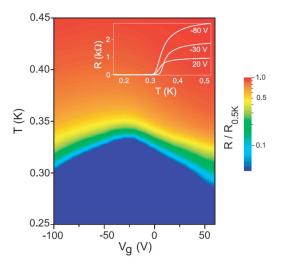


Figure 6. 2DTROX project: Resistance (R) is measured as a function of temperature (T) at different gate voltage (V_g) values. The colourscale indicates the ratio $R(T)/R_{0.5K}$, where $R_{0.5K}$ is the resistance at 0.5 K for each value of V_g. The critical temperature varies with V_g in a superconducting dome. Inset: A few curves at selected gate voltages are shown

Key publication (project 2DTROX 2017)

S. Sengupta, Tisserond, F. Linez, M. Monteverde, A. Murani, T. C. Rödel, P. Lecoeur, T. Maroutian, C. Marrache-Kikuchi, A. F. Santander-Syro and F. Fortuna, J. App Phys., **124**, 213902 (2018)

8. Spin resolved inverse photoemission

The conduction band is the keystone of many applications as it defines the possible electronic excitations. The conduction band receives the excited electrons in lasing processes, the photoexcited electrons in solar cells or the conduction electrons in transistors and in p-n junctions. A thorough understanding of the conduction band is therefore necessary in optoelectronics, spintronics or photovoltaics applications. From a fundamental point of view, there are also many questions that require accessing the conduction band. It is the case for reliably determining the gap in Mott insulators, in spin or in charge density wave systems.

Inverse photoemission is the most suitable experimental technique to measure the unoccupied band structure with k-resolution. Moreover, it is possible to exploit a spin-polarized source to gain insight on the unoccupied state spin. This technique involves sending an electron with a known incidence angle to a sample, in order to inject it in the unoccupied states of a system. When the electron relaxes, photons are emitted and detected in, for instance, Geiger-Müller detectors. The **SPOUSE** project has provided funding to improve the detection efficiency of the Inverse Photoemission setup at Laboratoire de Physique des Solides. The Geiger-Müller detector is now installed and operational in the experimental setup and the first spectra to validate the full operation of the system are being acquired (cf. Figure 7).

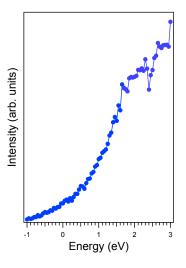


Figure 7. Preliminary spectrum of the inverse photo-emission of functionalized copper

9. Recent projects

Almost all the projects mentioned above correspond to financing decisions which were made in the period 2015 - 2017. In most cases, the more recent projects have yet to produce publishable results. Still, we wish to give an overview of some of these projects as well as the recent scientific trends which are visible in the LabEx.

In the area of topology the **KATOPO** project seeks to investigate novel non-trivial topological properties in a recently discovered family of correlated and magnetic systems, based on kagomé lattices. Another, theoretical project, **1DCOLDANYONS**, is at the interface between cold atom physics and topology and plans develop all necessary steps to adapt cold atoms to the quantum simulation of anyons, with a specific focus on Majorana fermions and parafermions.

At the interface between AMO and condensed matter physics we have also funded the **SPECTRAL** project which will introduce a new spectrscopic approach in order to observe the mobility edge in a system exhibiting Anderson localization (cold atom gas subject to a random, speckle potential). The **BATO** project is another cold atom project on out of equilibrium effects in a 1 dimensional gas. A single sample of the gas is trapped on an atom chip so that not only the mean distributions but also the fluctuations can be studied. The **OPTICCOM** project seeks to address questions of optical control of long range atomic interactions. The idea is to use optical fields to dress quantum states of colliding ultracold and molecules to prevent them from reacting at short distances.

The **GENLOOP** project is concerning quantum correlated materials, in particular the investigation of loop currents breaking discrete Ising-like (Z2) symmetries in Cuprates, beyond High T_c superconductors. These will be studied using resonant x-ray and polarized neutron scattering. The **EPIMOC** project is an investigation of multiple ordered phases in multiferroic materials. The technological interest of these materials lies in the possibility of controlling magnetism with an electric field, with applications in the domains of information, data storage and processing.

Two projects were related to plasmonics. The **KIDSPP** project seeks to develop a cryogenic detector for surface plamon-polaritons using a low temperature circuit. It nicely illustrates the beginning of a bridge towards the activity of the NanoSaclay LabEx. The **Jasmin-T** project is a study to develop a nonlinear medium that can perform mixing operations at THz frequencies using Josephson plasma excitations. The project may open the way to all THz signal processing.

We have also funded several projects for equipment of general use and which will be available for several research groups within PALM. Many of these projects involve the LabEx contributing to an investment with many different sources of funding, These include GRAVEX which aims at creating a state-of-the-art reactive ion etching facility that will be available to all members of the PALM Labex through its installation in the LPS cleanroom. The CRYOFAST project is to install a fast loading dilution refrigerator at the LPS which will be accessible to researchers for typically week long measurements without the traditional cryogenic maintenance requirements. On a smaller scale, the ÉCLAIR project is a collaboration between the LCF and LAC laboratoires to develop low power, external-cavity lasers with sub MHz linewidths in the 1000 nm to 1100 nm range for cold atom experiments.

Topic 2 "Complex systems: from out of equilibrium systems to biological matter"

Focus Topic 2 of PALM " Complex systems: from out of equilibrium systems to biological matter" gathers experimentalists, theoreticians and numerical modelers working on various objects (glasses, granular media, fracture, interfaces, suspensions, instabilities, chaos, turbulent fluids, soft matter, networks, and information, ...) but using the common language and tools of Statistical Physics. Understanding the emergent dynamics in out-of-equilibrium systems represents one of the major challenges for the next decade because they are ubiquitous and cannot be understood simply through small modifications of equilibrium physics. Moreover, they are directly connected to important societal needs such as energy, climate, environment or health.

This report covers the last two years of the initial phase of the Labex and the first call of the new phase. During the last two years of the previous phase, this Focus Topic has continued to support the community, but in a constrained situation characterized by a drop of the success rate at the call for projects related to the contraction of the available funds. Nevertheless, it was still possible to carry on a reasonable portfolio of interesting projects because most of them involved external resources. Surprisingly, most of the projects of the 2020 call still involved external resources, leading to a decrease of the financial pressure (meanwhile the typical amount of funds was restored) but without any notable change in terms of the number of projects. Following the recommendations of the 2017 meeting of the ISC (International Scientific Council), Focus Topic 2 has increased the interactions with the other scientific domains covered by PALM, and in particular funded a 2 year-post doc for project QSimMBDyn about out-of-equilibrium quantum many-body physics. This project is the follow up of a junior chair (L. Mazza) of a Focus Topic 1. We also funded project ShiLOM that that is an extension including the effects of disorder and irradiation in functional materials, a specific area of recurring interest for Topic 4. According to the perspectives detailed in the previous scientific report, this presentation splits the projects into the three sub-topic areas, though several of these projects span more than a subtopic and sometimes overlap with problems of concern of other branches of the Labex. The main scientific projects funded during the three project calls of the period 2018-2020 are described below.

1. Disordered and glassy systems

Junior chairs

Three Junior chairs were also awarded during the past three years in this thematic area. Actually, these funds were relatively small compared to the past ones because of the limited available budget of the projet calls of 2018 and 2019. These funds are aimed at produce a leverage and submit a more extensive project either to the labex, or to other funding schemes. The project QuanDynWOTran, by Maurizio Fagotti, recruited by CNRS at LPTMS in 2018, in collaboration with the theoretical group at IPhT (M. Schirò), is related to the Quench Dynamics without Translational Invariance. The characterization of the nonequilibrium time evolution of isolated quantum many-body systems is a main frontier of theoretical physics. Recently, some progress were made in understanding the dynamics in the presence of inhomogeneities. In particular, the so-called generalized hydrodynamics was developed, which allows access to the late-time dynamics in integrable systems, even in presence of interactions. The project is expected to have an impact on the out of equilibrium physics of complex interacting quantum systems, including transport phenomena in quantum dots, open driven and dissipative light- matter systems, a thematic area overlapping with the interests of the Focus Topic 1.

Key publication

M. Fagotti, *Locally quasi-stationary states in noninteracting spin chains*, Scipost Physics, 8, 3, 048 (2020)

V. Alba, B. Bertini, M. Fagotti, *Entanglement evolution and generalised hydrodynamics: interacting integrable systems*, Scipost Physics, 7, 1,005 (2019)

M. Fagotti, On the size of the space spanned by a nonequilibrium state in a quantum spin lattice system, Scipost Physics, 6, 059, (2019)

B. Bertini, M. Fagotti, L. Piroli, et al. *Entanglement evolution and generalised hydrodynamics: noninteracting systems*, Journal of physics a-mathematical and theoritical, 39/51/39LT01 (2018)

The second junior chair (project **TopDyn**) is carried by Franck Smallenbourg in collaboration with E. Trizac for Simulating the topological dynamics of network glasses. Indeed, many of the materials vital to our lives consist, at the microscopic level, of a disordered network of linked building blocks. Examples include for instance water, glass of windows, and cross-linked polymers. The macroscopic dynamics of these materials are determined by the microscopic network relaxation events that allow the network to relax stresses. At low temperatures, the time-scale associated with topology-changing events is large in comparison to the time scale of thermal vibration. As simulations need to cover both of these time scales, our ability to access the long- time dynamics of networked fluids is severely hindered by computational costs. This project proposes the development of a coarse-graining method that bridges this time-scale gap, permitting the simulation of lowtemperature networked materials on much larger length and time scales. The aim is to explore the interplay between microscopic network rearrangement mechanisms and the global dynamics of networked materials, also providing guidelines for the targeted design of new functional materials. The third junior chair (project EquiDystant) targets the non-Equilibrium Dynamics and metastable states: from classical to quantum systems and it is carried out by Laura Foini (in collaboration with Alberto Rosso). This project deals with aspects of non-equilibrium physics and with the effect of metastable states that arise in classical and quantum systems. It addresses a very general question, how a system relaxes starting from some highly excited state. The presence of metastable states can trap the system and lead to very slow dynamics and non-linear response, as for elastic interfaces in a random environment. From a different perspective the study of metastable configurations in disordered systems intimately related to glasses, should allow to understand the performances of many algorithms used in machine learning to optimize the parameters of the model, leading to the study of the relaxation and the mechanism of chaos in quantum many body systems.

Key publication

L. Foini, J. Kurchan, *Eigenstate Thermalization and Rotational Invariance in Ergodic Quantum Systems*, Physical Review Letters (2019)

L. Cugliandolo, L. Foini, and M. Tarzia. *Mean-field phase diagram and spin-glass phase of the dipolar kagome Ising antiferromagnet.* Phys. Rev. B 101, 144413 (2020)

Post-doc fellowship

During the past three projet calls, 7 projects were funded in this thematic cluster. In 2020 our focus topic funded a postdoc (project **ShiLOM**). Olivier Plantevin (PI), Catherine Corbel and Bernard Geffroy plan to investigate hybrid organic-inorganic perovskites that have become one of the most promising low-cost alternatives to traditional semiconductors in the field of photovoltaics and light emitting devices. These systems combine both attractive features of organic and inorganic materials within a single composite, for instance with stronger excitonic properties and brighter luminescence. Within these emerging materials, multiplecation mixed halide perovskites have been highlighted due to their facile band gap tunability by varying the halide composition and improved structural stability. The main focus of the project addresses the instabilities due to halide ion migration under photoexcitation that are studied using electron and ion irradiation for the introduction of point defects in a controlled manner. Point defects modify the electronic and light emitting properties of the material as well as the photo-induced halide mobility which is one of today's challenge for improved stability in opto-electronic devices.

Key publication (ShilOM)

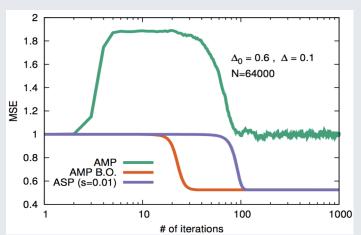
O; Plantevin, S. Valère, D. Guerfa, F. Lédée, G. Trippé-Allard, D. Garrot, E. Deleporte. *Photoluminescence Tuning Through Irradiation Defects in CH 3 NH 3 Pbl 3 Perovskites.* physica status solidi (b). 256. 1900199. 10.1002/pssb.201900199. (2019)

It also funded the post-doc Alberto Biella (project **QSim-MBDyn**: "Quantum Simulation of Many-Body Dynamics with Rydberg Atoms and Collective Light Scattering"). In this project, Leonardo Mazza and Marco Schirò are concerned by the developments in quantum engineering that have brought forth the possibility of studying collective quantum phenomena in hybrid systems of interacting matter and light. These systems, which are intrinsically driven and dissipative, raise a number of intriguing theoretical questions and allow to probe fundamental quantum many-body physics in uncharted non-equilibrium scenarios. The aim of this project

Highlight 4. Approximate survey propagation for statistical inference Fabrizio Antenucci, Pierfrancesco Urbani, Lenka Zdeborová

A generic inference problem can be described in the following way: given a set of measurements (that can be noisy or even non linear), how can we reconstruct the original signal from which they come from? What is the reconstruction error? Which kind of algorithms can we use? These questions can be addressed in simple generative models in which one generates a set of artificial data from a given signal through a known process and play the inference game. This is a probabilistic setting that naturally brings to disordered statistical physics models.

In the last work we have analyzed what happens when, in the inference game, the information about the statistical nature of the generative models is not used properly. In this case the student does not know perfectly the probabilistic informations about the teacher and we have shown that the reconstruction ability of a simple algorithm, called Approximate Message Passing (AMP), is degraded. This is due to glassiness in the statistical distribution (the posterior) over the signal. Therefore, we have introduced a new algorithm, that we have called Approximate Survey Propagation (ASP) that extends AMP to include glassy effects. We have shown that this algorithm performs much better than AMP. This is shown in the figure where we plot the Mean Squared Error (MSE) between the reconstructed signal (through the two different algorithms) and the true one. The orange line represents the MSE that can be achieved when the student uses properly the information on the teacher.



A. XFEL experiment results showing the development of Rayleigh-Taylor instabilities with spatial resolution of ~ 1 μm. The zoom shows strong PCI feature at the edge of RTI fingers. B. Example of Rayleigh-Taylor instabilities found in the Universe. This is a picture of the supernova remnants SNR E0102.2-72, aged of ~ 1000 years where an analogy with the experiment can be made leading to a better understanding of the evolution of the system

Fabrizio Antenucci, Florent Krzakala, Pierfrancesco Urbani, Lenka Zdeborová. Approximate survey propagation for statistical inference. Journal Stat Mech (2018)

Stefano Sarao Mannelli, Giulio Biroli, Chiara Cammarota, Florent Krzakala, Pierfrancesco Urbani, and Lenka Zdeborová. Marvels and Pitfalls of the Langevin Algorithm in Noisy High-Dimensional Inference. Phys. Rev. X 10, 011057 (2020)

Results obtained within project StatPhysDisSys of LabEx PALM coordinated by Pierfrancesco Urbani (IPhT)

is to develop a joint theoretical activity at LPTMS and IPhT on the modelling of these platforms, which are currently under experimental investigation at Laboratoire Charles Fabry (LCF), Institut d'Optique. The ambitious objectives of this project, which include the development of neuralnetwork algorithms for open many-body quantum physics, justify these complement funds to the Junior Chair previously awarded by the Focus Topic 1.

Key publication (QSim-MBDyn)

A. Biella, *et al.* Energy transport between two integrable spin chains. *Physical Review B* 93 205121 (2016)

See Highllight 4 (project StatPhysDisSys) on a related thematic area. Other highlights are also available on PALM website (SAMURAI 2017)

Key publication (project SAMURAI 2017)

F. Antenucci (CEA), S. Franz (LPTMS), P. Urbani (CEA), L. Zdeborová (CEA), *Glassy nature of the hard phase in inference problems*, Phys Rev X (2018)

Equipment

Two "Equipement" projects were also funded during this period. The project **FURIE** studies the "Fast equilibration in the underdamped regime" (Loïc Rondin of laboratory LAC

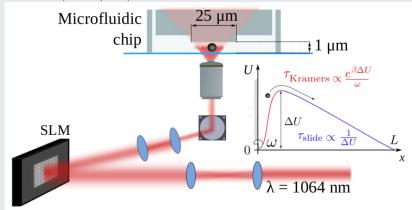
and E. Trizac). In this project the widespread of nanosystems in technology as well as in biochemistry has triggered essential developments around the physics of small systems, i.e. where involved energies are limited to a few tens of the thermal energy kBT. One iconic question is the arbitrary fast transition between equilibrium states since it is a crucial ingredient for the development of efficient nanoheat engines, or optimisation of AFM and NanoElectroMechanical Systems (NEMS). Recently, this problem was addressed through the development of engineering of swift equilibration protocols. However, the generalisation of such protocols remains limited to specific cases. The project aims at providing an experimental demonstration for arbitrary damping that is still missing studying the fast equilibration of an optically levitated nanoparticle both theoretically and experimentally where the funded Acousto-optics deflector is critical. This project opens perspectives on the development of fast non-isothermal states transitions and general control of out of equilibrium nanothermodynamics.

Key publication (project FURIE)

S. Faure, S. Ciliberto, E. Trizac, D. Guery-Odelin. *Shortcut to stationary regimes: A simple experimental demonstration*. American Journal of Physics 87, 125 (2019)

Highlight 5. Optimal thermal activation and barrier crossing Emmanuel Trizac, Marie Chupeau (LPTMS), Alexei Chepelianski (LPS)

Arrhenius' law (1889) is a cornerstone in our understanding of many kinetic processes in chemistry, thermodynamics or molecular biology. This empirical law stipulates that reaction rates depend exponentially on the energy barrier which separates the reactants from the final products; this is the so-called activation energy. A satisfactory theory was proposed 50 years later by Kramers for Brownian systems. Kramers' relationship introduces the coupling to the environment (the suspending fluid) via a friction parameter and confirms the exponential relationship between reaction speed and activation energy. It is therefore natural to think that the higher the activation barrier, the slower it is to cross, and therefore to conclude that the absence of the activation barrier would lead to maximum reaction rates. A collaboration between the LPS Orsay and the LPTMS, as well as the Cavendish laboratory in Cambridge has shown that this intuition based on the relationships of Kramers / Arrhenius was incorrect. In other words, it is not the free diffusion and therefore without any barrier which minimizes the time of first passage at a target point for a Brownian particle. The very existence of a barrier speeds up the process!



This figure shows the experimental setup to measure the escape rates of a Brownian colloidal particles in an external potential defined with holographic optical tweezers. It also shows the sketch of a theoretical potential profile where the increase of the Kramers escape time is compensated by a fast sliding time. The potential energy at the initial and escape points is equal, a general strategy is proposed to generate optimized 'accelerating' potentials with escape rates much faster than free diffusion.

M. Chupeau, J. Gladrow, A. Chepelianskii, U. F. Keyser, and E. Trizac. Optimizing Brownian escape rates by potential shaping. PNAS (2020)

M. Chupeau, B. Besga, D. Guéry-Odelin, E. Trizac, Artyom Petrosyan, and Sergio Ciliberto Thermal bath engineering for swift equilibration, Phys. Rev. E 98, 010104(R) (2018)

Results obtained within project SWEET 2016 funded by topic 2 coordinated by Emmanuel Trizac (LPTMS) andt Alexei Chepelianski (LPS)

See Highllight 5 (project SWEET 2016) on related thematic area

The second one, project ArTEMiS studies the "Atomic transport in nanocrystalline metals" (G. Baldinozzi of SPMS laboratory and Vassilis Pontikis of CEA) and it funds the acquisition of computing resources. The project aims at unravelling the atomic scale mechanisms of mass transport and recrystallization in nano-crystalline metallic samples via atomic scale simulations relying on near-transferable n-body potentials adapted to noble metals. It is legitimate to ask whether the grain growth in nano-crystalline metallic materials relies upon the same mechanisms observed in microcrystalline materials or the grain growth in nanocrystalline materials involves a different "new" physics. The available experiments do not support the idea that crystal growth in metallic nano-crystals can be simply extrapolated from the processes observed in micrometric crystals, but no definitive answer is available about the underlying physical mechanism justifying the need of computational experiments concerning atomic transport in nano-crystalline systems that will be compared with experiments and theoretical models, which have evidenced the unexpected existence in metallic nano-crystals of a linear grain growth below a critical grain size.

Key publication

G. Baldinozzi, P. Lecoeur, V. Pontikis, *Depth Profiling of Strain in Textured Tungsten Films,* Mrs Advances (2018)

V. Pontikis, G. Baldinozzi, L. Luneville, Laurence; et al., *Near transferable phenomenological n-body potentials for noble metal*, Journal of Physics-Condensed Matter (2017)

2. Soft matter, active matter and biological systems

Post-doc fellowship

During the past three years, 8 projects were funded in this thematic cluster. Two post-doc grants were awarded in the soft-matter area. The first one (project InterFreeze) concerns the study of the "Surfactant surface freezing: tuning mechanical properties" and is fostered by Anniina Salonen with the implication of S Rouzière, Philippe Fontaine, and Fabrice Cousin. The aim of this project is addressing freezing surfactant-laden surfaces that have recently been shown to give control over emulsion drop shapes as the balance between surface tension and crystal elasticity is varied. In parallel, the crystallisation of surfactants leads to versatile particles, which can confer solid-like properties to a gas water interface. The project bridges the gap between surface freezing and crystal formation to lead to a modulation of the surface structures and surface mechanical properties. Using the understanding of the interfaces for making foams with interesting mechanical and structural properties, the project hopes to shed light to the longstanding problem of linking local organisation, interfacial rheology and foam stability combining structural and mechanical characterisation of interfaces and the foams, which has justified the grant for the 2-year postdoc. The second post-doc grant concerns the

NanopiCo "Self-Assembly of Plasmonic project Nanoparticles in Confinement for Sensing Application" carried on by Cyrille Hamon and Thomas Bizien. This project aims at minimizing defects in nanostructures made of plasmonic (Au, Ag) nanoparticles organized into crystalline structures (i.e. supercrystals). Minimizing defects in plasmonic supercrystals is not only a fundamental challenge but is also relevant for Surface Enhanced Raman Scattering (SERS) spectroscopy. The project aims at achieving a hierarchical organization of gold nanoparticles over large areas (square centimeters) with micropatterned templates, which will confine the drying of the nanoparticles dispersion within specific areas. The post-doc carries out the nanostructuration of the single supercrystal and its assessment by Small Angle X-ray Scattering and SERS. The project aims at pointing out the limit to the formation of defects when the cavity geometry (size/shape) is commensurate with the thermodynamically favored shape of the supercrystals.

See Highllight 6 (project MUSA 2017) related to softmatter area

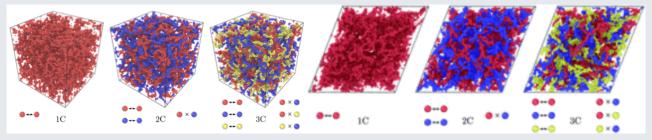
PhD grants

Three PhDs were funded over the period covered by this report. They involve several groups of PALM, but also collaborations with groups with specific expertise in biology outside the Labex perimeter (as for instance at I2BC). The first project **e-Bact** studies biofilms that are one of the most prevalent life modes of microorganisms in natural and industrial settings. A decade ago, the biofilm formation on electrodes immersed into sediments was found to produce electrical current but few fundamental studies were published aside and the mechanisms by which electrons are produced by bacteria and transferred to the electrodes are still unknown. The project aims at understanding experimentally the electroactivity of bacterial communities and how biofilms produce currents funding the PhD student, Marion Lherbette (PhD director Eric Raspaud), during three years. The second PhD grant Symbiose funds the PhD thesis of Julien Bouvard (Phd director Harold Auradou), and aims to uncover the role of the bacterial motility in plantbacteria symbiosis, focusing on the hydrodynamic aspects of the pre-infection approach phase. The system investigated here is the symbiotic partnership between leguminous plants and rhizobia, a motile nitrogen-fixing bacterium naturally present in the soil. While it is widely recognized that bacterium motility is a key factor in the infection rate, the detailed mechanism of the swimming of the bacteria near the plant roots, its chemotactic response to molecular signaling (flavonoids and other secreted plant compounds), and its competition with other fluid flow phenomena (drainage via root pumping or thin film capillary forces) are still open issues. This project develops dedicated microfluidic experiments to address experimentally the swimming properties of rhizobia and its role in the preinfection phase. The aim is to gain more insight into the physical (and particularly hydrodynamical) aspects of symbiotic interactions, a critical issue to optimize crop yields in combination with reasoned use of nitrogen fertilizer inputs in agriculture.

Highlight 6. Multi-component colloidal gels: interplay between structure and mechanical properties

Claudia Ferreiro-Córdova, Giuseppe Foffi (LPS)

Gels are very present in your daily life; the shampoo that you wash your hair with, the gelatine in your mince pies, or your toothpaste. In these examples, the gel is composed of a large amount of liquid which is entrapped in a three-dimensional network of molecules such as surfactants or polymers. Although their liquid content is much larger than their solid content, gels present solid-like mechanical properties such as the presence of an elastic regime at low strain. There is a particular type of gel where this network, instead of being formed by a sequence of molecules, is formed by chains of tiny solid particles (colloids). These are known as colloidal gels.



Snapshots of arrested phases for monogel, bigel and trigel. The interactions (attractive or repulsive) are also depicted for each species

In this project, the authors present a thorough numerical study where they models the formation of colloidal gels whose networks are composed of up to three different types of particle chains. Moreover, they correlate the resulting structures with their mechanical properties, enabling the authors to establish predictions on the performance of these gels for different applications. The insights presented in this work are of high relevance not only to advance the understanding of colloidal gels but also to the design of novel soft materials with tailored mechanical properties.

C. Ferreiro-Córdova, E. Del Gado, G. Foffi and M. Bouzid. Multi-component colloidal gels: interplay between structure and mechanical, Soft Matter, 16, 4414-4421 (2020)

Results achieved in the framework of the project MUSA 2017 funded by topic 2 and carried out by Giuseppe Foffi (LPS).

Key publication

T. Marzin, B. Desvages, A. Creppy, L. Lépine, A. Esnault-Filet & H. Auradou. *Using Microfluidic Set-Up to Determine the Adsorption Rate of Sporosarcina pasteurii Bacteria on Sandstone*. Transport in Porous Media.132 283-297 (2020)

V. Martinez, E. Clément, J. Arlt, C. Douarche, A. Dawson, J. Schwarz-Linek, A. Creppy, H. Auradou, and W. C. K. Poon. *A combined rheometry and imaging study of viscosity reduction in bacterial suspensions*. PNAS 117 (5) 2326-2331 (2020)

The PhD grants **NanoWeakGels** covers more specifically the soft matter area, the "Multi-scale Characterization of Bio-Hydrogels", studying the response of gels under stress. It focuses on the production of gels of nanoparticles and proteins for tuning materials properties through adaptable interactions. Colloidal gels under study consist in a homogeneous porous stress- bearing network structure, whose mechanical properties are varied in a controlled manner to rationalize the fate of these gels under stress, to elucidate the complex interplay between the flow of liquid through the pores (poroelasticity), and the fracture of the network. The PhD student develops a multiscale approach that combines indentation testing, image analysis, and characterization at the nanoscale (SANS, SAXS, cryoTEM).

Key publication

M. Léang, D. Lairez, F. Cousin, F. Giorgiutti-Dauphiné, L. Pauchard, and L-T. Lee. *Structuration of the Surface Layer during Drying of Colloidal Dispersions,* Langmuir, 35, 7, 2692–2701 (2019)

During the considered period, a Junior chair (seed funding **InterfAlgues**) was awarded to Gabriel Amselem to study Influence of a liquid / liquid interface on the motility of confined algae in collabor

ation with Mojtaba Jarrahi. The project investigates aspects of the oceans, soils and living beings: those are all habitats for microorganisms where swimming can be strongly influenced by the presence of a solid or liquid interface. These interactions have been widely studied for "pushing" micro swimmers such as bacteria. In the case of "puller" organisms, such as the algae Chlamydomonas reinhardtii, the influence of a solid interface on swimming has recently become available, but the effect of a liquid / liquid interface remains unexplored. The project studies the interaction between Chlamydomonas and liquid / liquid interfaces in microfluidic drops. The size and shape of the drops are systematically varied, and the spatial distribution of Chlamydomonas is determined in each condition. The emergence of collective effects is also quantified in conjunction with the effect of flows and stimuli on the distribution of algae. In addition to their fundamental character, these results can have application on the control of the accumulation of natural and artificial micro swimmers.

A Phase plate contrast for cryo electron microscopy imaging of soft and biological matter was also funded in 2020. The project **PP-SOMATEM** coordinated by Amélie Leforestier, Stéphane Bessanelli et al address the problem of characterizing soft matter and living matter systems that are fragile and sensitive objects, often characterized by complex self- assembled architectures. Cryo electron microscopy (cryoEM) is an essential tool to understand their structure and the interactions at work, complementary to scattering techniques. The project equipped the electron microscope of the LPS with a phase contrast device (Phase Plate), which spectacularly increases contrast. The equipment is used for several other projects, gathering teams of the LPS (SOBIO, MATRIX and MMOI, all members of PALM) and 4 labs of Paris-Saclay campus (I2BC, LIONS-NIMBE, LOB, MICALIS).

The focus topic has also renewed in 2020 the grant PhysBioPS for the conference cycle « Physique des Systèmes Biologiques Paris-Saclay » organized by M. Lenz, and by several other members of the Labex (Cécile Appert Rolland, Eric Raspaud...). This project aims to continue the structuring of the interface with Biology within PALM by continuing regular seminars and conducting new workshops. Since 2013, this initiative has been responding to these unification needs through a range of operations combining regular mobilization at the local level and visible events at the international level: internally, PhysBioPS offers a permanent and regular exchange platform promoting collaborations across borders between laboratories. At the level of the University of Paris-Saclay, PhysBioPS demonstrates the dynamism of the interface with Biology within PALM and promotes its consideration by the other constituents of the university. Nationally and internationally, PhysBioPS highlights this community as a cohesive entity of magnitude worthy of a first-rate multidisciplinary research center and covering many aspects of the Physics-Biology interface.

An example of research at the interface between statistical physics and biological systems is outlined in the hhighlight "Rotation stabilizes living matter".

See Highllight 7 (project SWEET) on the related thematic field

3. Fluids dynamics, instabilities, turbulence

Two projects were funded during the past three years in this area of Focus topic 2, but this repartition is a bit arbitrary because parts of the projects already presented develop scientific interactions with this area. The first one (project OPTFLO) involves a partial PhD grant for the study of the "Optimal paths for the flow of yield stress fluids". The project is carried out by Alberto Rosso and Laurent Talon and it studies yield stress fluids: they can can flow through the soil only above a critical pressure drop. Although ubiquitous and relevant for industry, the laws governing their flow are still misunderstood. Near the critical pressure drop, the liquid flows only along open channels showing strong analogies with the plastic depinning of the vortex lattice in a dirty superconductor or the excited states of directed polymers in random media. The project extends the methods developed in that context to describe the rheology of two protocols relevant for applications providing new clues on a longstanding problem in statistical physics: the glassy transition in finite dimension. The PhD student combines two different approaches: numerical simulations, optimization algorithms and directed polymer physics.

Key publication

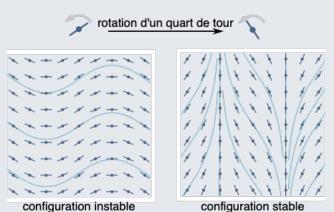
C. Liu, A. De Luca, A. Rosso, and L. Talon. *Darcy's Law for Yield Stress Fluids*. Phys. Rev. Lett. 122, 245502 (2019)

The project **MESOPLANET** within the fluids thematic area funds an IR Camera acquisition for the project "Influence of Mesoscale Structuring on Convection in Complex Fluids: from the Laboratory to the Planets" of Anne Davaille and

Highlight 7. Rotation stabilizes living matter A. Maitra, M. Lenz (LPTMS)

Learning of representations of data stands behind the recent progress in machine learning and paves our way towards artificial intelligence. Certain models for representation learning can be seen as a particular kind of a mean-field spin glasses. Methods stemming from physics of disordered systems turn out as very instrumental in understanding the behaviour of those model both from information-theoretic and computational point of view. This line of study brought up remarkable connections between physical phase transitions and appearance of computational hardness.

To account for this unexpected stability, two researchers as the Laboratoire de Physique Théorique et Modèles Statistiques have theoretically studied the behaviour of a special type of self-propelled object. They focused on objects that are able to autonomously rotate like spinning tops, a characteristic shared by some of the bacteria present in our intestine, as well as the cells that line the inside of our organs. In the presence of small imperfections in their initial arrangement, such particles are always subjected to a combination of the two perturbations illustrated below, and previous theories predict that either one of the two always grows catastrophically, eventually destroying the order of the flock. In their article, published in the journal Nature Communications, the researchers however show that the rapid rotation of their particles allow them to escape this fate by periodically transforming the unstable configurations into stable ones, which stunts their growth. This new mechanism may contribute to a better understanding of our cells, as well as lead to the design principles for artificial active systems able to manipulate objects at the micrometer scale.



The rotation of individual particles causes them to quickly alternate between an unstable bent configuration and a stable splayed configuration.

Reference : A. Maitra, M. Lenz, Spontaneous rotation can stabilise ordered chiral active fluids, Nature Communications 10, 920, (2019)

Results obtained in the framework of the project BioFib (Disordered assemblies of biofilaments: from aggregation to contractility) funded by topic 2 of PALM and coordinated by Martin Lenz (LPTMS)

Christiane Alba-Simionesco. Indeed, rocky planets, icy satellites, lava flows, bacteria solutions, colloidal dispersions and molecular glasses all share an important property: the variation of a control parameter, - such as temperature, light, concentration, or ionic content - , that can induce arrest and/or gelation of their microstructure and a drastic increase of their viscosity. When placed in thick layers under a gradient of the control parameter, they will develop convective motions but also form at the top surface a « skin » with solid-like properties which will affect the large-scale dynamics of the layer. This in turn affects the skin formation and texture. This interplay of the micro-meso-macro

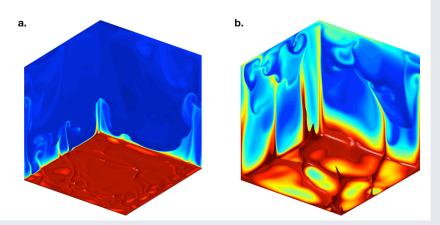
structures governs the evolution of rocky planets through their convective regime. The problem is experimentally modeled using colloidal silica suspensions (Ludox type) and it combines IR Camera acquisition with Neutron tomography, SAXS-SANS, DLS, and rheology.

See Highllight 8 (project ConvRad) on on the related thematic area

Highlight 8. Ultimate regime in radiatively driven convection V. Bouillaut, S. Lepot, B. Miquel, S. Aumaitre, B. Gallet (SPEC)

The heat flux transported by turbulent thermal convection has important implications for geophysical, astrophysical and industrial flows: one seeks a power-law relation Nu \sim Ray, where the Nusselt number Nu represents the dimensionless heat flux and the Rayleigh number Ra characterizes the internal temperature gradients. Decades of investigations of the Rayleigh-Bénard (RB) setup indicate that the heat transport is strongly restricted by boundary layers near the hot and cold solid plates. This prevents the observation of the "ultimate" scaling-regime of thermal convection, where bulk turbulence controls the convective heat flux independently of molecular viscosity and thermal diffusivity. This regime is characterized by a larger scaling exponent, $\gamma = 0.5$.

In contrast to the RB setup, many geophysical and astrophysical convective flows are driven by radiation: absorption of incoming light by a body of fluid induces local heating. We have developed a laboratory experiment that reproduces such radiative heating: a mixture of water and dye contained inside a tank with transparent bottom plate absorbs an incoming upward flux of light. By changing the concentration of the dye, we can tune the thickness of the heating region. For large dye concentration, we heat up the fluid in the immediate vicinity of the bottom plate, in a similar fashion to the RB setup. By contrast, for low dye concentration we heat up the bulk turbulent flow directly, therefore bypassing the boundary layers. This allows us to continuously transition from the RB boundary-layer scaling to the ultimate scaling regime of turbulent convection [1,2]: the exponent γ increases from 0.3 for large dye concentration to 0.5 for low dye concentration. We have proposed a model for the heat transport in this novel radiatively driven convective flow. The model underlines the peculiar role of the Prandit number (ratio of viscous diffusivity to thermal diffusivity), which we confirmed through an extensive study of the parameter space by means of state-of-the-art Direct Numerical Simulations [3].



Snapshots of the temperature field from Direct Numerical Simulations. **a.** The absorption length is much smaller than the thermal boundary layer. The temperature gradients are located in the thermal boundary layer very near the bottom boundary, with narrow plumes seldom penetrating the bulk of the fluid domain. **b.** The absorption length is much larger than the thermal boundary layer: the region of warm fluid extends more in the vertical direction, with taller and wider plumes penetrating the bulk turbulent region.

[1] S Lepot, S Aumaître, B Gallet, Proc Natl Acad Sci (2018) 115 (36) 8937-8941; DOI: https://doi.org/10.1073/pnas.1806823115

[2] V Bouillaut, S Lepot, S Aumaître, B Gallet, J. Fluid Mech. (2019), vol. 861, R5, doi:10.1017/jfm.2018.972

[3] B. Miquel, V Bouillaut, S Aumaître, B Gallet J. Fluid Mech. (2020), vol. 900, R1, DOI: https://doi.org/10.1017/jfm.2020.485

Project ConRad : S. Aumaitre B. Gallet (CEA), A. Davaille (FAST)

Results achieved in the framework of the project ConRad 2017 funded by topic 2 and carried out by Sébastien Aumaitre, Basile Gallet (SPEC) and Anne Davaille (FAST)

Topic 3 "Ultrafast Dynamics: from radiation sources to multiscale responses"

For the PALM Focus Topic 3 community, 2018-2020 has represented a transition phase in its environment, both in terms of administrative and scientific infrastructures.

In the new academic context after January 2020, the PALM Ultrafast Dynamics topic continues to promote collaborative projects within its community, which is very lively

and comparably strong both in the Université Paris-Saclay and in the IPP. In order to adapt to this new context, the Focus Topic 3 bureau composition has also changed, with a partial turnover of its members that guarantees an increased overlap with the Paris-Saclay Physics Graduate School (in particular, but not only, with Pôle 4 of PhOM).

In terms of research infrastructures, during this period the Equipex projects ATTOLAB and CILEX have completed and commissioned their light sources, and have seen their transition towards a new operation phase where the facilities are open to external users. For ATTOLAB, the first user experiment results have been obtained also thanks to PALM support under various forms, as hereafter detailed (*Highlight 11*). APOLLON has also been supported by PALM, and the first user experiments are currently under way.

Overall, Topic 3 has continued its strategy, encouraging the development of new activities by financing novel equipment, supporting young scientists (in particular continuing its support of External Junior Chairs like in the project **MARMOTT**, that aims at developing new research lines at ATTOLAB), and helping its community pursue advanced projects at international facilities like XFEL's.

PALM has also accompanied the general tendency towards a growing importance of theory of out-of-equilibrium states of matter (which is present in all PALM topics but is particularly crucial for Topic 3), by supporting theoretical projects and also by increasing the number of theorists (3) in the bureau of Topic 3.

We hereby present the main actions and results in 2018-2020, organized in five subtopics: 1) Sources 2) UHI/Plasma 3) Gas Phase 4) Condensed Matter 5) Chemical and Biological Matter.

1. Ultrafast laser systems and secondary sources

The development of advanced laser sources and secondary radiation generation is one of the keys to unravel novel ultrafast dynamics phenomena. These last years, several trends can be identified: sources at higher repetition rates (1 kHz up to 1 MHz) delivering more average power, few-cycle sources across the spectrum from the visible to the mid-infrared, sources with an increased control over the parameters such as carrier-envelope phase stability, or optical contrast. These features are often translated to secondary sources properties, opening up possibilities in terms of the processes that can be studied.

PALM has supported several projects in this topic (MIRExpress, FROMAGE), often *providing the seeding funding* required to seek larger budgets that are often necessary in this highly technological domain, in particular on currently hot topics such as spatio-temporal metrology, imaging (STAMPS), and contrast: for instance, it has been possible to improve the temporal contrast on APOLLON by three orders of magnitude (2IMPACTS).

PALM plays an essential role to initiate and accelerate collaborations between laser scientists and physicists that benefit from the use of unique ultrafast laser sources on the Saclay area.

See Highlight 9 (project STAMPS by Hamed Merdji)

Key publication (project 2IMPACTS)

Lucas Ranc, Catherine LeBlanc, Nathalie Lebas, Luc Martin, Jiping Zou, François Mathieu, Christophe Radier, Sandrine Ricaud, Frédéric Druon, Dimitrios Papadopoulos, "*Improvement of the temporal contrast-ratio in the ps range of the multi-PW Apollon laser front-end*", Optics Letters, in press (2020)

HIGH REPETITION RATE FEW-CYCLE SOURCES

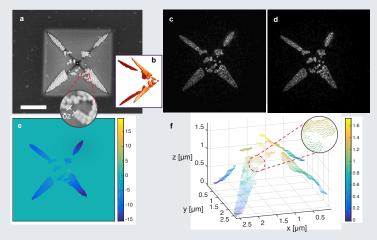
Ultrafast sources based on ytterbium-doped materials are unique in terms of compactness, efficiency, and average power they can deliver. They are used ubiquitously in industrial applications for these reasons. However, the pulse duration is limited by the spectral gain bandwidth to values typically longer than 200 fs.

The **CellComp** project consisted in investigating nonlinear optics in gas-filled multipass cells as a technical solution to temporally compress the pulses with high transmission: compression from 300 fs down to 7 fs (about 2 optical cycles at 1030 nm) with an energy efficiency higher than 60% has been demonstrated. These efficient compression techniques turn industrial-grade ultrafast lasers into ideal drivers for high harmonic generation in gas and solids and applications in attoscience.

Highlight 9. 3D nanoscale imaging with X-ray flashes using computer vision H. Merdji (LIDYL) et al.

Lensless microscopy with X-rays, or coherent diffractive imaging, is a promising approach in imaging. While two-dimensional images can already be created quickly and efficiently, 3D images are still a challenge. Researchers from Hannover, Hamburg, Lisbon and Paris-Saclay have now demonstrated a new imaging technique that enables reconstruction of a three-dimensional image based on a single laser pulse, by combining computer vision and lensless imaging algorithms. The results have been published in Nature Photonics.

At a nanometre scale, the ability to gain insights into the 3D properties of artificial or biological systems is often critical. This information is, however, difficult to retrieve as most techniques provide only two-dimensional projections along the imaging axis. Nowadays, intense ultrashort XUV and X-ray pulses allow realizing nanometre scale studies and ultrafast time-resolved 2D movies. Unfortunately, these existing methods are not easily extended to single shot 3D images. As a rule, a 3D image of an object is generated mathematically from hundreds of individual images. We have now succeeded in significantly accelerating this process by developing a method in which two images of an object can be taken with two twin coherent X-ray beams from two different viewing directions, which are then combined to form a spatial image - similar to how the human brain forms a stereo image from the two slightly different images of the two eyes. The method of computer-aided spatial vision is already established in the field of machine vision and robotics. Here it is used for the first time in the field of imaging with X-rays in 3D at a nanometer scale (see figure).



3D stereo imaging of an arrangement of nanoparticles. a-b, SEM image and respective iso-surface rendering of the test object composed of 50-nm-diameter gold spheres lining the inside of a pyramid-shaped notch lying a 100-nm-thick silicon nitride membrane. The pyramid base has a width of 2.5 μ m and 1.8 μ m of height. The scale-bar length is 1 μ m. The inset in **a** shows a zoom emphasizing a detail of 105-nm depth, δz. c-d, 2D CDI reconstructions, corresponding to 7º-apart views of the sample. Each view reaches a spatial resolution of 42 nm. e, Disparity map of the stereo views in *c-d*. The colour bar represents the disparity in pixels. f, 3D reconstruction of the nano-pyramid, retrieved directly from the disparity maps, without 3D interpolation for surface rendering. The colour bar represents the depth, in μm . The circle displays a zoom of the detail corresponding to the one shown in **a** as an inset. The image is inverted at it is seen from the other side.

J. Duarte, R. Cassin, J. Huijts, B. Iwan, F. Fortuna, L. Delbecq, H. Chapman, M. Fajardo, M. Kovacev, W. Boutu and H. Merdji. *Computed stereo lensless X-ray imaging*, <u>Nature Photonics</u> volume 13, pages 449–453 (2019)

Results achieved in the framework of the project STAMPS funded by topic 3 and carried out by Hamed Merdji (LIDyL).

Key publication (project CellComp)

Lavenu, L., Natile, M., Guichard, F., Délen, X., Hanna, M., Zaouter, Y., & Georges, P., *High-power two-cycle ultrafast source based on hybrid nonlinear compression*. Optics Express, 27(3), 1958 (2019)

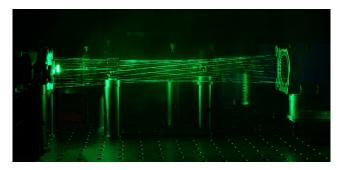


Figure 8. A green laser beam propagates in a multipass cell used for nonlinear temporal compression down to the few cycle regime (project CellComp)

HIGH-HARMONIC GENERATION FROM SOLIDS

Considerable progress in nano-fabrication and ultrafast laser technology have led to the emergence of a new research line, attosecond nanophotonics. Boosting laser fields to the strong field regime in nanostructured photonic devices was shown to generate nano-localized sources of energetic photons or particles, opening up a vast number of applications. Among these phenomena, high-harmonic generation in solids opens new prospects for petahertz optoelectronic devices or compact all solid state EUV sources (projects **HILAC and STAMPS**).

Key publications (projects HILAC and STAMPS)

Gauthier, D., Kaassamani, S., Franz, D., Nicolas, R., Gomes, J.-T., Lavoute, L., Merdji, H., *Orbital angular momentum from semiconductor high-order harmonics.* Optics Letters, 44(3), 546 (2019)

Franz, D., Kaassamani, S., Gauthier, D., Nicolas, R., Kholodtsova, M., Douillard, L., ... Merdji, H. *All semiconductor enhanced high-harmonic generation from a single nanostructured cone*. Scientific Reports, 9(1) (2019)

PLASMA BASED XUV LASERS

Seeding a high-order harmonic pulse to an XUV plasma amplifier is a promising way to generate a high-energy, ultrashort pulse laser beam from a compact experimental system, as compared to large-scale free-electron laser facilities. Recently a dual wavelength operation has been demonstrated in a high-density krypton plasma amplifier seeded with a fs harmonic pulse (project **SONATA**). The two lasing transitions share a common level, which could allow a refined control of their relative intensity and delay.

Key publication (project SONATA)

F. Tissandier, J. Gautier, JP. Goddet, A. Kabacinski, S. Sebban, J. Nejdl, G. Maynard. *Two-Color Soft X-Ray Lasing in a High-Density Nickel-like Krypton Plasma*, Physical Review Letters, 124 (2020)

2. High field laser-matter interaction, plasmas

Ultra-High Intensity (UHI) physics studies the interaction of matter with ultrashort light pulses (3-30 fs) at intensities exceeding 10¹⁸ W/cm². At such intensities, any kind of target is strongly and quasi-instantly ionized to form a plasma. The interaction between the laser pulse and this plasma leads to a rich and original physics. Among its most significant features, electrons in the laser fields reach relativistic velocities on a fs time-scale, and the plasma dynamics is dominated by the collective motion of electrons, driven by the electromagnetic laser field. The latter offer a unique opportunity to control the plasma dynamics by shaping the phase and the amplitude of the laser pulse. Behind a fundamental interest for studying relativistic plasma, UHI physics opens up new perspectives for generating X-ray or particles sources with unique properties. Applications of theses sources range from probing matter on ultra-small time and space scales, to societal applications such as radiotherapy or industrial radiography. Using longer, kJ lasers pulses, laser-plasma interaction can also be used to reproduce in the laboratory astrophysical phenomena: Highlight 10 demonstrates how this approach can be an invaluable tool to interpret astrophysical data, with interesting results obtained at the XFEL with PALM support.

We present here some other examples of research carried out over the past three years on these topics with our labex's support (chairs, post-docs, equipment).

LASER WAKEFIELD ACCELERATION AT KHZ REPETITION RATE

Electric fields in plasma generated with a UHI laser have amplitude of several hundreds of GV/m which allow to accelerate electrons up to 1 MeV over only 10 microns, or up to 1 GeV over 1 cm. Several teams of the LABEX PALM are working on this topic which was recently funded through two projects (ECOLE-ALP and the junior chair OPTIWAVE).

In the OPTIWAVE project, a near-single-cycle, kHz repetition rate laser source has been developed and used for laser-wakefield acceleration at LOA. The control of the Carrier Envelope Phase (CEP) of the laser allowed studying light waveform effects in wakefield acceleration, showing that in this regime the CEP has to be finely tuned for maximizing the beam charge (Figure 9).

Key Publication (project OPTIWAVE)

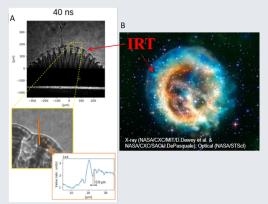
M. Ouillé et al. *Relativistic-intensity near-single-cycle light waveforms at kHz repetition rate.* Light: Science & Applications 9, 47 (2020)

See Highllight 10 (postdoc project IMARES)

Highlight 10. A new path to study astrophysical instabilities and turbulence in the laboratory

Paul Mabey and Michel Koenig (LULI)

The development of experimental methods allowing to obtain accurate information on dense plasmas (> 10^{20} cm⁻³) unreachable using conventional optical techniques, is fundamental in High Energy Density Physics (HEDP), including laboratory astrophysics, inertial confinement fusion research and materials science. They are, for example, based on X-ray absorption of the dense plasma to track density fluctuations. However, the observation of small density structures, due for example, to the emergence and evolution of instabilities, requires extremely high spatial resolution (< 5 µm). Currently, with x-ray produced sources, this value lies between 15 to 30 µm at best, although innovative x-ray techniques giving sub micrometric resolution coupled to a large field of view (~ 1 mm²) are mandatory. During the IMARES project, a collaboration between LULI, LOA and CEA/DIF led to the development of a new X-ray diagnostic to get unprecedented spatial resolution down to ~ 1 µm using a LiF crystal as a detector with also Phase Contrast imaging (PCI). This allowed them to obtain the first turbulent spectrum in HEDP over almost two order of magnitudes at the SACLA XFEL facility. Their technique opens a new path towards a better understanding of chaotic processes, astrophysical instabilities (see Fig. B) and more generally on physical phenomena which are too difficult to model due to the various scale involved.



A. XFEL experiment results showing the development of Rayleigh-Taylor instabilities with spatial resolution of ~ 1 µm. The zoom shows strong PCI feature at the edge of RTI fingers. B. Example of Rayleigh-Taylor instabilities found in the Universe. This is a picture of the supernova remnants SNR E0102.2-72, aged of ~ 1000 years where an analogy with the experiment can be made leading to a better understanding of the evolution of the system

Michel, Th. et al., « Laboratory Observation of Radiative Shock Deceleration and Application to SN 1987A », Astrophysical Journal 888 25 (2020) Mabey, P. et al. Characterization of high spatial resolution lithium fluoride X-ray detectors.

Review of Scientific Instruments 90, doi:10.1063/1.5092265 (2019).

Albertazzi, B., Mabey P. et al. Experimental characterization of the interaction zone between counter-propagating Taylor Sedov blast waves, Physics of Plasmas 27, 022111 (2020)

Results achieved in the framework of the project IMARES funded by topic 3 and carried out by Michel Koenig (LULI)

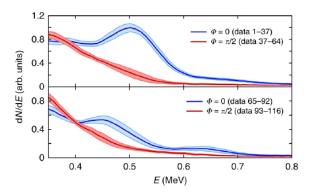


Figure 9. Average electron energy distribution for different CEP values

ELECTRON ACCELERATION AND XUV HHG FROM ULTRASHORT SURFACE PLASMONS

In the framework of a collaboration between LIDYL and the University of Pisa and Consiglio Nazionale delle Ricerche, evidence of surface plasmon enhanced emission of energetic particles and XUV harmonics has been demonstrated. These findings open up new possibilities for new applications, like for instance a useful source of multi-MeV electrons for applications requiring high charge fluxes.

Key Publication (project ECOLE-ALP)

A; Macchi, G. Cantono, L. Fedeli, F. Pisani & Ceccotti, T. *Electron* acceleration and XUV harmonic generation from ultrashort surface plasmons. Physics of Plasmas 26, doi:10.1063/1.5086537 (2019)

SIMULATIONS OF UHI INTERACTION IN THE QED REGIME

The analysis of the UHI physics strongly relies on Particle-In-Cell (PIC) simulations which solve self-consistently Maxwell equations and equation of motion for ion and electron macro-particles. The Junior Chair **SimPLE** led to the development of a new, cutting-edge PIC code, named SMILEI. This open-source code, which is adopted by a growing community, has been intensively used to study Quantum-Electro-Dynamics (QED) occurring when the laser intensity approaches 10²⁹ W/cm². Several experimental schemes – to be tested in the near future - have been proposed for reaching this regime at the Apollon facility, either by colliding an ultra-intense laser pulse with a multi-GeV electron beam generated by wakefield acceleration, or by focusing attosecond pulses from plasma mirrors.

Key Publications (project SimPLE)

Derouillat, J. et al. SMILEI: A collaborative, open-source, multipurpose particle-in-cell slec-consistently simulatescode for plasma simulation. Computer Physics Communications 222, 351-373, doi:10.1016/j.cpc.2017.09.024 (2018)

Niel, F., Riconda, C., Amiranoff, F., Duclous, R. & Grech, M. *From quantum to classical modeling of radiation reaction: A focus on stochasticity effects.* Physical Review E 97, doi:10.1103/PhysRevE.97.043209 (2018)

Niel, F. et al. From quantum to classical modeling of radiation reaction: a focus on the radiation spectrum. Plasma Physics and Controlled Fusion 60, doi:10.1088/1361-6587/aace22 (2018)

3. Gas Phase Matter

Since the typical time scales for electron motion in matter is the attosecond, the new attosecond sources of XUV radiation, as demonstrated at ATTOLAB, have opened fascinating possibilities to study in real time processes such as electron-electron correlation, ultrafast electron relaxation, electron-nuclei couplings in various species. At Paris-Saclay, a very active community investigates the dynamics of gas phase at attosecond time scales, essentially with XUV–IR interferometric measurement.

XUV-IR ATTOSECOND INTERFEROMETRY

Within PALM, a unique know-how exists on "electronic wave packets quantum interferometry", such as the so-called reconstruction of attosecond beating by interference of twophoton transitions (RABBITT). In the past three years, it has been extended in two main directions: the full description of RABBITT signals in oriented or isotropic systems ; and the development of the "Rainbow RABBITT" technique, which allows to probe the dynamics of resonances as they build up. Barreau et al. have measured the spectral phases of Ne **XUV-MIR** autoionizing states from attosecond interferometric observation (Figure 10) and full-electron ab initio calculations, by using an extension of the Fano model of atomic resonances.

See Highllight 11 (postdoc project ImDynCo)

Key Publications (project IMAPS)

L. Barreau et al. Disentangling Spectral Phases of Interfering Autoionizing States from Attosecond Interferometric Measurements. Physical Review Letters 122 (2019)

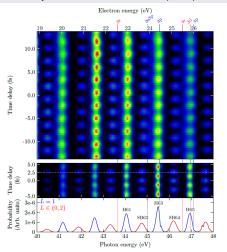
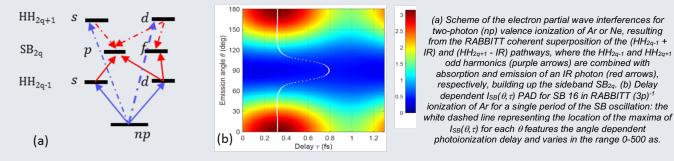


Figure 10. RABBITT spectrogram of Ne photoelectron as a function of the delay _ between the XUV and the IR pulses, measured (upper panel) and TD-XCHEM calculated (central panel). The lower panel shows the contributions of states of different symmetries to the calculated photoelectron spectrum for a time delay of 2:5 fs. The positions of the Ne resonances are indicated by blue (¹P^osymmetry) and red (¹S^e and ¹D^e symmetries) vertical lines.

Highlight 11. Angle resolved studies of time-delays in XUV-IR two photon ionization at ATTOLAB using electron-ion coincidence momentum spectroscopy

J. Joseph, F. Holzmeier, J.C. Houver, D. Dowek (ISMO), D. Bresteau, C. Spezzani, T. Ruchon, J.F. Hergott, O. Tcherbakoff, P. D'Oliveira (LIDYL)

The advent of attosecond technologies with ultrashort XUV pulses, has paved the way to real-time observation of the electron dynamics governing the fundamental processes of photoionization or photoemission [1]. At the new ATTOLAB facility on the Paris-Saclay campus, new results for angle resolved valence ionization of Ar and Ne in the XUV-IR two photon RABBITT (Reconstruction of attosecond beating by interference of two photon transitions) scheme have been demonstrated. Electron-ion coincidence 3D momentum spectroscopy has been implemented at the FAB10 beamline which generates Attosecond pulse trains (APT) at 10 kHz repetition rate. Together with a general formalism synthesizing the photoelectron angular distribution (PAD). These results provide a benchmarking of the COLTRIMS gas-phase endstation on FAB10 [2]. Future experiments will address real-time photoionization studies of small molecules, where the time-delays will be angle resolved in the molecular frame (MFPADs) [3], complementary to spectrally resolved MFPAD performed at SOLEIL [4].



We dedicate this work to the memory of our colleague and friend Bertrand Carré, coordinator of the Attolab Equipex project.

[1] R. Pazourek, S. Nagele and J. Burgdörfer, Attosecond chronoscopy of photoemission, Rev. Mod. Phys. 87, 765 (2015)

[2] J. Joseph et al, Angle-resolved studies of XUV-IR two-photon ionization in the RABBITT scheme, J. Phys. B. (2020)

[3] P. Hockett, E. Frumker, D.M. Villeneuve and P.B. Corkum, Time delays in molecular photoionization, J. Phys. B 49, 095602 (2016)

[4] K. Veyrinas et al, Dissociative photoionization of NO across a shape resonance in the XUV range using circularly polarized synchrotron radiation, J. Chem. Phys. 151, 174305 (2019)

Results achieved in the framework of the project ImDynCo funded by Topic 3 and carried out by the team led by Danielle Dowek (ISMO) and Thierry Ruchon (LIDYL)

DISSOCIATIVE IONIZATION

Tracking in real time the formation and dissociation of chemical bond is one of the ultimate goals pursued by physical chemists. One of the ways to reach this goal is by studying the dissociative ionization of molecules. PALM has supported this activity in various forms: by financing postdocs (Fabian Holzmeier within ImDynCo has studied the role of vibrational degrees of freedom during the dissociation of a chemical bond at the FERMI XUV FEL) as well as external visitors. During a three months stay of Prof. A. Z. Khoury at LIDYL (CHABLIS project), his team and T. Ruchon's group investigated non linear phenomena involving light beams carrying Orbital Angular Momentum, in both the perturbative and non perturbative regimes. The established connection between the two teams is now exploited to generalize these properties to the highly non linear regime of high harmonic generation. Furthermore, a tight collaboration between theorists (Robert Lucchese) and experimentalists (Pascal Salières) made it possible to define optimal generation condition for ultrashort circularly polarized high harmonics: this will advance studies of chiral sensitive light matter interaction such as chiral recognition. Finally, a new two-color scheme has been financed to study the dissociation dynamics for aligned small molecules (CoMoDyn project).

Key publications (projects ImDyCo and CHABLiS)

Holzmeier, F. et al. Control of H-2 Dissociative Ionization in the Nonlinear Regime Using Vacuum Ultraviolet Free-Electron Laser Pulses. Physical Review Letters 121, doi:10.1103/PhysRevLett. 121.103002 (2018)

Barreau, L. et al. Evidence of depolarization and ellipticity of high harmonics driven by ultrashort bichromatic circularly polarized fields. *Nature Communications* **9**, doi:10.1038/s41467-018-07151-8 (2018)

W. T. Buono , A. Santos, M. R. Maia, L. J. Pereira, D. S. Tasca, K. Dechoum, T. Ruchon, and A. Z. Khoury Phys. Rev. A 101, 043821 (2020)

4. Condensed matter

Recent years have seen a growing interest around the ultrafast properties of solids optically excited far from equilibrium. By shining the sample with intense ultra-fast pump pulses one can trigger non-equilibrium transient states, whose properties can be intrinsically different from the equilibrium ones. Our understanding of these transient states of quantum matter is progressing thanks to novel experimental approaches combined with the development of original theoretical methods. The activity in the PALM community covers several research lines (electron and structural dynamics, theory) on various systems and materials (charge density waves, semiconductors, 2D materials, Dirac and topological systems).

Over the last years, PALM contributed to this activity by financing young scientists (PhD students, postdocs, and young principal investigators): in particular, we would like to point out the External Junior Chair project **MARMOTT** (funded in 2020), supporting the project of a young researcher (Romain Géneaux) for the development of attosecond scale studies of Mott insulators on the ATTOLAB platform. Selected results are presented here below.

ULTRAFAST ELECTRON DYNAMICS

In the postdoc project **UDINI**, advanced spectroscopic measurements in both time and frequency domains have been used to investigate the ultrafast scattering of hot carriers at the surface of two dimensional materials and ultrafast charge transfer at the interface of heterostructures. These are the key processes that ultimately determine functional limits and properties in potential applications, such as switching and optoelectronic devices, energy storage and nanodevices.

See Highllight 12 (postdoc project UDINI)

PALM also supported young principal investigators, providing seeding money for a new setup in the project **UPSTAIRS.**

ULTRAFAST STRUCTURAL DYNAMICS

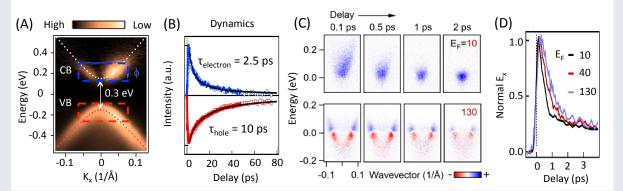
Ultrafast x-ray diffraction and ultrafast electron diffraction (UED) are ideal techniques for obtaining valuable information on structural dynamics at the atomic scale (Figure 11Figure 11Figure 11). The use of UED in pump-probe experiments has proven to be very efficient for studying the dynamics of photoinduced phase transitions by measuring the relative changes of the diffraction pattern following photoexcitation. During her PhD (PALM project **SLIDING**) Izabel González-Vallejo performed UED experiments on high quality single crystals of silicon and revealed a giant photoinduced response which can only be explained in the framework of dynamical diffraction theory, taking into account multiple scattering of the probing electrons in the sample and thus going beyond the well-known Debye-Waller effect.

Highlight 12. Time resolved ARPES studies of out-of-equilibrium 2D materials Zhesheng Chen, Luca Perfetti (LSI), Jean-Pascal Rueff (SOLEIL) and Marino Marsi (LPS)

Time-resolved ARPES makes it possible to directly visualize the band dispersion and the hot carrier dynamics in photoexcited solids with both high energy and time resolution. This opens unprecedented opportunities to manipulate the electronic structure of solids, using controllable parameters such as photon pulses or surface doping. In our project, we demonstrated this approach for selected 2D materials, using time-resolved ARPES as well as methods based on hard X-ray photoelectron spectroscopy to follow the lifetime and dynamical evolution of their excited states, and interpreting the results with theoretical models and calculations.

In black phosphorus, the photoexcited conduction band can be visualized at delays of 1ps as shown in Fig. A. Despite the low bandgap value, no relevant amount of carrier multiplication and negligible bandgap renormalization could be detected at excitation density 3-6×10¹⁹ cm⁻³. In Fig. B, the corresponding cooling processes of hot electrons and holes are monitored. Astonishingly, a Stark broadening of the valence band takes place at an early delay time because of inhomogeneous screening of near surface fields after photoexcitation [1].

The band gaps of black phosphorus and indium selenide as function of electron doping are monitored by time-resolved ARPES and soft x-ray ARPES. Moderate-gap semiconductor to band-inverted semimetal transition is observed in black phosphorus [2] and a ~120 meV band gap reduction is found in InSe semiconductor [3]. The electronic states and distribution function of hot electrons in the accumulation layer of InSe are directly monitored by time resolved ARPES. We investigated the low energy excitations of a quasi-2D electron gas with variable carrier density (Fig. C and D). The comparison of the experimental results to model calculations of screened Fröhlich interaction allows us to identify and quantify the effects of a remote electron-phonon coupling.



[1] Z. Chen, J. Dong, E. Papalazarou, M. Marsi, C. Giorgetti, Z. Zhang, B. Tian, J.-P. Rueff, A. Taleb-Ibrahimi and L. Perfetti, Nano Letters, 19 (1), 488-493 (2019)

[2] Z. Chen, J. Dong, C. Giorgetti, E. Papalazarou, M. Marsi, Z. Zhang, B. Tian, Q. Ma, Y. Cheng, J.-P. Rueff, A. Taleb-Ibrahimi and L. Perfetti, 2D Materials, 7, 035027 (2020)

[3] Z. Chen, J. Sjakste, J. Dong, A. Taleb-Ibrahimi, J.P. Rueff, A. Shukla, J. Peretti, E. Papalazarou, M. Marsi, L. Perfetti, Proc. Natl. Acad. Sci. USA 202008282; DOI: 10.1073/pnas.2008282117 (2020)

Results achieved in the framework of the project UDINI funded by topic 3 and carried out by Jean-Pascal Rueff (SOLEIL), Luca Perfetti (LSI) and Marino Marsi (LPS)

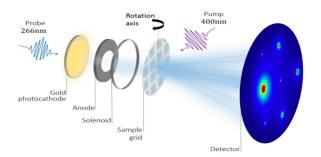


Figure 11. The ultrafast electron diffraction setup at LOA

Key Publication (project SLIDING)

I. González Vallejo et al, Observation of large multiple scattering effects in ultrafast electron diffraction on monocrystalline silicon, Phys. Rev. B 97, 054302, (2018) https://doi.org/10.1103/PhysRevB.97.054302

THEORY OF NON-EQUILIBRIUM QUANTUM MATERIALS

On the theoretical front a major open frontier of condensed matter is the development of novel conceptual and methodological tools to describe the out-of-equilibrium physics of electrons and phonons in optically excited solids. The PALM community has contributed to this development, both from the point of view of ab-initio studies as well as from the point of view of many body calculations on model Hamiltonians [Peronaci2018]. The FEMTONIC project, for example, aims at a detailed understanding of the energy relaxation processes, an important step in the search for new materials. Using a combination of state-of-the-art ab initio calculations and time-, energy-, and angle-resolved spectroscopy experiments, it is shown that the main mechanism governing the hot-carrier relaxation in GaAs is the electron-phonon interaction. The temperature dependence of the relaxation time is also calculated using and the agreement between theory and experiment is excellent.

Key Publication (project FEMTONIC)

Sjakste, J. *et al.* Energy relaxation mechanism of hot-electron ensembles in GaAs: Theoretical and experimental study of its temperature dependence. *Physical Review B* **97**, doi:10.1103/PhysRevB.97.064302 (2018)

The **UFEX** project (Ultrafast Processes and Excitonic Effects), recently funded in the 2020 call, aims to provide an efficient and precise theoretical description of ultra-fast processes in condensed matter. The influence of excitonic effects in semiconductors will be studied in relation with pump-probe experiments conducted at the ATTOLAB facility.

5. Chemical and biological systems

The understanding of chemical and biological fundamental processes benefits greatly from the development of advanced ultrafast spectroscopy set-ups combined with theoretical and computational studies. Experimentally, novel studies of ionized species in G-Quadruplex DNA structures

provided access to transient species have and conformational motions (OSPEG), while in the XUV domain, ultrashort pulses can characterize disordered biological structures and their dynamics (BIOPIX). From the theory perspective, efforts are directed in two major directions: achieving an ab initio description of the systems of interest, (OSPEG, Dyn-OC2H4), and constructing realistic models in order to capture elusive quantum-mechanical effects that might be important even in biological environments at ambient conditions. The action of PALM in this domain reflects this general tendency, through the support of young principal investigators (OSPEG, Dyn-OC2H4) and of postdocs (NanoDyn, BIOPIX): we hereby present recent results as examples of this action.

AB INITIO CALCULATIONS AND TIME-RESOLVED OPTICAL STUDIES OF G-QUADRUPLEXES

Four-stranded DNA structures (G-quadruplexes) are intensively studied because of their involvement in many biological processes and as promising architectures for molecular electronics. Quantum-chemistry calculations based on TD-DFT, together with a QM/MM (Quantum Mechanics / Molecular Mechanics) description of the complex environment, allow for the interpretation of timeresolved optical spectroscopy on DNA (absorption, fluorescence, circular dichroism), in particular of the evolving transient species (Figure 12) and the associated conformational DNA changes following UV photo-excitation.

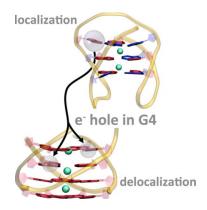


Figure 12. Time-resolved experiments and calculations were used to study the spectral properties of the ionized species created by UV light in G-quadruplexes. The figure shows that adopting an antiparallel structure, such as human telomere, the electron hole is localized on a single guanine. In parallel structures, the hole can be delocalized over two guanines.

Key publications (project OSPEG)

L. Martinez-Fernandez, P. Changenet, A. Banyasz, T. Gustavsson, D. Markovitsi, and R. Improta, Comprehensive Study of Guanine Excited State Relaxation and Photoreactivity in Gquadruplexes, J. Phys. Chem. Lett. 10, 6873-6877, doi:10.1021/acs.jpclett.9b02740 (2019)

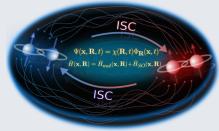
A. Banyasz, L. Martínez-Fernández, R. Improta, T. Ketola, C. Balty and D. Markovitsi, Radicals generated in alternating guaninecytosine duplexes by direct absorption of low-energy UV radiation, Phys. Chem. Chem. Phys. 20, 21381-21389, doi: 10.1021/acs.jpcb.9b02637 (2018)

Highlight 13. Spin-orbit interactions in ultrafast molecular processes F. Talotta (ICP & ISMO); F. Agostini & D. Lauvergnat (ICP), S. Morisset & N. Rougeau (ISMO)

Internal conversion and intersystem crossing are competitive non-radiative ultrafast relaxation processes determining the fate of photo-excited molecular systems. Theoretical and computational studies aiming to provide a realistic description of these processes need to account, consistently, for both effects. The goal of Dyn-OC2H4 is to propose, implement and test a novel algorithm for internal conversion and intersystem crossing based on the study of the collision dynamics of O(³P) and ethylene.

Photo-induced ultrafast phenomena or collision reactions involving electronic excited states are often studied based on trajectory-based molecular-dynamics methods. After the electronic excitation, the molecule can relax to the ground state via radiationless channels such as the spin-allowed - internal conversion, i.e., through a path involving electronic states with the same spin multiplicity. Analogous ultrafast phenomena can be observed in systems with "large" spin-orbit coupling, where the non-radiative - spin-forbidden - process is then called intersystem crossing, if it involves states of different spin. Encountering intersystem crossings might seem likely only in the presence of heavy nuclei, since the spin-

orbit coupling is a relativistic correction to the molecular Hamiltonian. Nonetheless, intersystem crossings have been observed in processes involving light-element species, like the collision reaction of O(³P) and ethylene, thus proving that the strength of spin-orbit coupling depends on the shape of the electronic potential energy landscape and, consequently, on the molecular geometry. Therefore, a theory that is able of treating internal conversion and intersystem crossing on equal footing, without an a priori knowledge of the relative importance of the two effects, is highly desirable, especially for the study of ultrafast dynamics in complex molecular systems.



In Dyn-OC2H4, we developed a new theoretical and computational framework to study internal conversion and intersystem crossing on equal footing, based on the exact factorization of the electron-nuclear wavefunction. See references below.

F. Talotta, S. Morisset, N. Rougeau, D. Lauvergnat, F. Agostini. Spin-orbit interactions in ultrafast molecular processes, Physical Review Letters 124. 033001 (2020)

F. Talotta, S. Morisset, N. Rougeau, D. Lauvergnat, F. Agostini, Internal conversion and intersystem crossing with the exact factorization, J. Chem. Theory Comput., doi: 10.1021/acs.jctc.0c00493 (2020)

Results achieved in the framework of the project Dyn-OC2H4 funded by topic 3 and carried out by Federica Agostini and David Lauvergnat (ICP, UPSaclay) and Sabine Morisset and Nathalie Rougeau (ISMO, CNRS).

NEW THEORETICAL AND COMPUTATIONAL Δ FRAMEWORK TO STUDY INTERNAL CONVERSION AND INTERSYSTEM CROSSING

The collision reaction of ground-state oxygen O(³P) with ethylene C₂H₄ encloses all the relevant and most challenging features of excited-state dynamical phenomena. The ab initio simulation of the process requires to capture the coupling among electronic states with different spin multiplicity, i.e., intersystem crossings, along with standard avoided crossings and conical intersections among singlet states (internal conversions). In the framework of Dyn-OC2H4 a new theoretical and computational strategy to

describe intersystem crossings and internal conversions on equal footing has been devised, and is based on the "mixed" description of the molecular systems adopting quasiclassical nuclear trajectories that are coupled to quantummechanical electrons.

See Highllight 13 (postdoc project Dyn-OC2H4)

The procedure is currently being applied for the first, fully ab initio investigation of the collision process of atomic oxygen and ethylene

Topic 4 "Emergence, Evolution, Rapid Reaction"

The board of the "Emergence and Interfaces" axis has been renewed during the period 2018-2020 in order to cover the widest possible field of competences.

It should be noted that the ultra high resolution imaging projects of biological systems "in vivo" or "in vitro" have reached a stage of strong maturation and are currently in a dynamic of development, such as the **DEEPIM** project, for in-depth microscopy of biological tissues.

See Highlight 14 (project DeepIM by Frédéric Druon)

In this period, where the available funds were less than in previous periods, the projects supported concerned the following fields 1) new materials and their characterization 2) physico-chemistry 3) biophysics 4) plasmas 5) metrology 6) study of interfaces. These projects have deepened the collaborations or weaved other ramifications between Palm and Saclay Plateau teams.

1. New Materials and their Characterization

Developments in materials science require advanced analytical methods which are made possible by the rich instrumental environment available within the perimeter of the University of Paris Saclay and the Institut Polytechnique de Paris. Promising results have been obtained by the **REMI** project which investigates the possibility to control the Eu³⁺

environment in different metaphosphate or polyphosphate glasses uner irradiation.

See Highlight 15 (project REMI by Nadège Ollier)

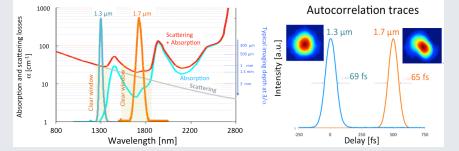
The **HOPIRR** project studies the role played by defects in the optoelectronic properties of perovskites, paving the way for defect engineering.

See Highlight 16 (project HOPIRR by Olivier Plantevin)

Highlight 14. First demonstration of dual-color 3-photon non-linear microscopy

F. Druon, K. Guesmi, K. Jurkus, P. Rigaud, M. Hanna, P. Georges (LCF), E. Beaurepaire, L. Abdeladim, P. Mahou, W. Supatto (LOB), S. Tozer, J. Livet (Institut de la Vision).

One of the most challenging topics in optical microscopy consists in imaging deep inside biological tissues with high resolution. In addition, there is an ongoing trend toward the development of microscopes enabling the monitoring of several parameters on simultaneous independent channels. Since its introduction in the 90s, multi-photon imaging has made tremendous progress and has become the gold standard for deep/live fluorescence microscopy of biological tissues. This approach currently delivers subcellular resolution imaging in intact tissues at depths of a few hundreds of micrometers. However, the imaging depth remains a crucial limitation in heterogeneous and scattering tissues such as the brain and nervous tissues. To overcome this limitation and access to deeper areas, one very promising approach consists in using three-photon instead of two-photon excitation, while shifting the excitation to the SWIR (Short-Wavelength InfraRed) range. Indeed, scattering decreases with increasing wavelength, following a typical 1/ λ^3 law. However water absorption should be avoided to prevent tissue from heating; so 1300 and 1700 nm were recently shown (C. Xu et al, Cornell Univ., NY) to be optimal spectral exitation regions, offering the best compromise in terms of minimal scattering and absorption (fig). Efficient three-photon microscopy however requires MHz pulse trains of µJ-range pulses with sub-100fs durations. In 2017, we introduced and developped a novel laser source exceptionally suited for this pupose, providing 70 fs pulses at a repetition rate of 1.25 MHz and with energies in the µJ range. This new source is based on a robust OPCPA (optical parametric chirped pulse amplifier) injected by a highpower Yb-fiber system. One unique feature of our innovative design is that it emits simultaneously two beams at the two optimal 1.3 and 1.7 µm wavelengths. These wavelengths are suitable for exciting respectively GFP and RFP, two of the most widely used biological labels. We used our source to image dual-labeled chick spinal cords, and therefore achieve the first demonstration of dual-color 3PE microscopy, along with simultaneous detection of third-harmonic generation signals on a third channel (see figure). Moreover, through-skull in vivo imaging in adult zebrafish brain has been performed using simultaneous dual color 3PEF and THG z. Besides providing innovative multicolor 3P excitation, our laser design outperforms alternative available sources in each 1300-and-1700-nm band. We also demonstrate the suitability of our dual-source for simultaneous in-depth high-quality multicolor 3P imaging of GFP-RFP labeled tissue along with label-free third-harmonic generation. This work is therefore the first demonstration of dual-color 3-photon imaging based on fluorescent proteins.



Optimal transparency spectral ranges for 3-P microscopy in biologically tissues such as brain. The blue axis represents the typical related maximum imaging depth. The blue and orange curves at 1.3 and 1.7 μm correspond to the measured spectra from aour laser source. (right) Corresponding autocorrelation traces and beam profiles at maximum energy.

Guesmi, Abdeladim, et al, Dual-color deep-tissue three-photon microscopy with a multiband infrared laser (2017)

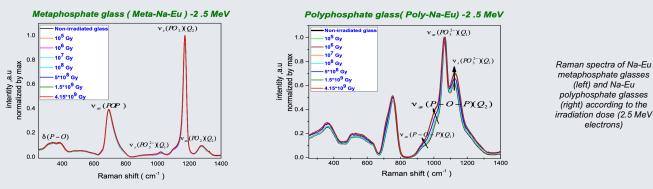
Patent application 1755167 (filed June 9th 2017): Source laser ultrabreve pour l'excitation multiphotonique multicouleurs dans l'infrarouge moyen

Results achieved in the framework of the project DEEPIM funded by topic emergence and carried out by Frédéric Druon (LCF) and Emmanuel Beaurepaire (LOB)

Highlight 15. Europium environment modification by electron irradiation in phosphate glasses

M. Mahfoudhi, N. Ollier (LSI), M. Lancry, T. Billotte (ICMMO)

Phosphate glasses present a lot of advantages for optical applications mainly due to the high content of Rare Earth (RE) ions that can be incorporated in their network. In this PhD work, we investigate the possibility to control the Eu³⁺ environment in different metaphosphate and polyphosphate glass compositions under irradiation. We study the mechanism leading to the evolution of the glass by comparing the impact of High energy electron and fs laser. Using SIRIUS Accelerator, glasses were irradiated with electrons of 2.5 MeV at various doses. We observe in figure 1 that there is no important change of the metaphosphate glass structure whatever the integrated dose contrary to polyphosphate glasses that show significant change (glass depolymerization) of the vitreous network from 108Gy.



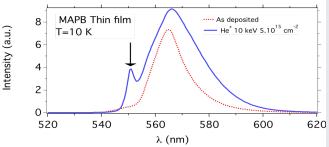
M. Mahfoudhi, N. Oilier, Tuning Eu²⁺ amount and site symmetry in phosphate glasses under irradiation by electron energy and integrated dose. Optical Materials 95, (2019)

Results achieved in the framework of the project REMI funded by topic emergence and carried out by Nadege Ollier & Kees Van-Der-Beek (LSI)

Highlight 16. What is the role played by defects in opto-electronic properties of hybrid perovskites?

O. Plantevin, D. Guerfa, S. Valère (CSNSM), E. Deleporte, H. Diab, G. Trippé-Allard, F. Lédée (LAC), D. Garrot (UVSQ, GEMaC)

Defects are usually seen as imperfections in materials that could significantly degrade their performance. However, defects could be extremely useful since they could be exploited to generate innovative materials and devices. Defect engineering is applied to hybrid organic-inorganic perovskites (HOP) with 3D and 2D structures, with strong light emitting properties. HOP materials have become one of the most promising lowcost alternatives to traditional semiconductors in the field of photovoltaics and light emitting devices. The objective is to use ion irradiation as a tool for the introduction of point defects in a controlled manner. Both strain and defects energy levels will modify the electronic and light emitting properties of the materials. We want to study how these properties are modified in order to get knowledge about the role that defects might play in these materials where "self-healing" mechanisms were proposed.



Photoluminescence measured at 10 K of a thin film of (CH₃NH₃)PbBr₃ before (dashed) and after Helium ion irradiation at an energy of 10 keV and a fluence of 5.10¹⁵ cm⁻² (continuous line). The excitation is a continuous Argon laser at 488 nm

(left) and Na-Eu

electrons)

We use Helium ion irradiation in the range 10-30 keV as a tool for the introduction of point defects in a controlled way. At low fluences, mainly point defects are created that introduce energy levels and modify the electronic and light emitting properties of the materials. Contrary to usual semiconductors, like crystalline silicon for instance, where irradiation defects act as recombination centers for the electron-hole pairs and quench very efficiently the luminescence, we observe here an enhancement of the optical emission at low temperature as shown in Figure 1 for a thin polycrystalline film of (CH₃NH₃)PbBr₃. We can deduce from this observation that irradiation defects act as active optical centers, essentially in the low-temperature orthorhombic phase as seen in the dependence of the total photoluminescence yield. Another effect of the ion irradiation directly observable is the emission through new excitonic processes, as indicated by the arrow in Fig.1 showing a new feature at 550 nm after Helium ion irradiation. The temperature dependence of the spectra is under analysis and evidences light amplification after ion irradiation at low temperature. These behaviours are very intriguing and need further studies for a better understanding of the specificity of defects and their impact over opto-electronic properties in HOP materials.

O. Plantevin, D. Guerfa, S. Valère, E. Deleporte, D. Garrot, H. Diab, G. Trippé-Allard, F. Lédée, Photoluminescence of defects in hybrid organicinorganic perovskites, (under preparation)

O. Plantevin et al., Photoluminescence Tuning Through Irradiation Defects in CH3NH3Pbl3 Perovskites. Physica Status Solidi B-Basic Solid State Physics 256, (2019)

Results achieved in the framework of the project HOPIRR funded by topic emergence and carried out by Olivier Plantevin (CSNSM), Emmanuelle Deleporte (LAC) and Antonio Tejeda (LPS)

The **HOP-GIFAD** project is a device capable of monitoring, under vacuum and in real time, the growth of thin layers of hybrid organic-inorganic perovskites (HOP), exploiting the capability of the GIFAD (Grazing Incidence Fast Atom Diffraction) method. This will provide very detailed information on the growth mode and phase transitions. This technique, developed at ISMO and validated on the crystallization dynamics of an organic monolayer, will allow the elaboration of very good quality HOP layers while providing a better understanding of the tetragonal-cubic phase transition observed above 50°C.

2. Physical Chemistry

Physical chemistry is very present in the Labex Palm community. Some of the experiments benefit from ultrafast laser installations and are part of the Focus Topic 3-Ultrafast Dynamics (e.g. **SPACE** project). Other investigations are part of studies that seem more traditional, but which are

pushed to the best of the state of the art, giving remarkable results and answering questions that are still relevant today.

The **MACO-GT** project is dedicated to the study of large, open-layer astrophysical molecules in order to feed the databases that will allow astrophysicists to search and detect them in the spectra of radio telescopes. It began with the spectroscopy of the CH2OH* radical.

See Highlight 17 (project MACO-GT by Laurent Coudert)

Key publication

O; Chitarra, M-A. Martin-Drumel, B. Gans, J.-C. Loison, S. Spezzano, V. Lattanzi, H. Müller, and O. Pirali, *Enabling CH2OH interstellar detection : Re-investigation of the rotation-tunneling spectrum of the radical*, Astronomy and Astrophysics (2020)

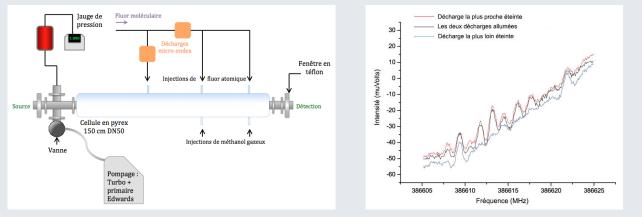
The other projects focus more directly on the study of molecular radicals or excited states of molecules in dilute phase or in interaction with a condensed phase.

Highlight 17. Large open-shell molecule of astrophysical interest L. Coudert, B. Gans, M.-A. Martin, O. Pirali (ISMO, UPSud)

This project aims at building high-resolution spectroscopic data bases for open-shell molecules of astrophysical significance. Spectroscopic results are still missing for such molecules because they are experimentally and theoretically more difficult to deal with than closed-shell molecules. These data bases should allow us to interpret radio astrophysical spectra and in some cases to carry out their first detection in the interstellar media. The present project includes experimental developments and theoretical research. One of the target molecules is the non-rigid open-shell radical CH₂OH⁺, which was recently detected in the lab.

Results: Our sub-millimeter-wave spectrometer has been upgraded and the spectra of several new molecules could be observed for the first time including ethynethiol (HCCSH) which is a metastable isomer of thioketene [1].

With the help of Jean-Christophe Loison (ISM, Bordeaux), we built a cell to produce the CH₂OH[•] and CH₃O[•] radicals by H atom abstraction, using methanol and atomic fluorine as precursors. This cell, shown on the left panel of the figure below, is 150 cm long and atomic fluorine, produced by a 2450 MHz microwave discharge, is injected through several holes so as to optimize radical production. The experimental signal of CH₂OH[•] was optimized varying discharge and gas flux conditions. The sub-millimeter-wave spectrum recorded near 386610 MHz is shown on the right panel of the figure below. The best signal is obtained with two injectors as the hyperfine structure of the $J = 8.5 \leftarrow 7.5$ transition can then clearly be seen.



A major result has since been obtained with this new experimental setup as more than two hundred new transitions of CH₂OH[•] could be recorded and assigned in terms of rotational-spin quantum numbers [2].

Theoretical results concerning the potential energy surface of CH_2OH were also obtained. It displays 8 saddle points including four equivalent C_1 symmetry minima, two local maxima, and two C_{2v} absolute maxima. The 2 lowest lying vibrational states display tunneling splittings of 0.035 à 44.809 cm⁻¹. These results are being used to develop a theoretical model allowing us to account for the spin-rotation coupling, the large amplitude motion effects and the hyperfine coupling.

[1] Gas phase detection and rotational spectroscopy of ethynethiol, HCCSH, Lee, Martin-Drumel, Lattanzi, McGuire, Caselli, and McCarthy, *Mol. Phys.* **117**, 1381–1391 (2019)

[2] Enabling CH₂OH interstellar detection: Re-investigation of the rotation-tunneling spectrum of the radical, Chitarra, Martin-Drumel, Gans, Loison, Spezzano, Lattanzi, Müller, and Olivier Pirali, submitted to Astronomy & Astrophysics (2020)

Results achieved in the framework of the project MACO-GT funded by topic emergence and carried out by Laurent Coudert (ISMO)

The excitation of triplet states of organic molecules remains a challenge that the **SPECTROTRI** project proposes to take up, with molecules deposited on a helium drop or a para-H2 matrix.

Singlet oxygen is of crucial importance in dynamic phototherapy. Its formation by interaction with organic molecules in a triplet state will be studied in project TESLA in a cooled ion trap, using negative ions analogous to porphyrins.

The photoionization of radical species of astrophysical interest will allow, thanks to the SPIRUV project, to obtain new data on the ro-vibronic structure of radical cations.

The **Discover** project will be distinguished within the framework of the policy of the fight against global warming. It proposes to test a novel method using ionizing radiation to convert carbon dioxide into oxalate. This proposal allows a very clever use of radiation from nuclear waste, as carbon dioxide dissolves very easily in the water of the spaces where it is stored.

The **SPACE** project aims at obtaining vibrational and electronic structure data with unprecedented precision on several prototypical molecules of the chlorophyll family in view of apprehending some essential details of the charge separation within the reaction center Photo system II.

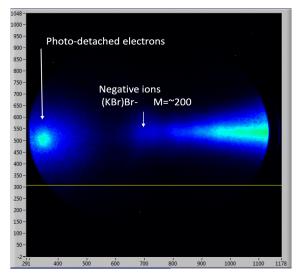


Figure 13. simultanous trace of (KBr)nBr– anions - and the photo ejected electron by a 355 nm laser

Key publication

F. Grollau , C. Pothier, M. A. Gaveau , M. Briant , N. Shafizadeh , and B. Soep , Action spectroscopy of spin forbidden states in the gas phase: A powerful probe for large non-luminescent molecules J. Chem. Phys. 152, 144306(2020)

3. Biophysics

The **3DLIghtChain** project proposes a biomimetic approach for the determination of the structure of a small membrane subunit (p22phox) of the superoxide-generating NADPH oxidase using mainly a lipidic cubic phase medium

as the crystallization environment. These phases constitute an excellent biomimetic tool for the organization, containment and crystallization of membrane proteins. Currently there is no consensus on the topology of the small p22phox protein within the lipid bilayer. Hydrophobicity profiles reveal an organization with 2, 3 or 4 transmembrane helices in addition to an extended extracellular loop. The objective will be to obtain crystals of peptide segments specifically selected from the p22phox sequence in order to determine its crystalline structures with X-rays. The project will focus on the factors contributing to the success of the crystallization of the selected transmembrane peptides in the mesophases with the aim to reconstitute the p22phox protein in its entirety and thus remove the ambiguity on the 3D organization of this protein.

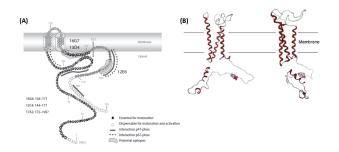


Figure 14. Topologies of the p22phox protein : (A) p22phox model with two transmembrane domains based on several biochemical analysis. (B) in silico prediction of p22phox with three transmembrane domains.

4. Plasmas

Projects supported cover the fields of cold and hot plasmas. The composition and temporal evolution of cold plasmas are determined by collision processes involving neutrals and ions, for a part of radical or excited species, for which the products and efficiency are poorly characterized. The ERACOP project aims to develop emerging techniques to determine in a controlled manner the elemental reactivity between these species on two instrumental devices at LCP. It also aims, beyond the diagnosis by laser spectroscopy, to use an innovative technique of high-resolution mass spectrometry based on the PTR-FTICR method developed at LCP on transportable devices to analyze compounds generated in cold plasmas, in particular plasmas studied at LPGP for the decontamination of gaseous effluents (removal of VOCs and hydrocarbons). We bring together the skills of several teams for a better understanding of these complex media by identifying the processes or species important for their stability and optimization.

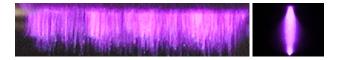


Figure 15. Atmospheric pressure air plasmas exhibiting different structures: filamentary in a dielectric barrier discharge (left) and more diffuse in a very high voltage corona discharge (right)

The study of heat transport in the presence of a controlled external magnetic field for plasma conditions relevant for ICF and astrophysics is the object of the MAGHEDP project which proposes experiments answering fundamental problems of magnetized plasmas . The three main objectives of this project are (i) to evaluate what is the limit of local to non-local transport for given plasma parameters as a function of the magnetic field amplitude, (ii) to measure the transport coefficients in the presence of the magnetic field and to compare them with existing models and (iii) to determine, in the dense (solid) phase, the dependence of the heat wave velocity on the amplitude of a B field. Different types of plasma conditions (density, temperature) will be produced, from low to high density, and from low to high temperature, taking advantage of plasmas developing in front, inside and behind a solid target irradiated by high power lasers.

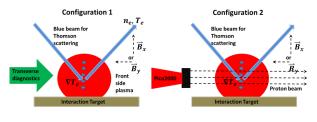


Figure 16. Experimental set-up with two different configurations envisioned for the project

5. Metrology

Cold atom interferometry has allowed in the last decades the development of extremely sensitive and accurate inertial sensors for measuring the gravity acceleration, Earth's gravity gradient or rotations. They appear very promising for a wide range of applications such as inertial navigation, geodesy, natural resource exploration, or fundamental physics. Up to now, cold atom interferometers involve the manipulation of a single atomic species. The project CAIMAN, aiming to handle three atomic species (⁸⁷Rb, ⁸⁵Rb and ¹³³Cs) simultaneously in the same instrument, will allow to take a big step in the field of cold atomic inertial sensors. A strong point of using different atomic species in the same instrument, compared to a single species experiment, is the ability to increase the number of complementary measurements without disturbance that could arise from spontaneous emission, the lasers manipulating one species having no influence on the other species.

The experimental apparatus is now in operation. An innovative fibered laser system allowing the manipulation of the three atomic species has been developped and has allowed as a first step the cooling and trapping of cesium atoms. In the short term, the next step will be to cool and trap simultaneously the three atomic species at the same position.



Figure 17. (Left) Fibered laser system (Right) Vacuum cell of the multi-species interferometer

Despite considerable efforts from many laboratories, the generation of an agile and high spectral purity radiation in the terahertz (THz) region, arbitrarily defined as 0.3-10 THz (roughly 10⁻³³³ cm⁻¹), remains not available. The project **TERAMET** propose to exploit recent progresses in the frequency stabilization (down to the Hz level) of DFB lasers at 1500 nm, patented@LiPHY, Grenoble, together with the commercially available rapid low-temperature grown InGaAs photomixers to generate a radiation in the 0.3-3 THz range using the photomixing technique. The new spectrometer will benefit from mature technology in the telecom range to provide an extremely high agility and spectral purity in the THz domain, opening new possibilities for ultra-high precision THz molecular spectroscopy.

6. The Study of Interfaces

The **CoEuRS** project allowed the identification of a sort of "solid" properties in liquids. It highlighted an elastic response under mechanical deformation, or mechanically induced thermal effects (thermo-elastic effect), previously unknown in (ordinary) liquids.

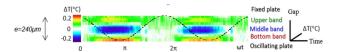


Figure 18. Thermo-elastic effect: By applying a low frequency (~ Hz) mechanical deformation, it is shown that a fluid confined between two surfaces emits a modulated thermal signal of the same frequency as the stimulus (thermography of a layer of 240µm polypropylene glycol subjected to a frequency of 1 rad / s).

It also demonstrated, for the first time, that the dynamics of the solid surface is profoundly modified by the contact of a liquid.

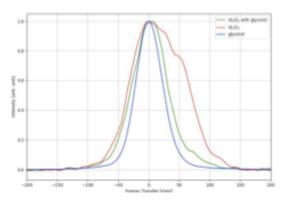


Figure 19. First High resolution IXS measurements at GALAXIES showing the energy transfer differences between the wetted alumina surface (green curve) and the dried alumina surface (red curve).

The project **HREELM** is dedicated to the realization of a prototype of a new microscope for surface studies: a high-resolution electron energy loss microscope. It will allow to image the distribution of surface vibrational states at the microscopic scale by combining a spatial resolution of a few tens of nanometers and a spectral resolution at meV. Surface vibrational states are of general importance in surface chemistry and physics as well as in material functionality and reactivity. Their knowledge in a wide energy range (from 0 to a few eV) with a resolution of the order of 5 meV gives access to the characterization of chemical functions, phonons and plasmons. Thus it is possible to

predict and know the couplings with the electronic properties of materials and the mode of interaction with the environment. **HREELM** is based on two technological innovations. (i) The use of a new brilliant electron source with high monocineticity will greatly limit geometric aberrations by avoiding the use of a monochromator and thus achieve the necessary spatial and spectroscopic resolutions, (ii) The use of electron optics will allow to keep these performances through imaging in HREELM. In 2019, the filing of a patent will protect the combination of the two innovations, which is essential to achieve the expected performance of the instrument.

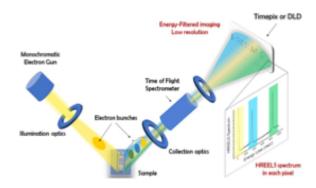


Figure 20. Electronic optics according to the principle seen in figure on the right. The use of time-of-flight spectroscopy will demonstrate the spectral resolution of the instrument.

Topic 5 "Higher Education"

During this period, support for higher education (510 keuros over the 3-year period) has been devoted to four main areas: building student labs, grants for master internships, predoctoral or doctoral training through one to three weeks summer schools and popularization of science in the PALM scientific area. A new trend in building ressources for distance learning has grown through several of these projects, which should prove more and more useful in the future. In addition, specific funds (50 keuros) were devoted to two doctoral schools organized within topics 2 and 3, and 4 PhD grants were awarded through the research topic calls for proposals.

In terms of access to the funding, the higher education call for proposals of the LABEX PALM is now recognized in our community as a source of funding to initiate projects with not too much time devoted to the grant application, saving energy to actually carry on the actions. This is essential as investing time in building new student labs or creating on-line education resources is not always as well recognized in careers as research publications. After a few years of running the annual project calls, projects initiated with the Labex PALM support have been able to attract funding from other sources, such as the IDEX initiative on lab platforms.

1. Master programs

Grants for master student internships within the LABEX have been distributed, for about 50 keuros per year, corresponding to 25 students funded per year, meeting a need from labs which cannot always find such funds within the project calls. For simplicity, these grants are distributed to the labs in proportion of the number of researchers in the PALM labs. To increase the attractivity of masters in the PALM domain, funding for visits of industrial sites or for research labs abroad has been continued and a contribution

Highlight 18. Rydberg spectroscopy of Cesium atoms C. Lopez (ENS Paris-Saclay)

The overall objective of this project is to give access for master students to an advanced research experiment around the Rydberg spectroscopy of Cesium atoms and their exploitation as an ion source. The first step that will open in the fall of 2020 is to perform spectroscopy of cesium atoms without Doppler broadening and to measure the hyperfine structure of the Cs energy levels. The influence of a magnetic field (Zeeman effect) can also be studied. An 852nm laser, a 1470nm laser and the necessary elements to realize the optical setup will be provided to the students at the beginning of the project. The ENS P-S has a Fabry-Pérot cavity which will be used as a frequency standard. One of the objectives will be to lead the students after a bibliographical research (or scientific documents provided) to build the optimal optical assembly to solve the problem and to make measurements with rigour.

The project can be developed in 4 stages, depending on the students' wish to go further in a specific direction:

- one photon Absorption Spectroscopy: using the 852nm laser and a cesium cell, spectrum recording and relative frequency measurements using a Fabry-Pérot cavity, highlighting the Doppler effect
- High resolution saturated absorption spectroscopy: modification of the optical setup, observation of hyperfine levels of Cesium, highlighting
 of the selection rule between hyperfine levels
- Two-photon absorption spectroscopy: adding the 1470nm laser and a second Cesium cell, installation of the 852nm laser servo-control (Lock-In+PID) on the hyperfine line.
- Study of the Zeeman Effect: addition of two coils around of the 1st Cesium cell to generate a controlled magnetic field of the order of a hundred millitesla, study of the influence of the magnetic field on one of the hyperfine levels of the D2 line of Cesium, influence of laser polarization, energy curves as a function of the magnetic field.

N.B.: the curves in figures 2 and 3 were obtained using the optical bench shown in figure 1 which the students will have to set up.

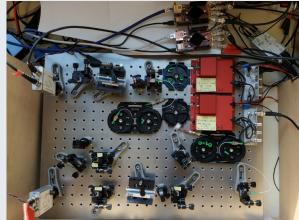


Figure 2: Absorption spectrum of the D2 Cesium line $(6S_{1/2} \rightarrow 6P_{3/2})$

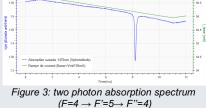


Figure 1 optical setup for the spectroscopy of the $6P_{3/2} \rightarrow 7S_{1/2}$ transition in Cesium with lock-in of the 852nm laser

Results achieved in the framework of the project CsRydberg funded by topic emergence and carried out by Colin Lopez (LAC)

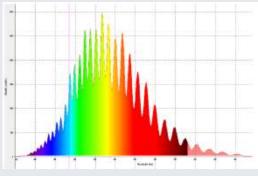
Highlight 19. Numerical processing tools for spectral analysis in optics

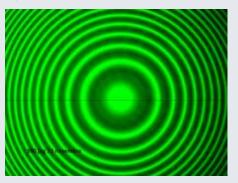
Gaël Latour, Jérôme Leygnier, Séverine Boyé-Péronne, Marion Jacquey

The ambition of the OPALES project was to set up digital tools such as digital spectroscopes and cameras on existing practical work mounts to access a better understanding of physical phenomena, and to facilitate data exploitation and analysis.

The equipment financed by the Labex PALM was deployed on two assemblies:

The OCT project (24h) is an original and ambitious project recently set up which consists in assembling and then adjusting a Michelson interferometer illuminated in white light before using it as a microscope producing 3-dimensional images with a resolution of the order of a micrometer. Purchased digital spectroscopes now allow students to first observe fluted spectra and to demonstrate the link between the interferogram (variation of light intensity as a function of the optical path difference) and the spectral width of the source. In a second stage, this tool is used as a diagnosis for the adjustment of their microscope.





Figures taken directly from reports by students of the Master 1 in Fundamental Physics at Orsay. a) Light intensity as a function of wavelength illustrating the splines of the spectrum at the output of the interferometer illuminated by a halogen lamp. b) Photo showing the spatial distribution of the light in the form of concentric rings at the output of a Fabry-Perot interferometer illuminated by a mercury vapor lamp

The discovery and use of a Fabry-Perot interferometer is at the heart of the second experimental project (8h) that received funding. Cameras are used to take images of the interference rings at the output of a Fabry-Perot (FP) interferometer illuminated by a mercury vapour lamp. These images are then processed on the computer by the students with ad hoc software to characterize the interferometer and analyze the spectral properties of the radiation incident on the FP.

Results achieved in the framework of the project OPALES funded by topic Higher Education and carried out by Marion Jacquey (LAC)

to the participation of teams of master students in the French Physicists' tournament has been initiated in this period.

2. Hands-on experience for master students

About half the funding has been devoted to building new labs for master students or modernize existing ones (15 projects over the 3 years for a total of 220 keuros).

The experimental platform on Condensed matter physics and Materials (PMCM) that is widely used by students from different masters in the PALM domain has benefited from our continuous support, and also attracted funding from other sources. The platform has moved in october 2019 in the new building "hbar" for Physics teaching (Bat 625) of the Paris Saclay campus, thus improving access for the students. New equipment for NMR analysis, for X ray fluorescence spectroscopy and Polarization microscopy for the study of materials have been installed with the support of the LABEX. A new web site is under construction to accompany the wider use of this platform.

An ambitious experiment on the spectroscopy of Rydberg atoms at ENS Paris Saclay, transferred from a research experiment at LPQM has been funded in 2019 and the first part on hyperfine spectroscopy of cesium atoms with one or two photon excitation will open to master students this fall of 2020.

See highlight 18

Support is also aimed at modernizing existing experiments, by adding numerical tools such as numerical spectrometers and cameras to facilitate data analysis by the students. This is particularly useful in particular when part of the teaching has to be done remotely.

See highlight 19

Several other student labs have been funded covering the different domains of the LabEx:

- structured illumination microscopy on a bioimaging platform at IOGS (to complement IDEX funds)
- high power ultrafast laser experiments for master students at LASERIX and LULI
- Training in cryogenic methods for doctoral students at CEA
- Experiments on condensed matter physics using the SOLEIL synchrotron source: one on the valence transition in a heavy fermion compound measured by inelastic X-ray resonant diffusion, the other on the study of growth processes with a structural study by X-ray absorption.

3. Predoctoral and doctoral schools

As planned in the previous report, two international schools for predoctoral and doctoral students were organized on the Paris-Saclay campus in the summer of 2018, at the initiative of the Labex PALM:

- microbiophysics: physical approaches to understanding microbial life (sept 2018) - organized by members of topic 2
- attosecond science: from ultrafast sources to applications (may 2018) organized by members of topic 3

They were supported by a specific budget of 50 k€ each, shared with research topics and gathered about 115 participants with 60- 80% Master, PhD students and post-docs)

Contributions were also been given to 10 schools over the 3 years (6 keuros on average per school), either on the Paris Saclay campus or outside (Les Houches, Cargèse, Beg Rohu), mostly to help reduce the cost of participation for Paris Saclay master or PhD students. Two editions of a predoctoral school were among them. In 2020, as for many scientific events, some schools took place online, some were postponed to 2021 and some had to be cancelled.

4. Popularization of science

A little more than 10% of our education funds were granted to actions in this domain. These include the creation of videos, an animated movie, and a scientific cartoon in collaboration between LabEx researchers and designers and artists. In addition, two projects aimed at building video resources for the master students and their teachers, which can also be accessible to a wider audience.

A scientific webseries called MANIP about research done by LabEx researchers now includes 4 videos visible on youtube (in french with english subtitles), plus a video on quantum intrication with the participation of Alain Aspect, also a member of the LabEx, created for the 80th anniversary of the creation of CNRS. This video as well as the last two episodes of the series benefited from the LabEx support in the period.

See highlight 20 (MANIP 2017 and MANIPBELL 2019)

Several media were built to explain to a general audience the complex topic of the 2016 Nobel Prize in Physics, namely topological concepts in physics. The main

Highlight 20. MANIP 2017 videos series on research conducted in the LabEx PALM Gaëlle Lucas-Leclin, David Clément, Hugo Cayla (LCF) and several researchers from the LabEx PALM

The MANIP project aims to produce a documentary web series, each episode focusing on a different experiment described by a physicist. The objective is to present different fields of research in photonics to the general public and to make portraits of researchers. Each episode lasts about

objective is to present different fields of research in photonics to the general public and to make portraits of researchers. Each episode lasts about 10 mn and integrates specifically designed illustrations and animations to clarify the principles involved in the experiments. The Labex's funding covered the realization of four episodes: episode 1: Karen Perronet-LCF (Biophotonics); episode 2: David Clément-LCF (Cold Atoms); episode 3: Thierry Channelière-LAC (Quantum Information); episode 4: Elizabeth Boer-Duchemin-ISMO (Plasmonics). An additional special episode on the history of quantum intrication with the participation of Alain Aspect (created in 2019 for the 80th anniversary of the creation of CNRS) and highlighted by the CNRS was partially funded by the LabEx PALM.

All episodes can be seen on a dedicated playlist on the Institut d'Optique YouTube channel: https://www.youtube.com/playlist?list=PLW1LMV6eX05t4y_kMHOAU-1qodzn3jgX0



Results achieved in the framework of the project MANIP2017 and MANIPBELL2019 funded by topic higher education and carried out by David Clément and Gaëlle Lucas-Leclin (LCF-IOGS)

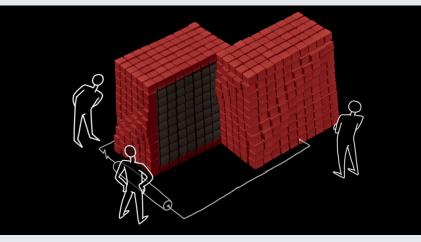
Highlight 21. The Hairy Nobel: an animated film about topological phases in matter J. Bobroff (LPS) with the Physique Autrement team; animated movie realized by Charlotte André

Topology in solids is at the heart of much current research, since the discovery of its key role in the Quantum Hall Effect. It has opened up a vast new experimental and theoretical field, from topological insulators to Majorana fermions, from skyrmions to quantum computers. It was honored in 2016 with the Nobel Prize in Physics. However, it remains one of the most difficult subjects to popularize. We built a multimedia project (animated film, website, images, posters) to stage and explain the topology. The project benefited from our expertise and our collaborations with video artists, graphic designers and web designers. On the scientific side, labex researchers involved in these themes, notably at the LPS (P. Simon, M. Goerbig, G. Montambaux) as well as the team of D. Carpentier and P. Delplace (ENS Lyon). This project will be widely disseminated via our networks (internet, academic world, science museums, national education) and our own actions (conferences, science festivals, media interventions) and is available free of charge in French and English, notably to the community of researchers in this field.

Below an illustration extracted from the movie. The whole film, and associated material (posters, reusable images, making-of movie), can be found at these links:

english version: https://www.youtube.com/watch?v=gEnDNUfGQTQ

french version: https://www.youtube.com/watch?v=iHPZ7TL9npUAII episodes can be seen on the following youtube channel: https://www.youtube.com/playlist?list=PLW1LMV6eX05t4y_kMHOAU-1qodzn3jqX0



Results achieved in the framework of the project TopoPourTous funded by topic higher education and carried out by Julien Bobroff (LPS)

production was an animated movie called "the Hairy Nobel" ("Le Nobel Chevelu" in french).

See highlight 21 (TopoPourTous)

The cartoon called "Glace de Spin" (Spin Ice in english) has just been finalized at the end of may 2020. It aims at explaining the physics but also the researcher at work. An extract is presented in highlight #5 below.

See Highlight 22 (MANIPBELL)

Finally of the two projects funded to create on-line teaching resources, the VitaMecaQ project, funded in 2018, created videos and tutorials for the teaching of quantum mechanics to students trained in physical chemistry, but can be used more widely for other students. It is available on youtube:

https://www.youtube.com/channel/UCodSDTjV0Xdu5xv TbvbWXSg/videos

A project funded in 2020 plans to create videos to illustrate notions in optics, other topic important for many students

working in the LabEx. Finally, support for a LabEx PALM prize in the Olympiades de Physique, an annual physics contest for high-school students contributed to advertize our scientific domains to future students.

5. PhD fellowship

Since 2018, 5 PhD grants have been funded by the LabEx.

See PhD grant

PhD Grant

Project: e-BACT Candidate: Marion Lherbette) Laboratory: LPS PhD Advisor: Eric Raspaud Date: SPET 2018 to AUG 2021 Subject: Bacterial biofilm electroactivity

Project: SYMBIOSE Candidate: Julien Bouvard Laboratory: FAST PhD Advisor : Harold Auradou Date: OCT 2018 to SEPT 2021 Subject: Bacterial motility for symbiotic interaction

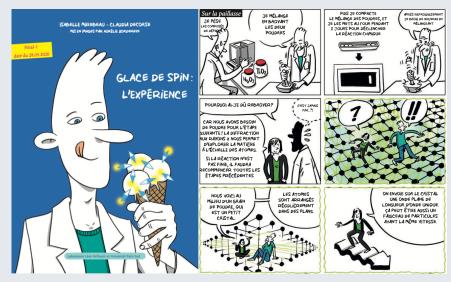
Project: 3DlightChain Candidate: Sana Aimeur Laboratory: ICP PhD Advisor : Laura Baciou Date: OCT 2020 to SEPT 2022 Subject: Biomimetic approach for determination of the structure of the superoxide-generating NADPH oxidase light chain subunit

Project: NanoWeakGels Candidate: Souhaila N'Mar Laboratory: FAST PhD Advisor : Frédérique Giorgiutti-Dauphiné Date: OCT 2020 to SEPT 2022 Subject: Multi-scale Characterization of Bio-Hydrogels

Project: OPTFLO Candidate: Federico Lanza Laboratory: LPTMS PhD Advisor : Alberto Rosso Date: OCT 2020 to SEPT 2022 Subject: Optimal paths for the flow of yield stress fluids

Highlight 22. A cartoon to explain Spin Ice and the dayly work of research Isabelle Mirebeau and Claudia Decorse (LLB) and Aurélie Bordenave

The project consisted in creating a cartoon to stage two "life-size" research experiments in condensed matter. The first concerns a liquid inserted in a mesoporous matrix, the second a frustrated magnetic compound called "spin ice". The cartoon is primarily aimed at students (Master's, Bachelor's) and scientists in the broadest sense. The goal is to make this public grasp the reality of a manipulation, from A (synthesis) to Z (interpretation), by underlining the importance of collaborations (between chemists and physicists, between labs and large research instruments). The cartoon will be disseminated on the WEB sites of the concerned labs (LLB, ICMMO,...), then in paper version, during conferences, science fairs, courses or TD. It has been realized by Aurélie Bordenave (scientific draftswoman with a state diploma) and Isabelle Mirebeau (DR1 CNRS section 3), in collaboration with scientists of the Paris-Saclay campus.



Results achieved in the framework of the project BDMANIP funded by topic higher education and carried out by Isabelle Mirebeau (LLB)

Topic 6 Innovation and Technology Transfer

INTRODUCTION: MAIN FEATURES AND EVOLUTION OF TOPIC 3 SINCE 2018

The main action consists in an annual call jointly organized with LabEx NanoSaclay. That call aims at supporting projects which initiate a technology transfer phase, but which are still at an early stage (proof of concept studies, market studies, development of pilots). The positioning of the call is to be as close as possible to the start of maturation and to encourage first-time innovators (70% during this call period 2018-2020 of the funded researchers have not been funded in the previous ITT calls 2012-2017). The typical amount of funding per project lies between 30 and $60 \text{ k} \in$, and can be used either to leverage other fundings, or to strengthen the maturity of the innovation, the experience of the PI as well as the protection of the intellectual property if needed before confronting financing structures that require a return on investment. Since the first ITT call (2012) from Palm and Nanosaclay labex, other calls have been developed targeting technological transfers and start up creations.

Since 2013, University Paris Saclay is organizing a Poc in Labs call and has lauched a seed fund in 2017 managed by Partech ventures that is able to invest in start ups (with typical amount of pre-serie A fundings). The Poc in Labs call is close to the labex ITT call, but is not limited to the scientific perimeter of Nanosaclay and Palm labex. Discussions have begun in 2020 to seek whether synergies were possible and timely.

There is a SATT (technology transfer acceleration society) associated to the Saclay research cluster (Université Paris Saclay, Institut Polytechnique de Paris, HEC) that offers two calls (Poc'up and maturation). To be eligible to the Poc'up call, the technology must have a TRL (Technology Readiness Level) of 2-3 and an external market study is mandatory before the project. The maturation call of the SATT is at a more advanced step than the labex call and is similar to other national calls that are dedicated to technologies with a TRL greater than 3 (*e.g.*, CNRS maturation call, ANR Astrid maturation call, FUI calls from BPI France or Rapid projects from the DGE and DGA).

The ITT call from the labex is different since projects are evaluated by known peers of the PALM and Nanosaclay community, with no anonymous external reviews, which can be appreciated in the early steps of the technology transfer where for instance the intellectual property is not always properly secured. Contrary to the SATT, there is no need for a first external market study, and the lack of experience of the project leader is not a drawback, quite the contrary. The Labex funding are used to give researchers a leg up on their technology transfer journey, and is helpful for the PI to strengthen their expertise before applying to other calls.

During the 2018-2020 frame period, the moderators of the ITT board of both labex have been renewed in September 2019, as well as several members. So, the last call in the period has been organized by the new board, but in close interaction with the formers members so as to keep the very consistent methodology of the call. It is organized in two steps, in the first one, Palm researchers can submit a pre-proposal letter (one page) that is analyzed by the bureau so as to determine its eligibility to the call: projects that seems to be research projects or on the opposite already in an advanced step of technology transfer are invited to clarify their positioning before the full proposal submission. In the second step, full proposals are examined with regards to four criteria (originality of the project with regards to the existing technologies/markets/societal impact, ITT strategy, maturity level, implementation of the project/risks).

The two labex also have tried to promote innovation among researchers by organizing Innovation workshops on a regular basis. Previous "innovations days" have addressed for instance different avenues for innovation (2015) and the experiences of inventors and entrepreneurs (2017). The two Labex are looking forward to the organization of the third edition of these innovation days, which could not take place in 2020, and will hopefully be organized in 2021.

1. Funded projects

A total of 24 ITT projects have been funded over 45 preproposals submitted during the first round over the last 3 calls (2018-2020), for a total amount of 1100 k€. Thirteen of these projects are more relevant to PALM topics. Among these 13 projects' principal investigators, 30% have been previously funded by the ITT calls (2012-2017). In several cases, a PALM research project has led to a patent filing as well as to the submission of a proposal to the ITT call. Among the 13 Palm ITT projects selected in the 2018-2020 period, nearly half of them had emerged thanks to a previous Palm research project. For instance, the PALM research project **UGOSOP** (topic 3) funded in 2016 has led to one patent filing and the submission of the **PROTULGATE** project (see highlight 23) to the ITT call in 2018. The Palm research project deepIM (emergence topic) funded in 2015 has also led to one patent filing and the submission of the **DeepIM Cube** to the ITT call in 2020 (see highlight 26). The **HOP-GIFAD** project (emergence topic) in 2018 has led to the **GIFAD-HiPIMS** in 2019 and the **Lubiol** project (emergence topic) has led to the submission of **SEIEM** (see highlight 25) to the ITT call (in 2018). The **TisaLED** project (emergence topic) in 2012 has led to the filing of one patent in 2015 and to the **LEDsGO** project funded by the ITT call in 2019. The PALM research project **Magtep** (emergence topic) selected in 2012 has been followed by an ANR and a H2020 FET project, and then to the **SoITE-Hybrid** project

Highlight 23. A versatile industrial solution for optically synchronized OPCPA based high intensity laser systems

Dimitris Papadopoulos (LULI), Xavier Delen, Frédéric Druon (LCF)

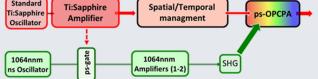
The Optical Parametric Chirped Pulse Amplification (OPCPA) technique is a key element in the architecture of high contrast ultrashort high intensity laser sources. Nevertheless, its implementation still remains challenging due to the strict synchronization requirements between the pump and the signal pulses. The goal of PROTULGATE is to provide solid proof that a novel method for the generation of these pump/signal pairs (demonstrated already in the frame of a preceding PALM project, UGOSOP, in 2016) can be effectively used in real world high intensity laser sources and provide an attractive, technically and financially, alternative for the high intensity laser industry.

In the first phase of the PROTULGATE project we developed, for demonstration purposes, a complete ultrashort CPA laser source (in an annex laser laboratory of LULI) integrating the novel pulse gating method used for the optical synchronization of the pump/signal pulses at 1064/800nm. We have been able to produce high fidelity multi-mJ, 15 ps pulses at 1064 nm frequency double at 532 nm with ~70% efficiency. This prototype system has been the subject of extensive tests and characterization proving the potential of the technique for use in PW class laser systems. In this direction and for the next phase of PROTULGATE we have scheduled (11/2020) the first integration tests of our system in the Apollon laser, as schematically described in the figure bellow. In parallel we have started the negotiations for a license of the patented technique with two industrial partners that have expressed a great interest in our results and the evolution of the project.

Current OPCPA implementation in the Apollon laser



PROTULGATE upgrade of the Apollon OPCPA source



D. Papadopoulos, X. Delen and F. Druon, Synchronisation effet Kerr, FR 18 53519 (Patent: 20/04/2018).

C. Alexandridi, F. Lemaitre, X. Délen, F. Druon, P. Georges, and D. Papadopoulos, *Kerr Shutter for the Generation of Optically Synchronized Pump-Signal OPCPA Pairs*, Laser Congress 2019 (ASSL, LAC, LS&C), OSA Technical Digest, paper JTh3A.14.

Results obtained in the frame of the project PROTULGATE (Development of a high intensity laser system prototype based on ultrafast gating) supported by the Valorization LabEx PALM (2018) realized by Dimitrios Papadopoulos (LULI) and Xavier Delen (LCF).

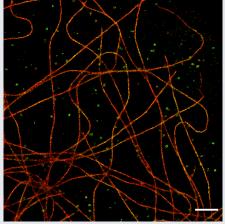
Highlight 24. New imagery for cell biology

Sandrine Lévêque-Fort, Aurélie Brousse, Clement Cabriel ISMO), Emmanuel Fort, Surabhi Sreenivas (Institut Langevin)

Optical microscopies for super-localisation of single molecules now make it possible to reveal cell organisation and molecular architecture at the nanometric scale, which until now have been inaccessible, thus bringing about a real revolution in cell biology. The basic principle of these microscopes is to constrain fluorescent molecules located in the same response function of the microscope to emit sequentially, staggered in time, in order to locate the position of each fluorophore with nanometric precision. Developments in these techniques have mainly focused on the gain in spatial resolution, making it possible to achieve accuracies below 10 nm.One major challenge is now to colocalize at this scale multple proteins to understand their function. Observations of multispecies is usually performed in classical microscopy by using molecule with non overlapping spectra which is not straighforward in single molecule, as a limited range of dyes presents an efficient blinking for the localization, and chromatic aberrations can hampered the results. We are thus currently investigating alternative solutions to reveal multiple dyes. In particular we focus on dyes which can be excited with a unique laser source and have emission only slightly shifted between 650 and 750 nm. We have already identify several compatibles dyes. By playing with alternative parameters than spectra we can for example identify easily different proteins, as shown here on figure, where Clathrin coated pits and tubulin can be distinguished with a very low crosstalk.

S. Sivankutty, IC. Hernandez, N. Bourg, G. Dupuis, S. Leveque-Fort, *Supercritical angle fluorescence for enhanced axial sectioning in STED microscopy*, Methods, 174, 20-26 (2020)

Results achieved in the framework of the project NanoImaBio supported by Inovation carried out by Sandrine Lévêque-Fort (ISMO)



Schematic representation of the PROTULGATE

integration strategy in the Apollon laser. In the upper

a) Super-resolved 2D Image were the false color allows to identify the different proteins associated to fluorophores with close emissions : in green AF647 labelling clathrin pits and in orange CF660 the tubulin network. (Scale bar funded by the ITT call in 2020. Regarding gender equality, 38 % of projects have a woman as principal investigator.

Most of these 13 projects are devoted to development of instruments, and an overview is given hereafter.

Three projects are related to intense lasers: the development of a high intensity laser system prototype based on ultrafast gating (**PROTULGATE**), which aims at developing industrials ultrashort chirped pulse amplification laser sources, for which one patent has been filed. Cleaning of pulses using parameter amplification and temporal reshaping (**CLEOPATRE**) and a last one is devoted to the metrology of high intensity femto laser based on the combination of fibered lasers (**HIBISCUS**), with a possible transfer of the technology to the SME phasics.

See Highlight 23 (project PROTULGATE)

Two projects are developing light sources: one project develops a compact LIDAR source by differential absorption, a portable instrument able to detect greenhouse gas (CH₄, CO₂) as well as H₂O thanks to their infrared signatures(**SACLAD**). The **LEDsGO** project develops concentrators and lasers pumped by LEDs. A light concentrator pumped by LEDs is a source of light with intermediate luminance between LEDs and lasers and it has been demonstrated that a Ti:saphire laser can be pumped by a LED.

Two projects are developing instruments for biological and medical applications. One project aims at developing high resolution imaging of molecules in biological cells, and another to develop an instrument for ex vivo and in vivo characterization of corneal transparency following pathology or laser treatment (CHARCOAL).

See Highlight 24 (project NanolmaBio)

One project (**LudiDRY**) objective is to develop a new design of refrigerator with inverted dilution able to reach very low temperature.

One project aims at real time diagnostic of thin films growth by pulsed magnetron pulverization thanks to fast atoms diffraction (**GIFAD-HiPIMS**) that combines two patented techniques (one for the growth of thin films, and the other for the grazing incidence fast atom diffraction technique). The SEIEM project is devoted to the development of an ultrafast electron gun for electrom-matter interaction studies (**SEIEM**).

See Highlight 25 (project SEIEM)

In April 2020, the following projects were funded: the above mentioned **HIBISCUS** project, **SoITE-Hybrid** project on nanofluid based solar-thermoelectric hybrid energy harvester, the **HREELM** project on the development of a high resolution electron energy loss microscope and has been used as leverage in a SESAME funding request (typical funding is 1 M€) and the **DeepIM Cube** project on a 3-band ultrafast laser prototype for deep and fast 3-photon microscopy..

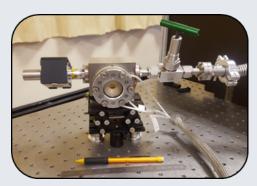
See Highlight 26 (project DeepIM Cube)

Regarding PALM ITT funding, most expenses are possible, except salaries of permanent staff: the LabEx provides basic budgets maybe small (50 k€), but very flexible, with a wide eligibility in the expenditures, and with a possibly reoriented nature of expenditure to accommodate the evolution of the action, in a fast way.

Highlight 25. System for Electron-Matter Interactions studies

Marie Géléoc (LIDyL), Jean-Philippe Renault (NIMBE)

Off-the-shelf electron sources cannot provide temporal nor energy resolution required by emerging applications. Sources issued from laboratories, more efficient, do not allow avoiding high nor ultrahigh vacuum, nor sometimes radioactivity. Building on the results of the PALM Emergence LUBIOL project, and on our feedback on our ultrafast electron-gun [1], we are working since 2016 to the conception, development and realization of an ultrafast electron gun (ps to fs) compact, robust, light and self-contained and mainly user friendly. The aim of the project is to realize a demonstrator of a mini field equipment which will be tested by first users from LabEx (CEA, LAC, SOLEIL). This new tool can be used for sample ionization or detectors calibration. Its modular construction is based on a photon source, the electron mini gun itself and its detector. A 1st prototype has been realized and allowed us to explore numerous technical solutions. 2019 was devoted to a patent application and to look for an industrial for the miniaturization and reliability of the HV feed-through. In 2019, the project was selected by Starburst Accelerator (a start up incubator for aeronautics and space sector), and presented at the Starburst Meet up event in April 2019. In 2020, intellectual property development is pursued and endeavor deal with reliability, integration and miniaturization of the different components in a prototype realized on the basis of a 1st feedback and on SIMION simulations, designed to operate over 0 to 10 keV.



1er prototype realized and tested successfully until 1 keV, from of off-the-shelf components.

Renault, J.P. et al. Time-resolved cathodoluminescence of DNA triggered by picosecond electron bunches. Sci Rep 10, 5071 (2020)

M. Géléoc, J-P. Renault, T. Oksenhendler, « Générateur pulse de particules chargées electriquement est procédé d'utilisation d'un générateur pulse de particule chargé électriquement, Demande de Brevet N° FR1907324 déposée le 2 Juillet 2019

Results achieved in the framework of the project SEIEM supported by Inovation carried out by Marie Géléoc (LIDyL)

Highlight 26. 3-band ultrafast-laser prototype for deep and fast 3-photon microscopy Frédéric Druon, Marc Hanna (LCF), Emmanuel Beaurepaire, Júlia Ferrer Ortas (LOB), Florent Guichard, Tiphaine Berberian, Alexandre Thai, Yoann Zaouter (AL)

The LOB and LCF recently demonstated an original laser source for 3-photon (3P) microscopy. This source is based on a high repetition rate fs fiber laser (commercial laser: Satsuma from the Amplitude Laser Group) to which was added an original frequency converter to reach the interesting mid-infrared (SWIR) wavelengths: 1.3 µm and 1.7 µm, that are in the water transparency windows. This dual-wavelength laser allowed imaging deep inside in vivo biological tissues with high resolution and including a novel paradigm based on multi-wavelength 3P microscopy[1]. This source as well as new approaches for deep multicolor 3P microscopy have been patented in 2017[2].

The "DeepIm Cube" project consists in the realization of a prototype of this laser source. This includes an industrial integration of the non-linear stage and an improvement of the technology to produce 3 simultaneous outputs (at 1 µm, 1.3 µm and 1.7 µm). Additionally to this third output, the technological improvements planned in DeepIm Cube will allow to obtain a better energy balance between 1.7 µm and 1.3 µm, together with a very high-industrial-standard reliability and stability and a high level of compacity, as shown in figure 1. This will be possible thanks to a collaborative work within the joint laboratory "DéFI" (Femtosecond Development and Innovation) between LCF and Amplitude Laser Group. The fast and efficient transfer of technology and skills between the LCF and Amplitude Laser will permit to test this new source at the LOB in order to demonstrate the potential of the source with enriched functional multimodal microscopy by the monitoring of several biological parameters on independent and simultaneous channels. The test of the "DeepIm Cube" source at the LOB is essential in order to convince biologists of the relevance of this new source for microscopy. Indeed, demonstrations with concrete biological results are, in the current microspopy market, more relevant than laser performances to convince potential customers and to be able to bridge the chiasm between early adopters and the mainstream market.

The work carried out within the framework of DeepIm Cube project addresses several cutting-edge research topics -in laser development and in vivo microscopy- together with important industrial issues with high-potential products for in vivo brain imaging.



(left) Laser system developed within DeepIm project: on the top left is the YDFA Satsuma laser, the rest of the table is dedicated to the OPA. (right) YDFA + OPA laser system developed by Amplitude Laser consisting of a fs YDFA Satsuma laser (black color) on which is positioned a platform in which the non-linear stage is integrated.

[1] Khmaies Guesmi, Lamiae Abdeladim, Samuel Tozer, Takuma Kumamoto, Pierre Mahou, Karolis Jurkus, Philippe Rigaud, Karine Loulier, Patrick Georges, Marc Hanna, Jean Livet, Willy Supatto, Emmanuel Beaurepaire, and Frederic Druon, « Dual-color deep-tissue three-photon microscopy with a multiband infrared laser » Light: Science & Applications, 7,doi:10.1038/s41377-018-0012-2 (2018)

[2] Druon, Hanna, Guesmi, Rigaud, Beaurepaire, Supatto, Mahou, Abdeladim (CNRS Ecole Polytechnique, IOGS) : *Dispositif et procédé de microscopie multiphotonique*, patente 9 June 2017, N°. BR76726_BR76726

Results achieved in the framework of the project DeepIm Cube supported by Inovation topic of PALM and EquipEx Morphoscope2 carried out by Frédéric Druon (LCF)

2. Leverage effect

A possible indicator of the leverage effect would be the number of filed patents linked to PALM projects. However, this indicator is difficult to measure, because the maturation time of a technology transfer is larger than the time of the PALM project. Some patents have been filed or even delivered before the PALM funding, some can be filed a long time after the end of the project, in a context of multiple fundings. And there is no similar easy-to-trace system of acknowledgement as like for publications. Concerning the projects supported through the innovation call, the leverage effect is specific to each situation. Some projects continue mainly by other pre-maturation or maturation funding (ANR, SESAME, SATT, RAPID, CNRS maturation program). For instance, the PALM project **dichro50**, funded in 2015, was later funded by a SATT funding that led to a technology transfer to the SME Cryoconcept. The project **HREELM** selected in 2020 as already been used to support a SESAME funding request from region lle de Fance.

Two start-ups had been created following projects funded during previous ITT calls, DAUMET after **3DPAuW** project and Teratonics after the two ITT projects **CASIMO-STRIPP** and **AMEFI-STRIPP**. Teratonics has been awarded the 2019 I-Lab for its patented nondestructive testing solution based on untrashort terahertz pulses and has received funding from French Tech seed Paris Saclay.

The **EXYT** project has led to the technological transfer of the INSIGHT system to the start up SourceLAB in 2019. This product provides a metrologic system for ultra short lasers (https://www.sourcelab-plasma.com/laser-shaping/beam-shaping-catalog/insight/).

Patents 2018-2020

FR3062545 (2018) Inner Nano-engineering of Hollow Optical Fibers and Capillary tubes by Plasma, by Tiberiu Minea (FAST) PALM Project INNOPLAS 2014

FR3067524 (2018) **Dispositif et procédés de microscopie multiphotonique**, by Frédéric Druon, PALM project DEEPIM 2015

FR3065805 (2018) **Method for spatio-spectral characterization of a polychromatic pulsed laser source** by Fabien Quéré (LIDyL) PALM project EXYT 2017

FR3067457 (2018) Method and system for controlling the speed of a laser pulse by Fabien Quéré (LIDyL) PALM project EXYT 2017

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