Département d'évaluation
de la recherche

Self-assessment document

Research unit

—
EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Unit name:	**Institut de Chimie Moléculaire et des Matériaux d'Orsay**
Acronym:	**ICMMO**
Hceres scientific domain and sub-domain:	**Physics-Chemistry**
Director's name (current contract):	**David AITKEN**
Director's name (future contract):	**David AITKEN**

INSTITUT DE CHIMIE MOLECULAIRE ET DES MATERIAUX D'ORSAY

EVALUATION CAMPAIGN 2018-2019

GROUP E

Self assessment document Teams

Appendices

Research unit

Self-assessment document

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Application type:

Renewal (w/o important modifications) ■ Restructuration ☐ *Ex nihilo* creation ☐

List of supervising institutions and bodies of the research unit:

Current contract:	Next contract:
Université Paris Sud **CNRS**	**Université Paris Sud / Université Paris Saclay** **CNRS**

Inter-disciplinary evaluation for the research unit (or for one or more internal team):

Yes ☐ No ■

Number of teams for the next contract: **9**

Requested label (UMR, EA etc.): **UMR**

SELF-ASSESSMENT DOCUMENT

1- Presentation of the unit

Introduction

In 1980, the federative *Institut de Chimie Moléculaire d'Orsay* (ICMO) was created under the direction of Professor Olivier Kahn to encourage closer contact between 6 CNRS-associated research units (UMR) hosted by Université Paris Sud (UPSud) on the Science Campus in Orsay, working in various area of molecular chemistry. In 2002, two other local UMRs working in the area of materials chemistry were affiliated, giving rise to the *Institut de Chimie Moléculaire et des Matériaux d'Orsay* (ICMMO) Research Federation. On 1st January 2006, the 8 UMRs of the federation merged to become a single unit (UMR 8182) bearing the same title (ICMMO), organizing themselves into 9 scientific research teams aided by the unit's Common Services, under the direction of Professor Jean-Jacques Girerd. This structural set-up has continued to function successfully under the subsequent Directors Professor Jean-Pierre Mahy (2010-14) and Professor David Aitken (2015-present).

ICMMO operates on the principle that research team line-ups are established on the basis of mutual consent from within the collected scientific personnel, at each new contractual renewal; this flexibility allows the most appropriate combinations of scientific expertise to address an evolving portfolio of challenges. For the present contractual period there are 9 research teams, each of which is given a significant degree of autonomy to identify its scientific objectives during the period and to secure and implement the appropriate means for achieving those objectives. At the same time, the day-to-day organization of the ICMMO unit serves to facilitate cross-team interactions and to nurture scientific links based on common interests. The 9 research teams benefit from the strong centralized support of the "10th team" known as the Common Services (CS), which provide administrative, technical and scientific support in the form of both human and material resources.

Geographically, ICMMO has a single-site location on the Orsay Science Campus of the UPSud. Buildings 410 and 420 are entirely occupied by the unit, while one small group is hosted in building 430 and some of the administrative services in building 415.

Workforce and resources of the unit

The Excel files "Données du contrat en cours" and "Données pour le prochain contrat" are supplied separately.

WORKFORCE

At the beginning of this evaluation period (01/01/13), ICMMO had a total permanent workforce of 164, comprising 27 researchers and 34 support staff employed by CNRS, along with 81 teacher-researchers and 22 support staff employed by UPSud.

Over the 5-year period, the CNRS workforce has declined, although this is in line with the general trend observed on a national scale over the same period. Nonetheless, the number of CNRS researchers today (22) is barely more than half the figure when the unit was created back in 2006 (40). The workforce turnover has been 19 departures (10 researchers, 9 ITA) of which 11 were retirements. 9 recruitments (5 researchers, 4 ITA) were made, confirming that ICMMO remains an attractive research institute. One CR was successfully promoted to DR, and one DR was awarded Emeritus status.

The UPSud workforce has remained virtually constant, which is a telling achievement given that UPSud has implemented significant budget restrictions since 2014 resulting in the non-renewal of many posts which are vacated. The turnover at ICMMO has been 15 departures (9 academics, 6 ITRF) of which 8 were retirements, and 12 arrivals (6 academics, 6 ITRF). Four MCF were successfully promoted to PR (with three remaining at ICMMO), while 2 PR were awarded Emeritus status.

The non-permanent workforce has remained roughly constant. The number of non-student contractual staff reflects a healthy number of postdoctoral researchers but also the presence of several contractual staff recruited to assist with scientific and administrative tasks. Given that French legislation requires that the unit remunerate certain categories of student internships, the number of M2 students taken in remains reasonable. The figures given below are given for the 1st January each year, which is "low season" for internships; between Spring and Summer, the total workforce goes beyond 300 due to short-term student placements.

Workforce status[a]	2006	2010	**2013**	**2014**	**2015**	**2016**	**2017**	**2018**	2019[b]
CNRS									
Researcher (DR/CR)[c]	40	33	**27**	**27**	**24**	**23**	**24**	**22**	22
Engineer/Technician (ITA)	41	36	**34**	**33**	**32**	**31**	**27**	**29**	27
Total CNRS	81	69	**61**	**60**	**56**	**54**	**51**	**51**	49
Université Paris Sud									
Teacher-researcher (PR/MCF)[c,d]	73	77	**81**	**81**	**81**	**79**	**79**	**78**	78
Engineer/Technician (ITRF)	26	23	**22**	**20**	**22**	**24**	**23**	**22**	24
Total University staff	99	100	**103**	**101**	**103**	**103**	**102**	**100**	102
Total permanent workforce	180	169	**164**	**161**	**159**	**157**	**153**	**151**	151
PDRA/other contractual	27	29	**27**	**29**	**34**	**27**	**32**	**35**	
PhD students	63	78	**80**	**71**	**71**	**66**	**69**	**67**	
2nd Year Master students	19	11	**28**	**29**	**18**	**25**	**21**	**20**	
Total non-permanent	109	118	**135**	**129**	**123**	**118**	**122**	**122**	
TOTAL workforce	289	287	**299**	**290**	**282**	**275**	**275**	**273**	

a: figures are given for 1st January of each year; *b*: anticipated figures; *c*: including emeritus status staff; *d*: one MCF is an employee of Université Descartes, Paris.

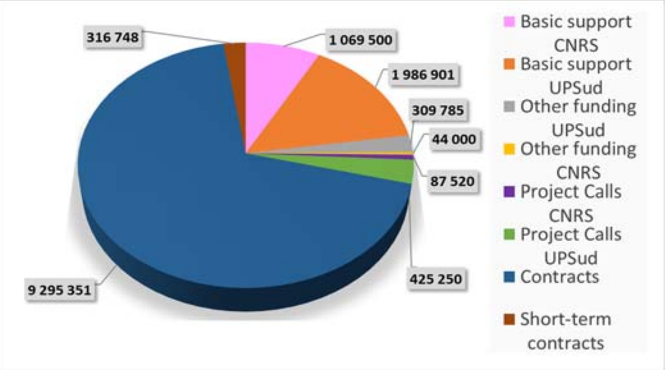
RESOURCES

An assessment is made here of the financial resources of the unit over the 5 year period 2013-17. (Figures for 2018 are not complete but the trend is similar). The annual budget varied from 2 to 3 M€ with a 5-year average of 2.71 M€. Basic support grants were received annually from the two institutions: CNRS support, remained more or less constant over the period, at around 200 k€/y. UPSud support, initially around 480 k€/y (2013-14), has been reduced to 345 k€/y (since 2015) as part of the establishment's economy measures.

Both institutions have been supportive regarding specific funding requests over the 5-year period. CNRS has made some contributions towards identified safety measures (44 k€) and has part-funded several scientific project through competitive call campaigns (88 k€). UPSud, through its calls for equipment acquisition and instrument platform support (ERM and MRM: *Equipements de Recherche Mutualisés* and *Moyens de Recherche Mutualisés*) has aided the unit to strengthen its Instrument Platform (425 k€).The Faculty of Sciences has been responsive to specific requests for financial help (60 k€), often to facilitate instrument or infrastructure repair, falling outwith call structures.

However, the most significant source of funding for research comes from contracts: over the 5-year period, a total of 9.6 M€, representing 71% of the total resources, came from national and international institutional funding mechanisms, charitable foundations and industrial collaborations. More details of these contracts (and the unit's strategy to obtain them) are given in the following section (Scientific policy) and full details are provided in appendix form. As an indication of the unit's performance, 94 contracts were operative, including 5 which were European-funded, in 2017.

	2013	**2014**	**2015**	**2016**	**2017**	**Total 2013 to 2017**
Basic support CNRS	213 000	231 000	221 500	196 000	208 000	1 069 500
Basic support UPSud	479 086	474 303	344 512	344 500	344 500	1 986 901
Other funding UPSud	77 297	40 240	42 220	42 600	107 428	309 785
Other funding CNRS	9 000	25 000	0	5 000	5 000	44 000
Project Calls CNRS	35 520	20 000	0	0	32 000	87 520
Project Calls UPSud	110 160	123 690	47 200	47 200	97 000	425 250
Contracts	1 568 533	961 074	2 212 280	2 321 607	2 231 858	9 295 351
Short-term contracts	96 176	85 305	27 103	62 452	45 712	316 748
Total	**2 588 772**	**1 960 612**	**2 894 815**	**3 019 359**	**3 071 498**	**13 535 055**



Scientific policy

The ICMMO research unit is affiliated to one of the best-rated French universities (UPSud) and to the largest French public sector research organization (CNRS). With a total staff of around 300, it is one of the largest chemistry UMRs in France. The declared central mission of the unit is to conduct the highest level of cutting-edge fundamental research in chemical sciences. As a university laboratory, the unit actively promotes training through research, playing host to a large number of PhD and Master students. Technology transfer of scientific discoveries via the university accompaniment structures is encouraged whenever appropriate. A familiar ICMMO ideogram is:

Training ← FUNDAMENTAL RESEARCH → Technology Transfer

ICMMO is internationally recognized. In the 2013 Shanghai Academic Ranking, **Chemistry at UPSud** was 5th equal in France (with 5 other universities), placing it in the top 151-200 bracket of world rating. By 2017, this ranking had risen to 2nd equal in France (with 2 other universities), in the top 51-75 bracket of world rating. ICMMO, as the largest chemistry unit of UPSud, has contributed significantly to this ranking.

RESEARCH

Towards the end of the previous contractual period (2010-14), a fair degree of reorganization of research team composition for the present contract was decided collectively. The transition was implemented progressively during 2013-14, correctly anticipating the approval of the AERES evaluation committee and validation by both CNRS and UPSud. To pursue their scientific projects, 4 of the previous research teams retained the same personnel line-ups while the 5 other teams redistributed their expertise. The success of this evolution can be judged by the scientific results and production which have been forthcoming from all 9 current research groups and are detailed elsewhere in this report.

For the present contract, emphasis has been placed on the combination of quantity and quality of scientific production in the form of publications in peer-reviewed journals. Encouragement to publish is made by the conditional distribution of recurrent institutional funding to the research teams and incentive material support on an individual basis, if appropriate. The in-house data base provides bibliometric data for all teams and/or individual scientists, and an internal audit (2017) was conducted to enhance awareness and evaluate progress in this respect.

The research conducted at ICMMO covers a wide area of chemical sciences. Disciplinary activities include biological chemistry, organic and inorganic molecular chemistry, materials chemistry, catalysis, electrochemistry, NMR spectroscopy and nano-sciences. In response to the "objectives" criteria of many funding calls, a significant number of ICMMO projects are oriented towards the application of chemical knowledge to meet contemporary societal challenges, these being chemistry for health, chemistry and the environment, or chemistry for new/smart functional materials. In this way, a considerable number of projects involve cooperation between two (or more) ICMMO research teams and/or external collaborations: locally, nationally or internationally.

An energetic approach to funding applications has been adopted. As an incentive, ICMMO levies only minimal overheads on successful submissions. The context of funding calls has evolved considerably during the last 5 years and a "project accompaniment service" has been introduced within the ICMMO to anticipate call dates and context, assess eligibility, assist in project preparation, and ensure close liaison with UPSud institutional structures (SCRED, DARI). ICMMO researchers have responded successfully to local calls from UPSud (ERM and MRM), Paris-Saclay Labexes (Charm3at, Lermit, NanoSaclay) and the recent Paris-Saclay *Strategic Research Initiative*; regional calls (DIM, SESAME, ASTRE); national calls (CNRS, ANR, ARC, Ligue Contre le Cancer) and international calls (mainly European). Over the assessment period, 8 applications were made for ERC grants by ICMMO scientists, sadly without success.

Participation in research networks is an indicator of ICMMO's prominent scientific position. Researchers have been active in 10 CNRS-supported national GDR (*Groupement de Recherche*), one international GDR, and 5 Campus France-supported bi-lateral international partnerships (PHC).

Recruitment of top-class research personnel is vital for sustaining ICMMO's reputation for scientific excellence. Since 2013, 4 CNRS researchers have been appointed following their success in the national recruitment competition (2 in Section 14, one each in Sections 12 and 16) and a fifth (Section 12) is expected to join the unit late 2018. A sixth (Section 14) has arrived through transfer from another unit. Teacher-researcher appointments have been rare due to the limited number of UPSud posts available. Nonetheless, 3 MCF (bioorganic chemistry, electrochemistry, polymers) and 1 PR (biological chemistry) have been recruited to the unit; the research profiles correspond to identified priorities within specific research teams. The attractiveness of ICMMO is underlined by the arrival of two scientifically productive MCFs from other units.

During the previous contractual period, a considerable degree of centralization of administrative and scientific support for research was achieved. This organization has been consolidated during the present, and two policies are worthy of particular mention. Firstly, investment priority has been given to maintain and develop the high-performance Instrument Platform which provides precious analytical facilities to all ICMMO scientists. Second, taking account of available man-power, a Synthesis Pole has been created in order to respond fairly and best serve the demands of the research teams for high quality chemical samples to be made available using in-house synthesis expertise.

TRAINING

ICMMO is committed to maintaining a strong link between training and research, and seeks to provide top-level training facilities to a large number of postgraduates student (PhD and Master) in all relevant areas of chemistry. Since 2013, 128 PhD theses have been defended successfully. At the time of writing, 67 PhDs are in progress in the ICMMO unit and 20 M2 students have internships. Trainees are fully-integrated within the research teams' laboratories and are provided with support from the Central Services, as well access to the Instrument Platform facilities, on the same basis as for permanent staff.

The high quality of PhD student recruitment is reflected in the scientific output (Table 4, appendix 4) although coherent ICMMO research project earmarking for ministerial PhD grants (*contrats doctoraux*) has not been fully achieved due to the divergence of policy of the Doctoral School in this regard. ICMMO attracts a sizable contingent of externally-funded international PhD students (36 in total), some of whom are enrolled for joint-diploma awards. These students came principally from China, Lebanon and Vietnam, while Brazil, Tunisia, Algeria, Pakistan and Italy were also represented. Over the assessment period, 6 PhD projects were fully funded by private enterprise, indicating the pertinence of the unit's research training for industry.

The ICMMO PhD community is represented electively on Council and an annual "Doctoral Day" is organized specifically to allow the unit's PhD students to present and discuss their research work. Postgraduate participation at scientific meetings is encouraged: research teams are expected to enroll their PhD students for presentations of their research work at national (or international) level, while the DU continues to lobby the Doctoral School to provide material support for this policy.

As well as playing host for all PhD vivas (which are open to the public), ICMMO provides classroom facilities equipped with video projectors for many Master lecture courses. More than 30 ICMMO personnel contribute directly to teaching in 10 of the 11 Master diplomas offered with a Chemistry speciality by the UPSay School of Basic Sciences, and the Chief Coordination of 5 of these Master programs is ensured (sometimes jointly) by an ICMMO teacher-researcher. Training is also provided in UPSay Master diplomas with Physics, Energy and Engineering specialties. Collectively, this constitutes an unrivalled investment in training at a research level.

Pursuit of excellence in research training means that the acquisition of the Habilitation (HDR) diploma is encouraged within ICMMO. Since 2013, 9 scientists have obtained the HDR status.

It should perhaps be added here that the majority of the ICMMO scientific staff (78 at the time of writing) are university teacher-researchers and have significant statutory implication in the teaching of chemical sciences, as well as the administration of teaching programs at UPSud: at all levels from L1 to M2 at the Faculty of Sciences, at the Orsay University Institute of Technology (IUT), and/or the PolyTech Paris-Sud Engineering School.

ICMMO personnel have also offered vocational training through the CNRS *Formation Entreprises* catalogue.

TECHNOLOGY TRANSFER

A number of innovations emerging from ICMMO research are amenable to technology transfer. To this end, the unit has maintained close interactions with the UPSud DARI (*Direction des Activités de Recherche et de l'Innovation*) and the Paris-Saclay SATT (*Société d'Accélération du Transfert Technologique*). Support is provided to secure protection of intellectual property, resulting in 21 patents being filed. Initiatives to promote technology transfer through the Paris-Saclay PIA instruments have been successful: *Valorisation* support via Charm3at and Lermit LabExes, IDEX pre-maturation (8 projects), and SATT maturation accompaniment (3 projects). Two of these projects have resulted in the creation of start-ups (Ajelis, Novecal) with whom ICMMO retains privileged relations. A third start-up (Click4tag) was co-founded by an ICMMO researcher and the creation of a fourth (Pattox) is anticipated later this year. A license was taken out on an ICMMO patent by Aryballe Technologies for the development of an "electronic nose".

Collaboration with industry has remained a fruitful section of the ICMMO portfolio. The list of industrial partners since 2013 includes: Acros Organics, Aperam, ArévaH2Gen, Auber & Duval, Chpolansky, EDF, Ethera, Greenfish, Michelin, PSA, Renault, Roquette, Sanofi, ST Microelectronics and Te-Ox. Personnel employed by start-ups are accommodated in ICMMO labs for defined periods in order to facilitate progress in joint research projects. (Te-Ox, Ajelis). An ICMMO technology contact cell exists locally, serving as an entry point for first-time contact with industries and to articulate round tables or other introductory meetings, on an occasional basis.

In 2013, the ICMMO *Chimiothèque* was created, in order to preserve the large and varied collection of chemical samples prepared by the research teams, and also to make this collection available to the scientific community at large; this was achieved when the ICMMO joined the *Chimiothèque Nationale* network (47 units) in 2014. The collection (480 products) has been evaluated in 5 HTS campaigns, including one in Australia (for new antibiotics) and one by Sanofi, from which 9 ICMMO molecules were selected as hits and are undergoing further evaluation.

2- Unit's environment

ICMMO is a driving force and a pivotal reference for chemical sciences in the local environment. Members of the unit have contributed to the construction and development of the dominant local structure, the IDEX-labelled **ComUE Paris-Saclay**, which is the intended precursor of the University of Paris-Saclay (UPSay) (see section 5 of this report).

Three members of the unit sat on the transitory UPSay Academic Senate (2013-15) and 7 are currently elected to its replacement, the UPSay Academic Council including one Vice-Presidency. ICMMO occupies a prominent position in the UPSay Chemistry Department, which federates 30 laboratories and serves as a cross-disciplinary (and cross-institutional) structure for the development of chemistry research, teaching and innovation, under the direction of Prof J. P. Mahy. The unit is also implicated in two other UPSay Departments: Life Sciences, Physics of Light and Matter.

ICMMO has been especially active in 3 UPSay "Laboratoire d'Excellence" (Labex) instruments. Most of the unit's scientists are affiliated to the Charm3at Labex, but others participate in Lermit or NanoSaclay. ICMMO personnel are at the forefront of the governance of Charm3at (Director) and Lermit (Deputy Director). These Labex structures have been an important source of funding for all research teams in the unit: for projects, for equipment and/or for training support. Through them, inter-Labex funding for new research projects has also been possible (*e.g.* Charm3at/PALM; Charm3at/SynOrg). The UPSay Labex structures also provide support to facilitate technology transfer, as was outlined above (end of section 1). The UPSay "Equipement d'Excellence" (Equipex) project Andromeda has also been a source of funds for equipment.

The 2016 UPSay Strategic Research Initiative (IRS), designed to support inter-disciplinary projects which address high-level science and technology challenges, earmarked 7 projects in which ICMMO scientists are involved. Two of these (MOMENTOM, NanoTheRad) received major IDEX funding, while the other 5 (Bioprobe, SysABCD, PhyChim^3, BME and ISC2D) are supported by the UPSay Department of Chemistry. Affiliation to a labelled IRS has led to funded partnerships with other Labex groups (BME/Labex LaPSIS)

ICMMO scientists working on new energy sources have been involved in the "Institut d'Excellence dans le Domaine des Energies Décarbonées" *Paris-Saclay Energy Efficiency* (PS2E), including a seat on the Mangemement Board, which has served as a springboard for contracts with industry (Air Liquide, EDF). Other local structures, the two Paris-Saclay "Advanced Research Theme Networks" (RTRA), *Digeteo* and *Triangle de la Physique*, have been a source of research resources.

The architecture and organization of the UPSay structures, coupled with an advantageous geographical location alongside other research centers in the south-west suburbs of Paris, have led to an unprecedented number of fruitful ICMMO collaborations with research groups in other affiliated laboratories, working not just in chemistry but also in biology, physics, engineering or pharmacy, *e.g.* ICSN, LCP, ISMO, BioCIS, IBBMC, IGM, ENS Cachan, ILV, CEA-Saclay, CentralSupelec, Polytechnique. Collaborations with neighboring scientific laboratories – ICSN, CEA, LCB – have been enhanced through the on-site presence of ICMMO personnel. Privileged access to high-performance platforms (complementary to ICMMO's own), such as SOLEIL, CLUPS, CLIO, IMAGIF, is another asset.

3- Research products and activities

Scientific output

The total number of ACL publications[1] of ICMMO research in peer-reviewed scientific journals over the period 01/01/13 to 30/06/18 is **889**. This equates to an ACL/ETPC/y of **2.70**. The average Impact Factor for those publications was **4.461**. These are highly satisfactory bibliometric data. 51 of these papers involved two or more ICMMO research groups, testifying to good cross-team interactions. The Instrument Platform contributed to no less that 245 of the published papers, of which >70% are ICMMO research team productions.

Across-the-board expertise in selective chemical synthesis and the elaboration and evaluation of new materials is the ICMMO hallmark. The unit's scientists continue to produce and characterize an impressive number of molecular structures and materials types, often singularized by their novel architectures, structural complexity, or remarkable properties. An exquisite array of selective and efficient preparative methodologies have been developed in order to foster this production. Each of the 9 research teams will present below a detailed account of its scientific output. Here, a concise overview of the unit's collected research contributions is organized around three focal areas.

Chemistry for and inspired by life sciences
A large number of molecules which are synthesized at ICMMO are targeted for their relevance to some aspect of life sciences.
Proficient methodologies for the selective (often stereoselective) synthesis of diverse amino acid and sugar derivatives have been established, while total syntheses of complex natural products have been a highlight. Bioinspired systems designed to mimic functional peptide secondary structures or to serve as artificial enzymes have been synthesized successfully.
Useful chemical tools have been prepared to address specific life sciences issues, such as ultra-low detection biosensors, electronic tongues, natural product-derived antibacterial polymer films, and click-mediated labels for oligosaccharide recognition in living systems. Sophisticated NMR spectroscopic tools have been developed to characterize the behavior of the numerous biomolecules and analogues prepared at ICMMO. Progress in medicinal chemistry areas has been made, *e.g.* through the development of new approaches for vectorization of anticancer drugs.

Sustainable development chemistry
ICMMO scientists have provided significant innovations to make chemistry "greener".
A major area of activity is fine catalysis. Efforts focused on pertinent present-day transition-metal catalyzed transformations (*e.g.* alkene hydroamination) have been fruitful. Important progress has been made using complexes of low-cost metals as catalysts such as calcium (*e.g.* for cyclization reactions) and iron (*e.g.* for mild oxygenation of organics). New or improved organocatalyzed reactions have been described, in some cases with very high enantioselectivity.
Metal-based catalytic systems have been developed as ambitious devices for artificial photosynthesis or for photocatalytic oxidations, while photochemical cycloaddition reactions have been developed as tools for organic synthesis. Further contributions to sustainable synthetic technologies include studies on the use of alternative solvents (*e.g.* PEG, ionic liquids), reagent or catalyst immobilization, and applications of electrochemical synthesis.
Research on renewable energies has advanced through new developments for hydrogen production via proton exchange membrane water electrolysis or direct photo-electrochemical dissociation of water.

Functional molecules & materials chemistry
ICMMO has consolidated its established track record in the area of functional molecules and materials.
Significant advances have been made in the use of magnetism in the preparation of magnetic switches and spintronic systems (whether molecular or nano-sized), and in the use of light to control spin-crossover of nanoscale materials as well as photochromic organic systems. The creation of chiral structures in an achiral material using a femtosecond laser has been demonstrated.

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[1] In this document, we consider an ACL (*Article dans une revue avec Comité de Lecture*) as a peer-reviewed scientific paper, which includes ICMMO in the authors' affiliations, published in a journal which indexed in the Web of Science database (Thomson-Reuters) with an impact factor. For simplicity in our bibliometric assessment, all ACL journals are considered as having the 2015 Web of Science Impact Factor. The ACL/ETPC/y indicator is the number of ACL papers per full-time equivalent researcher per year; all full-time staff have been included in this calculation regardless of their individual output.

Specialist work on oxides has been pursued. Lithium cobalt oxide electrodes show promise in the development of micro-batteries. Sophisticated hybrid sensors incorporating nanostructured stannic oxide electrodes have been prepared. High-entropy oxides with remarkable ionic conductivity have been developed, while external factors which control thermoelectric properties or crystal growth of massive oxides have been identified. A program for detailed simulation of the behavior of oxides has been developed. Studies of the mechanisms of formation and evolution of microstructure and texture in metals have contributed to the optimization of their physical and mechanical properties and to the development of new multi-metallic materials.

Quantitative data

Quantitative data are given in the Excel file "Données du contrat en cours" supplied separately.

Selected production and research activities

It is gratifying to note that significant production and research activities have been forthcoming from all 9 ICMMO research teams. A showcase section of the most prominent 20% is presented below for each team and constitutes *de facto* the selection of the unit. A complete list of the unit's output is available on request.

Highlights

■ **Scientific results: top-level production, visibility, recognition.** ICMMO scientists published 889 peer-reviewed articles in the evaluation period, targeting high-impact journals (> 50 articles in journals with FI > 10, including 25 in *Angewandte Chemie*), leading to an average IF of 4.461. ICMMO scientists have delivered 279 invited lectures at national or international meetings and 319 seminars, of which 40% were outside France (in 29 different countries).

■ **Technology transfer.** Serving as excellent role models, scientific discoveries made by an ICMMO research group have led to the creation of 2 start-up companies thanks to exemplary cooperation with new local technology transfer structures. Agelis (2014) has won national innovation awards for its production of efficient absorbents for pollutants, while Novecal (2018) prepares precious-metal recovery systems.

■ **Outreach.** Many ICMMO staff communicate on science and research through lectures and demonstrations to schools and non-professional audiences, but a star role is played by the teacher-researcher (R Haumont) who has literally served chemistry expertise on a plate: he has established the award-winning *Centre Français d'Innovation Culinaire*, holds the University Chair "Cuisine of the Future", has given numerous public talks, radio and television presentations, and has published several books on molecular cuisine.

■ **A driving force in the construction of Paris-Saclay.** ICMMO research and ICMMO researchers play key roles in shaping and characterizing the new Université Paris-Saclay structures. This is shown by participation in Department and Labex management, animation of labelled Strategic Research Initiatives, and considerable success in funding calls from within these structures, and has led to excellent collaborative networking with other laboratories on the site.

■ **The ICMMO Instrument Platform.** A comprehensive, high-performance instrument park, unparalleled in the region, allowing state-of-the-art analysis of molecules and materials for ICMMO and collaborating scientists alike. The estimated current equipment value is 7 M€. Recent additions include a cryo-XRD instrument (2014-15), an NMR console upgrade (2016) and a state-of-the-art SECM-coupled AFM (2017); the showcase acquisition for the present contractual period, a 200 kV STEM, will arrive this year (2018).

4- Organisation and life of the research unit

Quantitative data

Quantitative data are given in the Excel file "Données du contrat en cours" supplied separately.

Management, organisation and scientific animation

GOVERNANCE

During the 2010-14 contract, the ICMMO Director (DU) was Prof Jean-Pierre Mahy. Prof David Aitken was Deputy-Director (DA) during that period and was subsequently appointed DU for the new 2015-19 contract, with Prof Anne Bleuzen as DA. The head of Administration (AD) of ICMMO since its creation in 2006 has been Ms. Catherine Charles-Pauwels. The ICMMO management structure, which functions in accordance with the unit's *Reglement Intérieur*, is as follows.

Direction. Governance of the unit is ensured by the Management trio: DU, DA, AD. Weekly meetings are held to treat all matters relating to the unit's operations and to implement decisions. The Head of Human Resources, Head of Finance and Head of Health & Safety/Infrastructure are regular invited participants at management meetings.

Directoire. The Management Board is composed of the Management (DU, DA, AD) and the leaders of the 9 research teams (RE). This Board meets on a monthly basis to discuss ICMMO scientific policy, staff recruitment and investment in equipment.

Conseil du Laboratoire. The unit's Council is composed of 15 elected members and 15 ex officio members (DU, DA, all REs, appointed members); the AD is a standing invitee without vote. Elected members represent three electoral colleges: researchers/teacher-researchers (C-EC), technical/scientific/administrative support personnel (ITA-ITFR), and PhD students. Council is consulted regularly (4-5 meetings/year) on the unit's scientific policy, training policy, funding and budget use, human resources, health & safety and the ICMMO working environment in general. Council's position can be expressed by vote and minutes of each meeting are published on the unit's intranet. The *Bureau du Conseil* composed of 8 members of Council is provided for, but rarely convened. Its purpose is to deal urgently with specific points normally treated by the Council.

Commission du Personnel. The Personnel Committee is composed of Management (DU, DA, AD), the Head of Human Resources (RH), 5 elected Council members (4 ITA-ITFR, 1 C-EC) and 2 REs. The committee meets around 4 times a year and has an advisory role for the DU and for Council regarding ITA-ITRF employment within the unit and is consulted on job profiles, career management, human resource deployment, bonuses, and working conditions for this staff category at ICMMO.

Commission de la Plateforme Instrumentale. The Instrument Platform Committee is composed of Management (DU, DA, AD), 5 elected Council members (2 ITA-ITFR, 1 C-EC), 1 RE, 2 finance personnel (Head of Finance + platform finance officer) and all staff in charge of the Platform's services. This committee oversees the Platform's operating and maintenance budget and establishes priorities for instrument upgrade, which are submitted biannually to Management.

CENTRAL SERVICES

The 9 scientific research teams in ICMMO benefit from considerable support from a centralized "10th team" in the form of the Common Services (SC), which are divided into three sections: Scientific & Technical Support (SST), General & Administrative Services (SAG), and a small Communication cell (COM).

SST has a staff of 16 (+ 1 CDD) and is managed by the DA. The well-equipped Instrument Platform is the largest part of this structure: it provides an instrument park for the analysis of a wide array of sample types originating from molecular and materials chemistry. A full inventory of the equipment is provided in Appendix 2. The platform encompasses 6 NMR spectrometers (including a 600 MHz instrument fitted with a unique proton/deuterium cryogenic probe); 3 mass spectrometers (including an HRMS facility); 4 X-ray diffractometers (single crystal, thin film, powder); EPR (X and Q bands, ENDOR); SQUID, XPS and FTIR instruments; 2 AFMs and 2 SEMs. One of the AFMs, acquired in 2017, is coupled with a SECM. The centerpiece acquisition of the present contract, a 200 kV LaB_6 STM, will arrive later this year (2018). A service is provided for all instruments by qualified technical staff, whereby ICMMO researchers or external collaborators are assisted in data measurement and interpretation. A second part of SST is the nascent Synthesis Pole, whose purpose is to provide practical support through the execution of predefined chemical synthesis projects as a service to the research teams of the unit. Since 2013 the pole operated through a series of fixed-term contracts until the first permanent staff recruitment was achieved at the end of 2014. Expansion of this service through further recruitment remains a priority for the unit. The SST is completed by a valued glassblowing workshop and other infrastructure supports.

SAG has a staff of 23 (+ 2 CDD) and is managed by the AD. In addition to dealing with general administrative affairs, SAG provides, across the board at ICMMO, a Project Accompaniment Service; an IT Service; an HR Service; a Health & Safety/Infrastructure Service and a Finance Service, each with a competent Head of Service reporting to the AD on a regular basis. Since 2011, ICMMO has an autonomous financial management status (*Délégation Globale de Gestion*) under the auspices of UPSud, which is accommodated by appropriate staff distribution. The unit has the responsibility for the administration of non-permanent recruitment (*c.* 100 per year). ICMMO draws up and monitors its own annual budget (3-4 M€) for both institutional and contractual credits, reporting to the UPSud Accounting Office at the end of the fiscal year. In 2016, new French regulations on the Budget Management and Public Accounting (GBCP) required that multi-year budget programming of research contracts be implemented.

COM is represented by the Communications Manager who reports directly to the DU and who chairs the ad hoc Communication cell of the unit. The COM portfolio includes the organization of meetings and events (see the next section), group visits, internal information dissemination and intranet, and liaison with external communication networks. A key objective, currently undertaken jointly with the Head of IT, is the complete renewal of the unit's website.

SCIENTIFIC ANIMATION

Internally, each research team organizes its own lab seminars with appropriate frequency and content. The ICMMO unit has a lively Chemistry Seminar Series, with 20-25 invited external speakers per year; disciplinary areas are varied in order to maintain wide appeal. Visiting academics and new staff members are included in the seminar programme. Periodically, ICMMO Scientific Days are organized, in which all scientists participate. The format is a series of presentations by each research team followed by round-table discussion, allowing fruitful scientific exchanges between teams and facilitating new joint research projects. The post-graduate student community organizes an annual ICMMO PhD Day, with a programme of oral communications and poster presentations from all teams and prizes awarded.

It is worth mentioning that other events (such as the summer barbecue or the New Year wishes), widely appreciated by all ICMMO members, foster team-spirit on the scale of the unit and provide a less formal opportunity for furthering scientific discussions. One notable event was the "*L'ICMMO a 10 ans*" symposium, attended by all members of the unit, to mark 10 years of existence with a series of personal reflections from different unit members.

BUDGET POLICY

Each research team has the responsibility of defining its research objectives which are commensurate with its resources. The unit's financial policy is to distribute a sizable part of the basic support grants from institutions to the research teams. Management retains an annual budget of 120 k€ to ensure the correct functioning of the Central Services and to maintain and develop the Instrument Platform. Research teams have full responsibility for the use of funds which are generated through successful scientific research calls and other contracts. The Central Services provide appropriate financial management and retains a modest fraction (currently 2%, only applied for eligible funds) as a contribution to the operating costs of the unit.

Parity

The Management trio for the present contractual period comprises of 1 man and 2 women. The other members of the Management Board are 8 men and 2 women. The gender split of the elected members on the present Council is 45% men, 55% women. On the previous Council, these figures were 55% men, 45% women.

Since 2013 the gender split for C-EC recruitment is 65% men, 35% women, while for ITA-ITFR recruitment these figure are 30% men, 70% women. (For the record, ICMMO is not formally represented in the employers' recruitment committees.)

Both CNRS and UPSud have been vigilant regarding work-related psycho-social risks, including sexual harassment, and have made efforts to prevent them through training and awareness sessions. ICMMO staff at all levels are encouraged to follow these sessions. Should an incident arise, the confidentiality of the unit's in-house HR service is the first port of call; efficient referral to the institutional HR services is ensured if required.

Scientific integrity

ICMMO and its personnel adhere to the guidelines on scientific integrity issued by CNRS Ethic Committee (*Promouvoir une recherche intègre et responsable*, 2014 and 2016 update). These apply, in particular, to the definition of legitimate co-authorship of scientific articles, including contributions made by scientific staff of the Instrument Platform. An "ICMMO article" is defined as one which contains practical or intellectual contributions made by an ICMMO scientist in the course of his/her activities as a member of the unit, and indicates "ICMMO" as well as the institutional names in the authors' affiliations.

Part of the scientific publication policy of ICMMO is to privilege well-reputed and prominent journals operated by established publishers. Many of these publishers apply software screening to submitted manuscripts to detect plagiarism.

In each research team, laboratory notebooks are used as standard policy by permanent and non-permanent personnel for recording details of research experiments on a daily basis and are cross-checked internally.

Should a conflictual situation arise as regards scientific integrity, referral is first made to the DU. Further referral may then be made to UPSud's appointed Scientific Integrity Advisor (SIA; Prof P. Berthet, ICMMO). Periodic presentations by the SIA to the ICMMO community on issues of scientific integrity will begin from 2018.

Health and safety

Safety is a top priority and is given full consideration within the unit's organization. ICMMO has 2 personnel members with *Assistant de Prévention* (AP) status, who advise the DU on all matters relating to H&S. Each research team has a H&S correspondent; joint meetings are held regularly with the APs and on occasions with the Science Faculty H&S and medical services. ICMMO has 12 workplace first-aid personnel, who follow annual qualification courses. The ICMMO PCR (competent person in radiation protection) transferred to another unit in 2016, and was replaced expediently by a new PCR (T. Nait) in 2017 following training and validation.

All new personnel arrivals are provided with a "welcome pack" containing safety instructions and guidelines for good laboratory practice. Workplace aptitude is validated by the local H&S correspondent and an AP. Twice-yearly, two-day mini-symposia on security awareness are organized for recently-arrived ICMMO personnel (up to 100 people annually); participation is compulsory. These events are animated not only by the APs but also by external experts from CNRS and UPSud. Efforts are made to provide English translations for non-French speakers. Further certified work awareness training is supplied using the CNRS NEO software application.

Annual "hands-on" training is provided by the APs for fire-extinguisher use and defibrillator use.

Security

Protection of Intellectual property. Recognition of hierarchical responsibility, and thereby operational transparency of research workplans and data manipulation, are a prerequisite for the signature of all internship or hosting agreements. In particular PhD students are required to sign and respect the content of the *Charte de Thèse* document of the Doctoral School.

IT services and digital data storage. All access to numerical data and network services within the unit requires individual authentication. The unit's servers are hosted in a dedicated space accessible only to IT staff, and the ICMMO network is isolated from the exterior by a firewall. ICMMO operates under the auspices of the Information Systems Security Policy of UPSud and the unit's IT staff work in full cooperation with the UPSud Computer Centre for immediate handling of any security incidents.

In 2015, the Chief Security and Safety Officer of the Ministry of Research considered that the activities and expertise present at ICMMO were sufficiently important for the unit to be designated a ZRR (*Zone à Régime Restrictif*), an area to which access is limited for the purposes of protecting the scientific and technical interests of the state. The unit has been required to compile and submit the appropriate files; designation of ZRR status is pending.

5- SWOT analysis

Strengths	Weaknesses
- Strong scientific output. Testified by the number and the quality (average IF) of scientific publications. **- High performance Instrument Platform.** The qualified staff make a significant contribution. **- Excellent integration in the local PIA environment.** ICMMO science contributes to and is strengthened by Labex, Equipex and other local structures. **- Attractiveness on a national and international level.** High-profile scientists recruited in competitive national CNRS campaigns, top-level teacher-researchers recruited to university positions. **- Efficient and reliable centralized administration.** The unit’s management is respected, both internally and by the supervising institutions. **- Technology transfer.** Good interaction with the SATT facilitates exploitation of research results when this is possible.	- **Nostalgia for bygone structures.** Created in 2006, the unit is still relatively young; a sentiment that “things were better in the old days” still lingers in some sectors. - **Difficulty in coherent planning.** The apparent lack of medium-term planning strategies of the part of the supervising institutions is prejudicial to the units performance. - **Lack of concertation with the Doctoral School.** The attribution of Ministry PhD grants takes no account of the unit’s scientific policy, despite the unit being the largest single participating laboratory.

Opportunities	Risks
- Université Paris-Saclay. It is the declared policy of the new institutional environment to provide the means and the motivation for scientific excellence. - **Reinforce Chemistry as a contemporary discipline.** Paris-Saclay as a springboard for the amalgamation of units under a single, fully-encompassing Chemistry Department. - **Consolidation of the Instrument Platform.** Coordination with complementary platforms in the same geographical sector, leading to an unrivalled high-performance multi-technique analytical park. - **Strengthen the Synthesis pole.** Governing bodies recognise the importance of a centralized dedicated fine-synthesis service for researchers. - **BPC, a brand new building.** More space, modern facilities, better organization. - **Emerging structures within Paris-Saclay.** The unit is well placed for inclusion in the “follow-ups” to the current Labex structures CHARM3AT, LERMIT and NanoSaclay.	- **Diminished technical / scientific support staff.** Contributions from ITA and ITRF staff remain essential for top-level research production. - **Reduction in research staff.** The continued regression in CNRS scientist numbers and non-renewal of vacant UPSud positions will have a detrimental effect on ICMMO research performance. - **The move to the new BPC building.** The cost and the duration of the move are uncertain, but it seems likely that research activities will be hindered and training abilities impaired (at least temporarily). - **Restrictions imposed in BPC.** *Cohabitation:* the coherence of the ICMMO unit might be challenged in the future BPC structure by the size and disciplinary orientation of the Faculty of Pharmacy. *Logistics*: Efficient functioning of ICMMO may be hampered by architectural impositions and legal restrictions applied in the future facilities. - **Bureaucracy.** The complexity of the emerging UPSay governance may result in an excessive number of administrative tasks of dubious benefit. This distracts scientists from their real professional value and has an endemic demoralizing effect.

6- Scientific strategy and projects

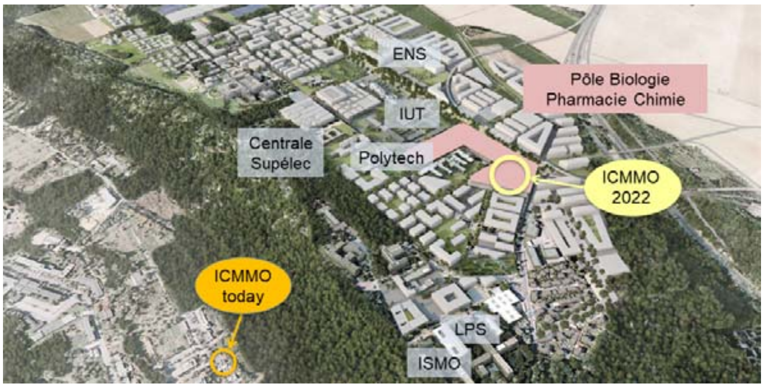
INSTITUTIONAL CONTEXT

At the time of writing, all indications point towards the creation of the Université Paris-Saclay (UPSay) on 1st January 2020. UPSay will therefore replace UPSud as the university institution to which ICMMO is affiliated. ICMMO has a clear ambition to continue to play a leading role in the constitution of the University of Paris-Saclay, and especially in the structuring of chemistry on this plateau. It will be ICMMO policy to be fully implicated in (and indeed central to) the structure and the organization of chemistry as a discipline under the auspices of UPSay. This can be achieved through cooperative policies (collaborations, equipment access, joint workshops and seminars) with neighboring chemistry units (ICSN, ILV, LCP) and the continued commitment and dedication of ICMMO staff in the development of the appropriate structures, for example in the leadership of the UPSay Chemistry Department (J.P. Mahy).

The UPSay context is expected to provide constructive opportunities for ICMMO. The declared policy of the new institutional environment - to encourage and support excellence - will serve as a podium for cutting-edge interdisciplinary project development, which ICMMO intends to shape. The continuity of the existing "excellence" structures and Strategic Research Initiatives in one form or another is widely anticipated, and ICMMO is well positioned to be a major contributor to emerging structures. These may take the form of federative Institutes on a Paris-Saclay scale, focussing for example on Health and Therapeutic Innovation or Catalysis Sciences.

The impact of ICMMO on the Paris-Saclay landscape will be reflected by its geographical move to new premises within the Pharmacy-Chemistry-Biology (BPC) Pole, which will be constructed in the heart of the Paris-Saclay Campus and certified "High Environmental Quality". The unit will occupy 10000 m^2 of space on three contiguous floors of a single building, shared with research units of the Faculty of Pharmacy. For ICMMO, the move is expected to provide improved working conditions for researchers (logistics, space, security) and better physical localization of the Central Services (SAG and SST), particularly the unit's Instrumental Platform. Specific laboratory facilities for technology transfer activities have been earmarked. The BPC pole will also be the primary location for Master Chemistry teaching, which will facilitate the implication of ICMMO in training through research. The "Campus Mission" steering committee of this project for ICMMO is headed by B. Poumellec, who will continue in this capacity; progress will also be closely monitored by the DU.

The location will bring ICMMO scientists in close proximity not only with pharmacists (who will also move to the BPC pole) but also with other chemists and physicists working in UPSay-affiliated laboratories on the Saclay plateau (ISMO, LPS, ENS, CentralSupelec, CEA). Staff with teaching duties at IUT or Polytech will be ideally located. Despite institutional differences, ICMMO chemists will retain constructive relations with colleagues affiliated to the Ecole Polytechnique.



MANAGEMENT

The management structure of the unit will remain essentially the same as that in operation during the 2015-19 contractual period. Governance will be ensured by the same Management trio, *viz.* Prof David Aitken (DU), Prof Anne Bleuzen (DA) and Ms Catherine Charles-Pauwels (AD). The management team's proposal of serving a second term of office was discussed during the Autumn season of 2017 and was approved in a statutory vote of confidence by the Council on 6th December 2017 (20 votes in favor, 7 against).

The unit's scientific policy, training policy, funding and budget policies and human resources policies will be discussed and decided in concertation with the existing consultative Management Board and Council structures as well as their emanations. The current frequency of meetings of these structures appears to be appropriate and will be retained (4-5 meetings/year for Council, 8-10 meetings/year for the Management Board). The unit's Central Services will continue to provide strong and reliable in-house support and ITA/ITRF recruitment priorities will take account of the importance of the Central Services.

The Instrument Platform and the Synthesis pole will play an important role in central support for ICMMO research and will continue to provide high level scientific services to the research teams across-the-board. Efforts will be made to maintain a pro-active communication cell and an enterprising technology transfer cell as privileged points of contact for the unit.

The Management will continue to lobby for coherence between the Doctoral School's recruitment procedures and the interests of all scientific groups within the unit.

RESEARCH TEAM ORGANISATION & PROJECTS

The reorganization of the unit's forces, which was implemented 5 years ago to provide the 9 current research teams, appears to have been successful in terms of the scientific production outlined above. For the next contractual period the research teams intend to continue working on the same organizational basis and with the same personnel line-ups Internal evolution (such as a change in the Team Leader in a few cases) will be indicated in the appropriate section of each teams' self-assessment document.

Each team will retain its scientific specialty in disciplinary terms, defining for the period a portfolio of objectives in line with its resources and its expertise. Specifically this means that the disciplinary areas implicated will include biological chemistry, organic and inorganic molecular chemistry, materials chemistry, catalysis, electrochemistry, NMR spectroscopy and nano-sciences. Joint projects between two or more teams will be encouraged by Management through small incentive packages and through the organization of thematic workshops on three focal areas: chemistry for and inspired by life sciences; sustainable development chemistry; and functional molecules & materials chemistry. Cross-team interest in societally important issues will be encouraged but it is not intended to formalize these themes as working structures (or alternatives to teams) within the unit. Funding will remain a critical issue and the current success rate in the context of the local environment (PIA / Paris-Saclay) is likely to incite ICMMO research teams to continue to work harmoniously with research groups affiliated to other units in the vicinity.

Each team's scientific projects for the next 5 years will be presented in the individual self-assessment documents which appear in the pages below.

Self-assessment document

Team 1 – CP3A

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Chimie Peptidomimétique et Procédés Alternatifs**
Acronym:	**CP3A**
Director's name (current contract):	**Marie-Christine SCHERRMANN**
Director's name (future contract):	**Marie-Christine SCHERRMANN**

SELF-ASSESSMENT DOCUMENT

1 Research products and activities

Scientific output

The "Chimie Peptidomimétique, Photochimie et Procédés Alternatifs" (CP3A) team was created at the beginning of this five-year period. It brings together a large part of the former "Synthèse Organique & Méthodologie" (SOM) team and the green chemistry group of the former "Procédés et Substances Naturelles » (PSN) team with common interests in the development of sustainable synthesis technologies using, among other things, clean and unconventional processes for the preparation of compounds having applications in the fields at the chemistry and biology interface. The research is structured in three axes:

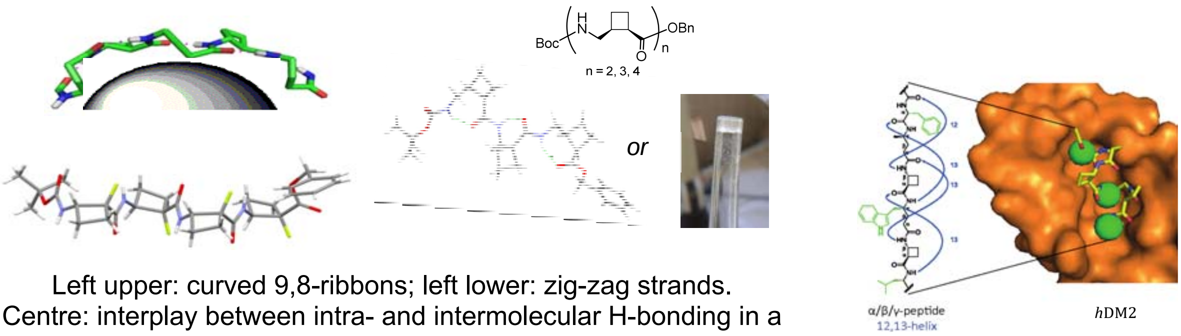
- Peptides and peptidomimetic foldamers
- Methodology in organic synthesis: photochemistry, organocatalysis and silicon reagents
- Green Chemistry and alternative processes

The CP3A team published 50 articles in peer-reviewed journals, corresponding to 2.19 articles / full-time equivalent researcher; the average impact factor was 4.63. Team members also reported their results through 13 invited lectures, 52 communications (14 oral and 38 poster presentations) and 21 invited seminars.

- Peptides and peptidomimetic foldamers

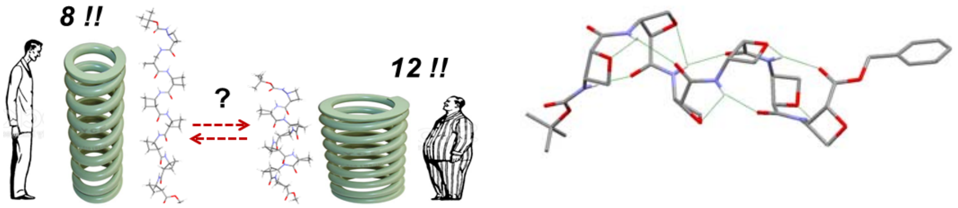
A preeminent activity of the group is the development of peptide-based foldamers, which has led to international recognition. Our speciality is the use of cyclobutane β- and γ-amino acids as monomers for the bottom-up rational construction of folded molecular architectures which are supported by non-covalent interactions (mainly H-bonds). Historically, we were the first to describe (in 2010) the 12-helix folding of homooligomers of *trans*-cyclobutane β-amino acid (*t*ACBC). Over the last 5 years we have diversified the composition of foldamer peptides that incorporate 4-membered ring building blocks and we have discovered and characterized new folding manifolds as well as design features for controlling folding preferences.

• We examined the oligomers of α-fluorinated *cis*-cyclobutane β-amino acid (*c*ACBC) and showed that they can adopt "zig-zag" strand conformers which barely rely on intramolecular H-bonds (*New J. Chem*. 2015). We discovered an unprecedented 9/8-ribbon conformational preference for a β/γ-peptide built using *t*ACBC and GABA (*Chem. Commun.* 2015); the topology of these oligomers is determined by a remarkable conformation/configuration code, which dictates that these ribbons should adopt a partially-curved architecture. We examined oligomers of a *cis*-cyclobutane-constrained GABA analogue and identified a concentration-dependent interplay between rare ribbon-like structures stabilized by intramolecular 7-membered ring H-bonds, and an organized supramolecular assembly leading to thermoreversible organogel formation (*J. Org. Chem.* 2017). We designed a "minimal constraints" template to induce a β/γ-peptide to adopt preferentially a 13-helix conformer, which is a structural mimetic of Nature's own α-helix in peptides and proteins (*Chem. Commun*. 2016). This led us to collaborate with Prof A. Wilson, Leeds, to demonstrate in 2016 the first proof-of-concept for the bottom-up design of functional α/β/γ-peptide foldamers which act as inhibitors of the p53-hDM2 protein-protein interaction (PPI) (*Angew. Chem. Int. Ed.*, 2016).



Left upper: curved 9,8-ribbons; left lower: zig-zag strands. Centre: interplay between intra- and intermolecular H-bonding in a constrained γ-peptide (ribbon-like or organogel). Right: peptide foldamer designed as an α-helix mimetic for PPI inhibition.

• Detailed studies were conducted of the aza-analogue of *t*ACBC, *N*-aminoazetidinecarboxylic acid (AAzC). We showed that this foldamer building block has a strong proclivity to adopt a "hydrazino-turn", a robust 8-membered ring H-bonded conformer feature which we characterized spectroscopically in detail thanks to fruitful collaborations with the NMR team (ICMMO) as well as Dr A. Zehnacker (ISMO, Orsay) and Dr M. Mons (LIDYL, CEA-Saclay) (*Angew. Chem. Int. Ed.* 2014). We used this secondary structure to destabilize the 12-helix adopted by *t*ACBC homooligomers: with an AAzC residue at its *N*-terminal, a (*t*ACBC)$_5$ segment can forced to adopt a "hydrazino-head" stabilized 8-helix conformation, while a (*t*ACBC)$_3$-AAzC-(*t*ACBC)$_4$ octapeptide segment also adopts an 8-helix predominantly (*Angew. Chem. Int. Ed.* 2015). Atomic-level fine tuning of a peptide foldamer architecture has thus been demonstrated and provides, by design, the longest known 8-helical β-peptides. We also studied homooligomers of the natural product oxetin, an oxa-analogue of *c*ACBC. We showed that the uncommon 10-helix conformer which was adopted was stabilized propitiously by a parallel network of previously-uncharacterized 5-membered ring H-bonds (*Chem. Commun*. 2018).



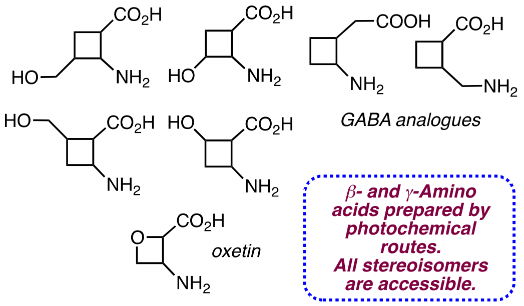
Left: residue-controlled switchover from 12-helix to 8-helix.
Right: series of bifurcated 5-ring/10-ring H-bonds which stabilize a 10-helix β-peptide conformer.

- In collaborative work, we have prepared bespoke peptides for the complexation of actinides (with E. Simoni, IPN-Orsay, *Inorg. Chem*. 2016) and we have prepared short peptide fragments for the preparation of truncated analogs of Neuropeptide Y, currently being evaluated as selective ligands for Y1 and Y4 receptors (with O. Reiser, Regensburg). We collaborated with A.-F. Burnol & T. Issad (Institut Cochin, Paris) in the development of an insulin-sensitizing compound for the treatment of diabetes, for which the synthesis requires meticulous control of a key peptide coupling step (*Scientific Reports* 2017). This cross-disciplinary project was supported by the "IdF-Innov" technology transfer service and led to a patent filing in 2017 with international extension in 2018.

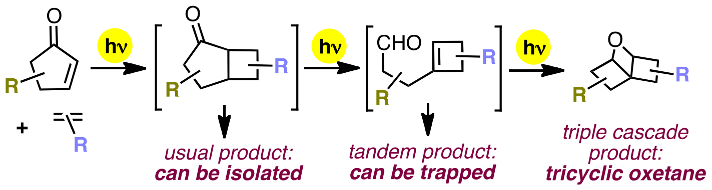
- Methodology in organic synthesis: photochemistry, organocatalysis and silicon reagents

- As we indicated in the previous section, functionalized cyclobutanes are used ubiquitously in the group and we have developed practical synthetic access thereto; today we possess the most extensive catalogue of such compounds prepared in-house synthetically. Recently we have expanded our library of β- and γ-cyclobutane amino acids using photocycloaddition chemistry to construct the 4-membered ring.

Practical synthetic access has been established to derivatives of ACBC bearing hydroxy or hydroxymethyl substituents at either C3 or C4 with full diastereoisomeric control, and resolution procedures have been implemented (*Org. Biomol. Chem.* 2014, *J. Org. Chem.* 2018). Ongoing work exploits the chemistry of the alcohol function to diversify the inventory of substituted ACBCs. A Paternó-Büchi photocycloaddition reaction was used to develop a short synthesis of all isomers of the natural product oxetin (*J. Org. Chem.* 2016). In part collaboration with Dr O. Yazbeck (Lebanese University, Beirut), several approaches for the syntheses of non-racemic cyclobutane γ-amino acids (rigid GABA analogues) have been examined and compared (*J. Org. Chem.* 2017).

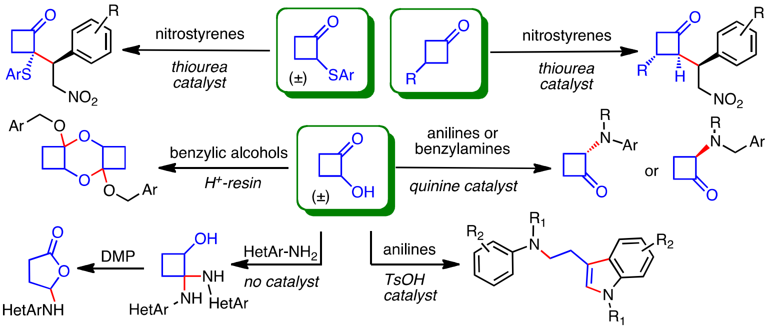


- The selective activation of molecules by the absorption of light can provide access to complex structures which are difficult to obtain otherwise, and we have probed the use of photocyclization reactions to explore molecular diversity. Studies have included pyrimidinedione photodimerizations, tandem retro-[4+2]/[2+2]-cycloadditions, and pinacol-type rearrangements of bicyclic Paternó-Büchi photoadducts (*Eur. J. Org Chem.* 2017).



A significant achievement was to harness the reaction between cyclopentenone and an alkene to give, in a fully controlled manner, a bicyclic adduct, a cyclobutene aldehyde or an unprecedented tricyclic angular oxetane, via single, tandem, or triple photochemical reactions, respectively (*Angew. Chem. Int. Ed.* 2018).

- Cyclobutanones are versatile small-ring building blocks for organic synthesis. A focus of the synthetic methodology program conducted in the group involves metal-free transformations of substituted cyclobutanones to provide access to more complex intermediates in a selective fashion. This work constitutes a long-standing collaboration with the research group of Dr. A. Frongia and Dr. F. Secci (University of Cagliari, Sardinia). Small libraries of 3-alkyl/aryl- and 2-arylthio- substituted cyclobutanones were desymmetrized and deracemized, respectively, in organocatalyzed Michael reactions with a panel of nitrostyrenes with good to (very) high regio-, diastereo- and enantio-selectivities (*Eur. J. Org Chem.* 2015, *Org. Biomol. Chem.* 2016). We have developed racemic 2-hydroxycyclobutanone as a useful synthon, by establishing: *organocatalyzed* enantioselective Amadori-Heyns rearrangements to give 2-aminocyclobutanones (*Adv. Synth. Catal.* 2014); *Brønsted acid-catalyzed* cyclodimerizations (*Org. Biomol. Chem.* 2017) and tandem reactions with anilines to provide direct syntheses of tryptamines (*Chem. Commun.* 2015); and *non-catalyzed* aminal formation, from which γ-amino-γ-lactones are prepared by oxidative ring expansion (*Org. Biomol. Chem.* 2017).



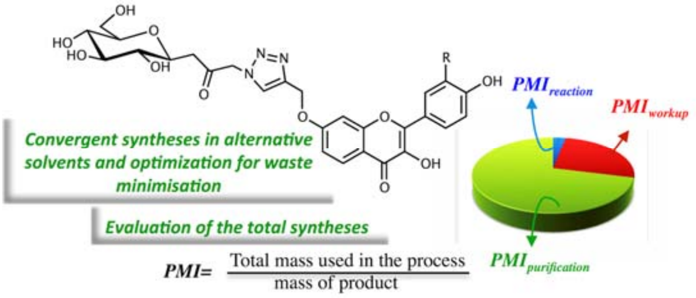
- The group has been interested in other methodologies for the synthesis of non-canonical amino acids. We have used a one-pot three-component methodology involving an α-silyloxymalononitrile as MAC (Masked Acyl Cyanide) reagent for the oxyhomologation of protected L-serinals to give a useful entry to *syn*-3-amino-2,4-dihydroxybutanoic acid and a panel of cyclic derivatives thereof. We have recently discovered how the habitual *syn* diastereoselectivity of MAC reactions can be switched to *anti*, for the first time, allowing access to orthogonally protected derivatives of *erythro*-β-hydroxyaspartic acid, a key constituent of a number of macrocyclic peptides (*Org. Biomol. Chem.* 2017).

- Green Chemistry and alternative processes

- Solvents generally constitute the most important part of the mass of a reaction medium and we are therefore interested in their substitution by non-polluting alternative media. We explored the use of PEG, non-toxic and easily recyclable alternative solvents, to achieve various transformations. Although different research groups have shown that PEG-catalyst recycling was very effective, determination of metal content in the product and in the PEG had never been carried out. We conducted this study on copper-catalyzed azide-alkyne cycloaddition (*New J. Chem*. 2015) and demonstrated, for the first time, that the amount of residual metal in the products was greatly reduced thanks to the chelating properties of PEG. In collaboration with S. Berteina-Raboin (University of Orleans), we have developed various syntheses of heterocycles in PEG_{400} as the solvent (*Eur. J. Org Chem.* 2014; *RSC Advances* 2016; *Molecules* 2018).

These synthetic methods in alternative solvents have been applied to the synthesis of flavonoids linked to a *C*-glucoside by a triazole; these multi-step syntheses were evaluated by new metric of green chemistry described below (*Green Chem*. 2016).

- In order to quantify syntheses in terms of green chemistry, various metrics have been proposed such as the Sheldon's E factor (mass of waste / mass of product). The determination of this factor whose calculation is based on the outflows is not easy for multi-step syntheses and it is more convenient to calculate the mass intensity (MI) whose determination is based on the inputs (mass materials used / mass of the product). With J. Augé (University of Cergy Pontoise), we demonstrated that MI could be calculated for linear and convergent sequences and we applied this calculation algorithm to the synthesis of PEG with 6 or 18 hydroxyl functions (*Green Chem*. 2013). Aiming to measure the impact of the operation that affects to a greater extent the mass intensity of the whole process (PMI), we determine this green metric for the reaction (PMI_R), the workup (PMI_W), and the purification (PMI_P) for the total synthesis. This analysis, applied to flavonoids linked to a C-glucoside by a triazole, revealed that for the total synthesis of these compounds, largest part of the material used was dedicated to treatments and purifications, this was particularly dramatic when chromatography was necessary (*Green Chem*. 2016; *Beilstein J. Org. Chem*. 2016).



• Green chemistry also aims to reduce energy consumption and increase process safety. In this context, mesofluidic systems represent a good alternative to conventional reactors because their high ratio (surface / volume) allows a better control of mass and heat transfer, the low volume of reaction increasing safety. Continuous flow chemistry is also a key technology for implementing organocatalytic reactions. We have described the preparation and characterization of a novel heterogeneous chiral organocatalyst by grafting cupreine onto silica and studying its performance for Michael addition (*RSC Advances* 2015). The conditions developed in flow allowed us to reach an overall turnover of 60 using 2-MeTHF as solvent, which is a relatively high value for organocatalysis.

Highlights

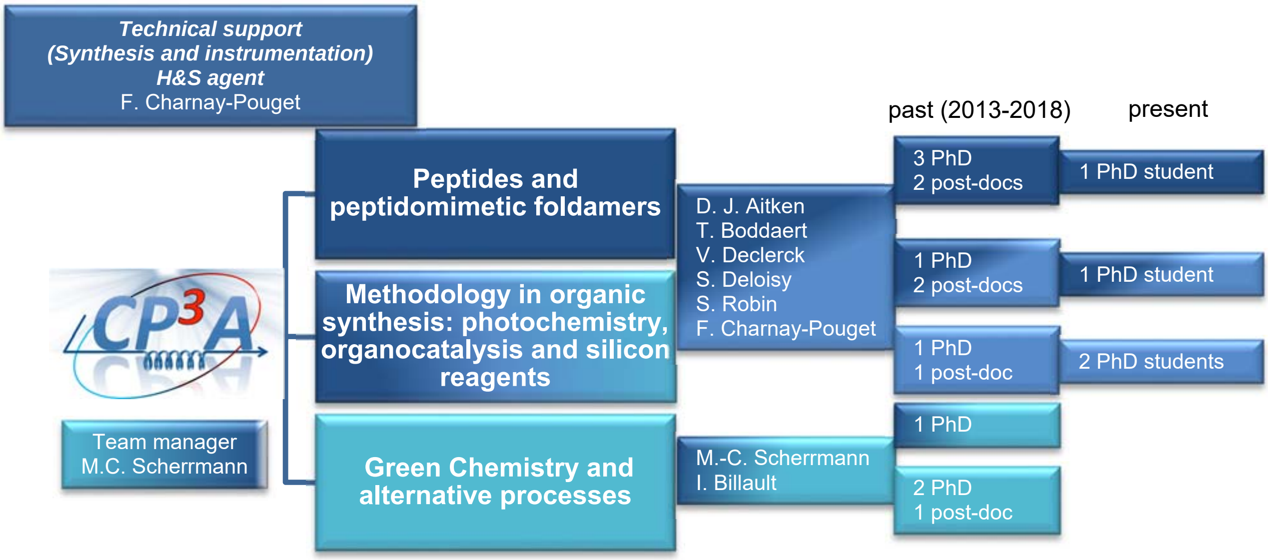
- **International recognition in foldamers**. The team has made significant contributions in the area of peptide foldamer science, including the discovery of rare foldamer topologies and the design of an unprecedented "bottom-up" functional α-helix mimetic. 15 high-quality papers were published, 7 invited conference lectures were delivered, numerous seminars presented, and 2 invitations were received to serve as Guest Editor for "foldamer themed issues" of peer-reviewed journals
- **Technology transfer**. A multi-disciplinary collaboration with a team of biologists at the Cochin Institute (Paris) was successful thanks to a critical contribution in the synthesis of a potential anti-diabetes agent, leading to "IdF-Innov" maturation support in 2016, patent filing in 2017 and an international extension in 2018.
- **Attractiveness at the international level**. A long-standing collaboration with academics from the University of Cagliari (Italy) resulted in the publication of 7 co-authored articles on organocatalysis and 2 on photochemistry. Two international PhD joint-diplomas were successfully achieved; 4 visiting foreign researchers, 3 visiting foreign PhD students and 4 visiting foreign Master students were hosted in the team.
- **Authoritative monograph in green chemistry.** In the increasingly important area of sustainable development, a comprehensive book dealing with the theory and the practice of green chemistry was co-authored by the Head of the CP3A team. "*Chimie Verte: Concepts et Applications*", CNRS Editions, 2016 (491 pages).

2 Organisation and life of the research unit (or the team/theme if relevant)

Management, organisation and scientific animation

The majority of the CP3A team members were part of the "Synthèse Organique & Méthodologie" (SOM) team of the previous contractual period, led by Prof. D.J. Aitken. Since the latter became Head of the Institute, it was decided collectively that CP3A team leadership should be entrusted to Prof. M.-C. Scherrmann.

During the period considered, 3 permanent members left the team either for retirement (L. Blanco, DR CNRS and J. Ollivier, CR CNRS) or for mobility (R. Piccardi, CR CNRS); these staff were CNRS researchers and were not replaced. Currently, the team is composed of 8 permanent staff (2 Profs, 2 MCF-HDR, 3 MCF and 1 AI) whose activities are dispatched among the 3 themes according to the following chart.



The use of the team's financial resources is decided collectively at monthly meetings of permanent staff, during which the team leader presents an up-to-date summary. Decisions are made in a collegial manner at these meetings concerning the purchase of equipment, participation at scientific symposia and the recruitment of trainees.

Scientific seminars are also organized for all the members of the team (permanent or not) during which the results of the various subjects are presented and discussed.

It should be noted that the members of the team, except an AI, are teacher-researchers, strongly involved in educational activities (I. Billault, responsible for the analytical chemistry platform in master 1; M.-C. Scherrmann, co-responsible for professional M2 Instrumentation and Methods of Molecular Analysis; S. Deloisy, responsible for the continuation of studies at the IUT; V. Declerck, head of organic chemistry studies at the Chemistry Department of the IUT; T. Boddaert, head of chemistry studies at Institut Villebon-*Georges Charpak*), as well as in administrative responsibilities (D. J. Aitken, director of the Institute and member of the Academic Council of Paris-Saclay; all the permanent staff are or were members of the ICMMO Council; D. J. Aitken, M.-C. Scherrmann, members of the Chemistry Department Council; M.-C. Scherrmann, member of the Bureau of the Research Commission and the Academic Council of Paris-Sud University; V. Declerck, S. Deloisy, I. Billault and M.-C. Scherrmann, members of the Consultative Commission of Specialists for Chemistry). These activities, as well as the quality of the scientific production, have been recognized by the national or university authorities through promotion for 4 members of the team during the last 5 years.

3 SWOT analysis

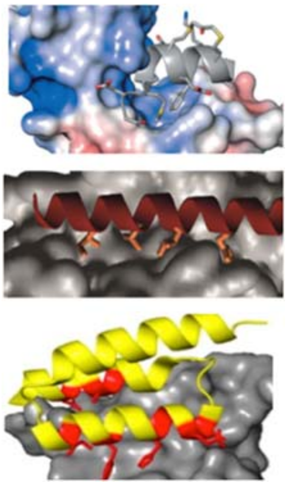
Strengths	**Weaknesses**
➢ The team is well positioned in the local environment and as a result, has a growing number of collaborations within the perimeter of Paris-Saclay University ➢ International attractiveness ➢ International recognition in the field of foldamers	➢ No CNRS researcher in the team ➢ Few contracts with industry ➢ Number of teacher-researchers with the authorization to supervise PhD research (HDR) ➢ Low success rate in calls for projects
Opportunities ➢ Integration in the Department of Chemistry of Paris-Saclay University ➢ Position of Paris-Sud University in the structuring of Paris-Saclay University with a strong objective of developing international collaborations ➢ Foster of a European network of synthetic organic photochemistry ➢ Contemporary incentives to develop environmentally friendly methodologies	**Threats** ➢ Too many administrative tasks ➢ Doctoral School 2MIB policy for awarding PhD grants ➢ Slow progress of the "alternative processes" theme due to limited manpower

4 Scientific strategy and projects

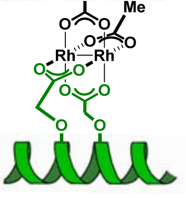
The organization of the team will remain identical for the next period (see section 2), as well as the research themes for which the objectives are described below.

- Peptides and peptidomimetic foldamers

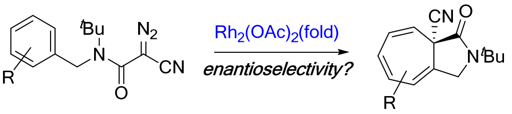
The group will continue its research on peptide-based foldamers. In the first two themes, the predictable constraints imposed by *trans*-cyclobutane β-amino acid (*t*ACBC) monomer building blocks will be exploited to construct helical foldamer manifolds which *function*, either in a biological sense or in a chemical sense. In the third theme, a search will be conducted for new types of H-bonding interactions which allow regular folding patterns to be adopted.



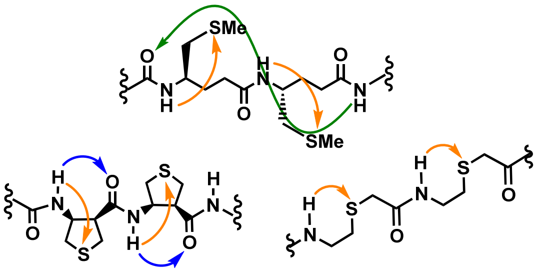
• Functional helical foldamers: bioactivity. This project will showcase a β,γ-peptide paradigm for the bottom-up design and modular construction of molecular architectures which mimic both the structure and the function of a natural α-helix. Three pertinent biological systems will be considered, with the explicit objective of demonstrating the power of the design approach for biomedical and pharma applications. The 1st target system is the RNase S-peptide/S-protein interaction, which implicates a (*i*, *i*+4, *i*+7) hot spot recognition triad near the N-terminal of the S-peptide sequence (upper). The 2nd target system is the PPI between BCL-x$_L$ and BIM, central to apoptosis regulation, which implicates a four-residue (*i*, *i*+4, *i*+7, *i*+11) hot-spot disposition (centre). The 3rd target, which has a central role in angiogenesis, is the PPI between Vascular Endothelial Growth Factor (VEGF) and its receptors (VEGFR); the novel strategy here will be to "trap" VEGF using truncated analogues of the deactivator peptide Z-VEGF by reproducing the N-terminal helix segment with a (*i*, *i*+1, *i*+4, *i*+5) hot-spot recognition repertoire (lower).



• Functional helical foldamers: catalysis. The use of β-peptides as ligands in functional metal complexes is unprecedented. In this project, regular helical β-peptide foldamers will be assessed as novel asymmetric ligands for enantioselective metal-catalyzed transformations. As a illustrative test case, dirhodium(II)-catalyzed intramolecular Buchner reactions of benzylic α-diazo-α-cyanoacetamides will be studied, in order to prepare useful bicyclic frameworks frequently encountered in natural products.



• New H-bonding paradigms for atomic-level foldamer design. A limiting factor in current peptidic foldamer design concepts is that the central non-covalent interactions are largely restricted to amide-type NH···O=C hydrogen bonds. Other types of non-covalent interactions are much less studied.

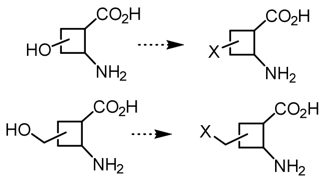


To date, NH···S interactions implicating aliphatic thioether aminoacids have not been integrated as design features for foldable molecular architectures. This project will examine foldamer building blocks with built-in NH···S hydrogen bond feature and to explore the ability of this feature to promote new folding patterns in backbones which do not normally fold, or alternative folding propensities of otherwise-folded oligomers. The principle is illustrated with the following three examples. To what extent can a γ^4-peptide 14-helix coexist in competition with short range interactions (top)? To what extent can a β-peptide strand be modified (lower left)? Does the thia-analogue of 5-aminopentanoic acid adopt a regular structure whereas the parent δ-amino acid does not (lower right)?

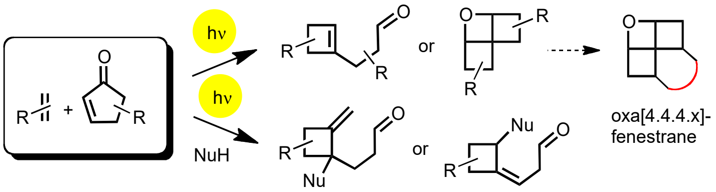
A second project in this area will be the conformational control of γ-amino acid analogs in which the γ-C is replaced by a nitrogen atom. These poorly-known β-hydrazino peptides should be able to adopt well-defined short-range secondary structure stabilized by an unprecedented β-hydrazino turn, a feature which will be fully characterized and implemented in new peptidomimetic foldamer edifices.

- Methodology in organic synthesis: photochemistry, organocatalysis and silicon reagents

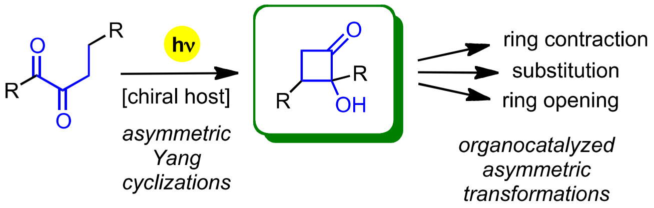
• Cyclobutane amino acids. Access to a significantly enlarged inventory of functionalized cyclic homologated β- and γ-amino acids will be achieved using the team's photochemical methodology for the construction of the four-membered ring cores. Divergent transformations of hydroxy- or hydroxymethyl-ACBCs will be conducted, providing ACBC libraries with programmable substituent identity at peripheral positions in a controlled fashion.



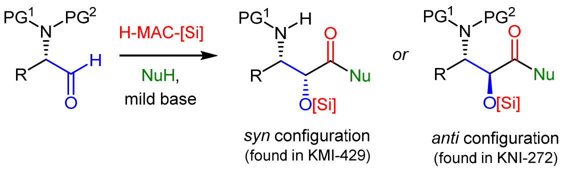
• Photochemistry in synthesis. The group will continue to develop organic photochemistry as an innovative tool for selective synthesis. As well as the use of photochemical [2+2]-cycloadditions to prepare cyclobutane amino acid libraries, efforts will be oriented towards photochirogenesis. In particular, enantioselective versions of the Paternó-Büchi reaction will be studied, along with the little-known thia-Paternó-Büchi reaction which implicates thiocarbonyl photochemistry. Enantioselective Norrish-II/Yang cyclizations will also be considered (see below). Work will continue on the development of the tandem and triple photochemical cascade reactions between a cyclopentenone and an alkene. The chemical reactivity of the cyclobutene aldehyde and tricyclic oxetane photoproducts will be explored, with a view to preparing novel molecular architectures (difficult to obtain using other methodologies) and to exploit these compounds for the preparation of useful multi-functional intermediates for fine organic synthesis. In one particular study, selected cyclopentenone substrates will be induced into tandem allylic nucleophilic substitutions leading to new methylene-cyclobutane aldehyde structures. In another part of this work, the possibility of using duly-substituted angular tricyclic oxetane scaffolds to prepare unique oxa[4.4.4.x]fenestranes will be considered.



• Organocatalysis and cyclobutanone chemistry. The fruitful collaboration with the research group of Drs. A. Frongia and F. Secci (University of Cagliari, Sardinia) will be pursued in the forthcoming contractual period (joint research proposals are in submission). Studies on the chemical reactivity of 2-hydroxy- and other 2-substituted-cyclobutanones will be expanded, notably as regards organocatalyzed asymmetric transformations, such as ring contraction, nucleophilic substitution and ring opening, will be examined. In parallel, enantioselective and environmentally-friendly approaches for the preparation of 2-hydroxcyclobutanones using photochemical approaches will be studied, such as Yang cyclization of α-diketones in a chiral host–guest environment. In the search for new categories of asymmetric organocatalysts, the extensive in-house library of homologated cyclic amino acids will be screened for their performance using benchmark reactions (aldolization, Michael addition, …).



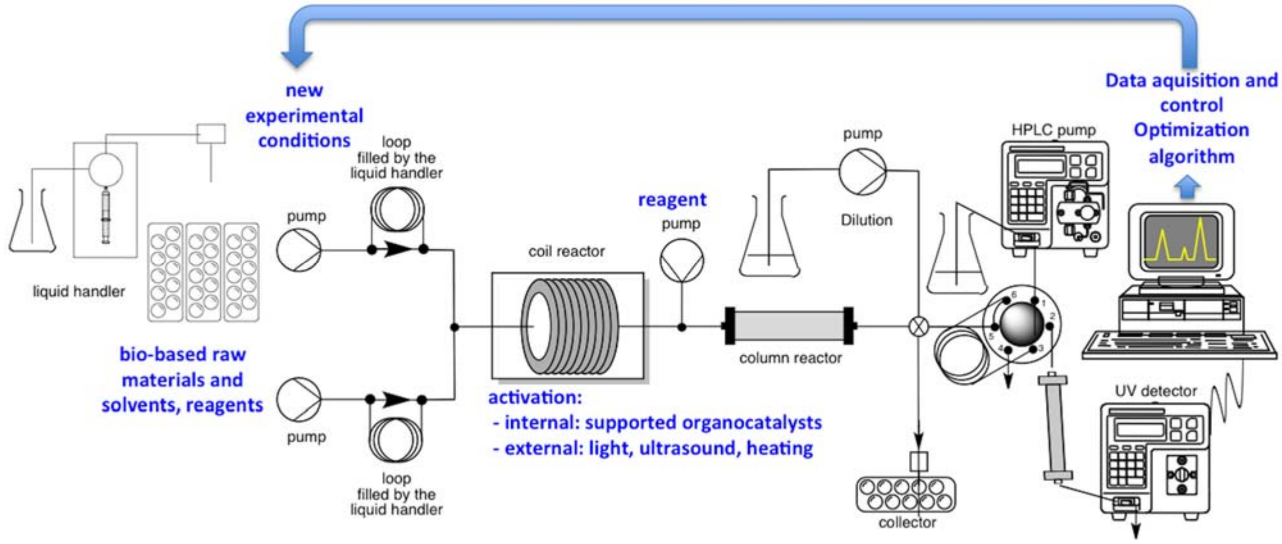
• MAC Methodology. The group's recent demonstration of the control of *syn*/*anti* diastereoselectivity during the 3-component MAC-methodology oxyhomologation of protected L-serinals will be capitalized. The influence of the side-chain identity, the silyl group of the MAC reagent (H-MAC-[Si]) and the presence of a Lewis acid will be evaluated, in order to optimize formation of either *syn* or *anti* derivatives from the same precursor in a generalized manner. This stereo-control in the transformation of other α-amino aldehydes will be confirmed through test-case selective syntheses of biologically active small peptides (*e.g.* KMI-429, a human aspartic protease BACE-1 inhibitor; KNI-272, an HIV-1 protease inhibitor). Efforts will focus on the elaboration of an unprecedented *enantioselective* variant of MAC methodology; a convincing application of this development will be the expedient asymmetric synthesis of the α-hydroxy-β-amino isopentanoic acid residue of microbacterins A and B, two peptaibols with significant cytotoxic activity against human tumor cell lines. Further extension of the methodology to β-amino aldehyde substrates will be elaborated in order to prepare α-hydroxy-γ-amino acids, again in diastereoselective fashion. This unprecedented strategy will be applied in the synthesis of the central 2-(α-hydroxy-γ^4-aminoalkyl)thiazoline fragment in the structure of the tubulysins, highly potent cytostatic natural products.



- Green Chemistry and alternative processes

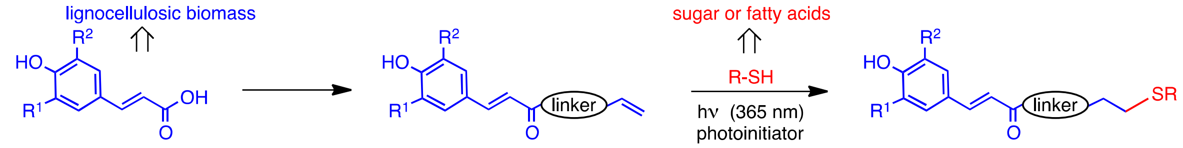
The research of the group will be focused on continuous flow synthesis to prepare new chemical structures through innovative eco-designed processes.

In order to determine the optimal operating conditions for the syntheses, we will continue a project, recently initiated in collaboration with Pr. N. Dragoe (SP2M), aimed to develop a fully automated system with an online HPLC analysis. This system includes a liquid handler used to fill variable volume loops with the reactants, pumps, reactors whose temperature can be precisely controlled, a fraction collector, an original dilution system for HPLC analysis. A Labview program that we have developed controls all these elements. The system will be complemented by HPLC data processing, design of experiment programming and adaptive feedback control. In comparison with the few platforms described so far, the originality of our system resides in the inclusion, in the programming of optimization, of metrics to evaluate the greenness of the process.



This automated platform is designed to be used with flow reactors of different geometry, variable flow rates, and temperatures ranging from −30 to +150 °C. It can therefore be used for the rapid development of various reaction sequences.

An example concerns the preparation of new biosourced antioxidants, acting as skin photoprotective products, from hydroxycinnamic acids in turn recovered from lignocellulosic biomass.



R^1 = H, R^2 = OCH_3 (**ferulic acid**)
R^1 = OCH_3, R^2 = OCH_3 (**sinapic acid**)
R^1 = H, R^2 = H (***p*-coumaric acid**)

These antioxidants will be obtained through (*i*) implementation of operationally simple yet efficient reactions endowed with high atom economy, (*ii)* control of the waste production during the reactions that will be evaluated by appropriate metrics, (*iii)* development of meso-fluidic processes for a smart use of the energy, enhanced security. Moreover, the antioxidant activity and UV spectral properties of the newly prepared compounds, both in pure form and in actual cosmetic formulations, will be fully evaluated (collaboration with Pr. A. Marra, Institut des Biomolécules Max Mousseron (IBMM), Montpellier and Pr. L. Coiffard, Service Cosmétologie, UFR des Sciences Pharmaceutiques et Biologiques, Nantes).

Self-assessment document

Team 2 - MSMT

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Méthodologie, Synthèse & Molécules Thérapeutiques**
Acronym:	**MSMT**
Director's name (current contract):	**Cyrille KOUKLOVSKY**
Director's name (future contract):	**Cyrille KOUKLOVSKY**

SELF-ASSESSMENT DOCUMENT

1 Research products and activities

Scientific output

The MSMT (Méthodologies, Synthèse et Molécules Thérapeutiques) team is involved in total synthesis, natural products chemistry, methodological development in organic chemistry and the access to molecular diversity. Next to this, we design and prepare chemical probes to interrogate biological systems whose bioactivities and therapeutic potential are evaluated within interdisciplinary collaborations. The team is located in two separate buildings.

There are currently several projects within the team which are presented below, with the corresponding permanent members:

Innovative Project in Natural Product Synthesis	Cyrille Kouklovsky, Professor Guillaume Vincent, CR CNRS
Innovative Project in Amino Acid and Peptide Chemistry	Cyrille Kouklovsky, Professor Valérie Alezra, MCF
Innovative Project in Phosphorous-Containing Biomolecules	Antoine Fadel, DR CNRS Nicolas Rabasso, MCF
Innovative Project in Glycosaminoglycan Chemical (glyco)Biology	David Bonnaffé, Professor Christine le Narvor, CR CNRS Aurélien Alix, MCF Maryline Macé, T Jérôme Hénault, AI

The team is member of both LabEx LERMIT and CHARMMMAT (D. Bonnaffé is deputy coordinator of the LabEx LERMIT).

Since 2013, several team members left the group; none of these persons have been replaced:

- Jean-Pierre Férézou, DR CNRS: retired (2015)
- Annie Pouilhès, IR CNRS retired (2015)
- Nadine Barroca, MCF: moved to the SM2B team at ICMMO (2014)
- Didier Gori, AI; moved to Aix-Marseille University (2016)

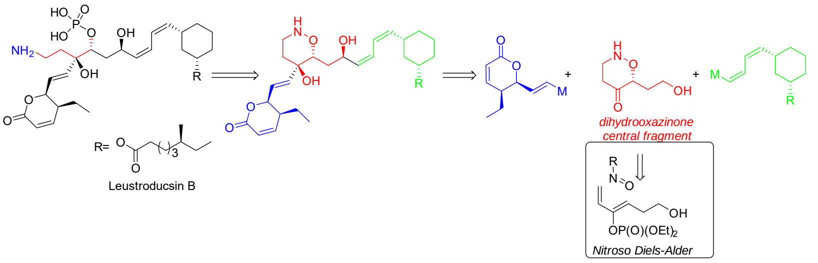
During the 2013-2018 period, the team has published 53 articles (average impact factor: 7.028; PRP/FTER/y: 1,72), 6 book chapters, and 2 patents (one licensed); team members have given 21 invited lectures, 38 oral communications and 46 invited seminars.

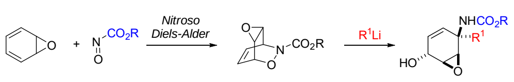
Innovative Project in Natural Product Synthesis

indole alkaloids-biomimetic synthesis-indole dearomatisation-cycloaddition-nitroso-stereoselective synthesis

The innovative project in natural product synthesis is divided in two topics: synthetic applications of the nitroso Diels-Alder reaction, and indole alkaloid synthesis.

Synthetic applications of the nitroso Diels-Alder reaction: We have been involved for many years in a comprehensive study of the nitroso Diels-Alder reaction and its synthetic applications in the total synthesis of natural products as well as in the access to original molecular scaffolds. Recent efforts have focused on the total synthesis of leustroducsin, for which an original strategy featuring a nitroso Diels-Alder reaction as the key step reaction has been designed. Although two of the three fragments have been prepared, the synthesis has yet to be completed. Furthermore, we are studying the use of original dienes for cycloaddition reaction: cycloadditions of benzene oxide led to cycloadducts for which a new fragmentation reaction has been designed, leading to highly functionalized scaffolds. Perspectives for this work are the study of the scope and applications of this sequence.

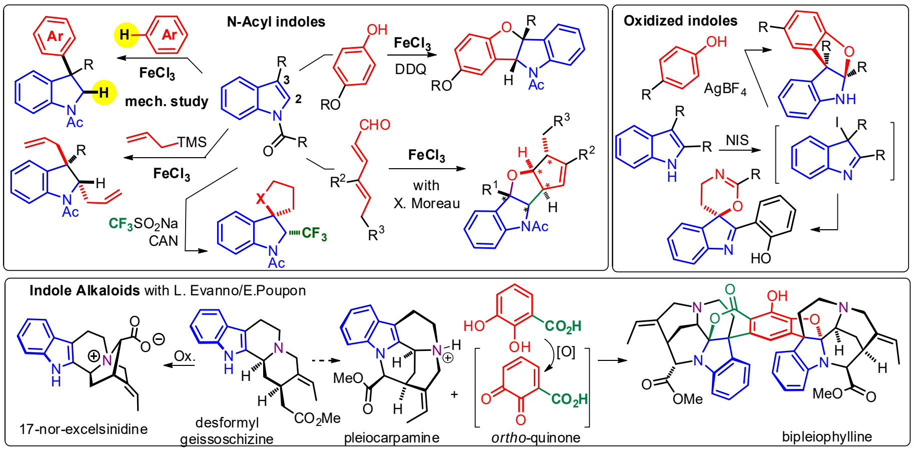




Collaborations: Huw Davies, (Emory University, Atlanta, USA)

Funding: 2 PhD grants (MESRI, ASN)

Indole Chemistry: Driven by our interest in indoline-containing natural products and also by the importance of the indole nucleus in drug discovery, we designed several dearomatization reactions of indoles through unusual Umpolung strategies. Activation of N-acyl indoles with $FeCl_3$ results in the reversal of the innate polarity of the C2=C3 bond with the generation of electrophilic indoles at the C3-position. We developed a regioselective hydroarylation of N-Ac indoles for which a comprehensive mechanistic study was realized. N-Ac indoles activated by $FeCl_3$ were also engaged in a [3+2] oxidative coupling with phenol, a 2,3-diallylation reaction and a iso-Nazarov-(3+2) annulation sequence from dienals. An iron-free radical mediated trifluoromethylative spirocyclization was also developed. Alternatively, C3-electrophilic indoles could be generated by oxidation with NIS which led to benzofuroindolines in presence of phenols and to 3,3-(1,3-oxazino)spiroindolenines via the cyclization of acetamides. Turning our attention towards natural products, the biomimetic synthesis of bipleiophylline, a highly complex indole alkaloid, was achieved in only 2 steps from natural pleiocarpamine through the development of a divergent oxidative coupling between indoles and 2,3-bishydroxybenzoic acid derivatives which involves transient *ortho*-quinones. Finally, while targeting the total synthesis of pleiocarpamine, we achieved the first total synthesis of 17-nor-excelsidine for which the key event is the oxidative cyclization of desformylgeissoschizine with formation of the key C-N bond.



Collaborations: Laurent Evanno and Erwan Poupon (BioCIS, Faculté de Pharmacie, Université Paris-Sud), Xavier Moreau (ILV, Université de Versailles), Isabelle Chataigner (COBRA, Université de Rouen), Vincent Gandon (ICMMO, Université Paris-Sud), Nour-Eddine Ghermani (Faculté de Pharmacie, Université Paris-Sud), Alejandro Perez-Luna (IPCM, Sorbonnes Universités).

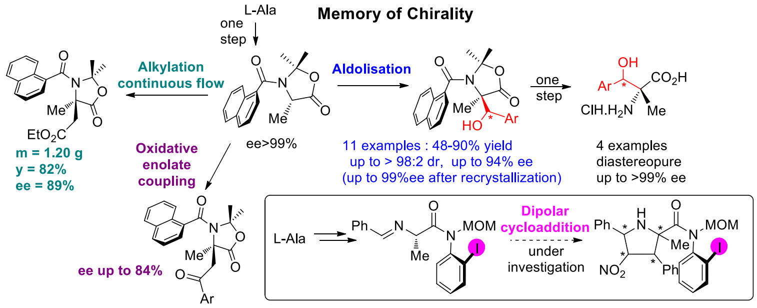
Funding: ANR PRC 2017-2021 ("ArDCo", 100 k€ / team with I. Chataigner and X. Moreau); ANR PRC 2015-2020 ("Mount Indole" 212 k€ / team with E. Poupon/L. Evanno, Coord. G. Vincent), China Scholarship Council (2 PhD 2016-2020 et 2017-2021), Marie Curie IIF 2015-2017 (2 years postdoc + 30 k€, Coord. G. Vincent), Labex CHARM3AT 2015-2018 (PhD with X. Moreau and I. Chataigner), Fondation pour le développement de la Chimie des Substances Naturelles 2012-2015 (PhD, Coord. G. Vincent); ANR JCJC 2012-2016 (CouPhIn, Coord. G. Vincent 160 k€), MESRI (2 PhD grants).

Innovative Project in Amino Acid and Peptide Synthesis

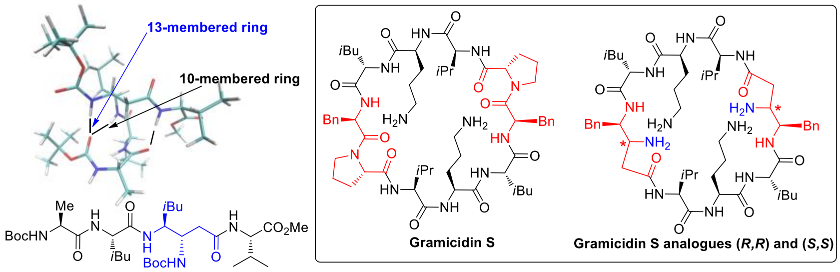
Amino acid-gamma peptide- asymmetric synthesis-memory of chirality-antimicrobial peptide

This project is divided in 2 topics: development of original asymmetric synthesis of quaternary α-amino acids by memory of chirality (MOC); synthesis of β,γ-diamino acids and their use to build γ-peptides.

Memory of chirality: In continuation of our previous work, we have developed an asymmetric synthesis of β-hydroxy quaternary α-amino acids by MOC aldolisation. This means that this synthesis use only the chirality of the starting α-amino acids to access to highly enantioenriched quaternary α-amino acids even though the initial stereogenic center is temporarily destroyed. The chirality is memorized by a chiral conformation of tertiary aromatic amide. Recently, we have also adapted our MOC alkylation reaction to continuous flow in collaboration with Pr. J.-i. Yoshida (Kyoto University, Japan). We are currently working on other types of reactions by MOC: oxidative coupling of enolates (radical reactions) and 1,3-dipolar cycloadditions.



β,γ-diamino acids and γ-peptides: We have used β,γ-diamino acids to build original peptidic structures. We have thus shown that a tetrapeptide adopted a folded structure stabilized by several hydrogen bonds, involving the β-nitrogen of the β,γ-diamino acid. We have also synthesized and tested (collaboration with S. Zirah) the antimicrobial activities of analogues of Gramicidin S. Our analogues are less active than the parent peptide but present almost no haemolytic activity.



Collaborations: Muriel Sebban (IRCOF, Rouen), Jun-ichi Yoshida (Kyoto University, Japan), Takeo Kawabata (Kyoto University, Japan), Paul Williard (Brown University, Providence, USA), Emeric Miclet (Sorbonne Universités), Jean-Valère Naubron (Spectropole, Marseille), Séverine Zirah (Museum d'Histoire Naturelle, Paris), Bertrand Poumellec (ICMMO), Angelita Rebollo (Sorbonne Universités).

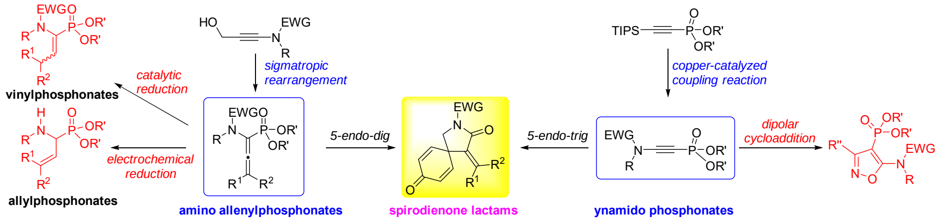
Funding: RBUCE-UP 2012-2013 (Cofund Marie Curie, 2 years postdoc + 35 k€, Coord. V. Alezra), China Scholarship Council (1 PhD 2014-2017), Marie Curie IIF 2013-2016 (2 years postdoc + 30 k€, Coord. V. Alezra), Inter-Labex CHARM3AT/SYNORG 2017-2018 (1 year post-doc + 10 k€, with M. Sebban), Sanofi 2012-2015 (140 k€, Coord. V. Alezra); 2 PhD grants 'MESRI) .

Innovative Project in Phosphorous-Containing Biomolecules

Allenes – Spirocyclic compounds – Electrochemistry – Ynamides
Cycloadditions – Aminophosphonates - Isoxazolines

Over the past few years, we have been involved in the chemistry of unsaturated aminophosphonates to explore their reactivities towards oxidation and reduction. Our previous work in this field led us to prepare α-amino allenylphosphonates with a large diversity of substituents and on a large scale. The partial reduction of allenylphosphonates to vinylphosphonates is a challenging task in order to control the stereoselectivity on the final compounds. We have been able to set up conditions (catalytic hydrogenation) that provide the α-amino vinylphosphonates. In depth investigations on this reduction led us to design specific substrates that could be converted either to the *Z* or the *E* vinylphosphonates. On the other hand, the electrochemical reduction of the same substrates leads to the α-amino allylphosphonates. When oxidized with cerium(IV), the α-amino allenylphosphonates are transformed to spirodienone lactams in good yields. Mechanistic investigations have been performed to extend this cyclisation to the largest variety of substrates. To enlarge the scope of this reaction, we have developed an alternative approach based on the 5-*endo*-trig cyclization of ynamido-phosphonates. The latter were barely known when we initiated this project and we have developed an easy phosphonates. The latter were barely known when we initiated this project and we have developed an easy access to these substrates through a copper catalyzed coupling reaction. On the way to the oxidation of this new ynamides we have used them as partners for cycloadditions to form isoxazole phosphonates as single isomers.

Our group has a long history with both aminophosphonates and small carbocycles. Continuing our research in this field we have developed a selective and easy access to β-amino cyclopropanephosphonic acid or isoxazolinephosphonates from vinylphosphonates.



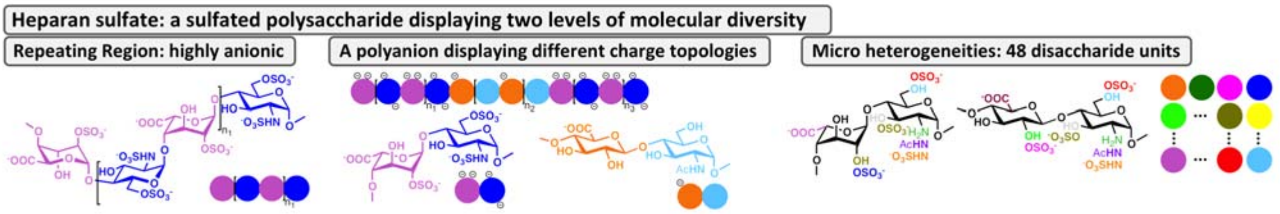
Collaborations: Joëlle Prunet (Glasgow University, Scotland); Pedro de Oliveira (LCP, Université Paris-Sud); Jalila Simaan (Université Aix-Marseille).

Funding: 2 PhD grants (MESRI, ASN), Maison de la Fondation de la Chimie (Financial support for the mobility of Pauline Adler during her PhD).

Innovative Project in Glycosaminoglycan Chemical (glyco)Biology

Synthetic organic chemistry – Glycochemistry – Glycosaminoglycans – Conjugation/click chemistry
Combinatorial chemistry – Self-assembly – Protein-ligand interactions – Drug Design
Therapeutic Innovation – Interdisciplinarity

We develop chemical (glyco)biology approaches to understand, at the molecular level, biological processes in which carbohydrates are involved, with the aim of bringing innovative solution for human health. In this regard, our strong implication in the Laboratory of Excellence in Research on Medication and Innovative Therapeutic (LERMIT) opened new collaborations opportunities within the Paris Saclay perimeter, complementing the existing ones, to develop glycosciences-based therapeutic innovation. Our expertise in glycochemistry (including chemical and chemoenzymatic oligosaccharide synthesis), (bio)orthogonal conjugation strategies and supramolecular chemistry gives a unique edge to our chemical biology research that is acknowledged at the national and international levels (8 invited plenary or keynote lectures and 12 oral communications by group members since 2013; DB invited professor at Academia Sinica, Taiwan, in 2014). We concentrate on Glycosaminoglycans (GAGs), especially Heparan Sulfate (HS). These linear and sulfated polysaccharides interact with and modulate the activities of numerous extracellular proteins, including established therapeutic targets such as growth factors, cytokines, chemokines and bacterial or viral proteins. A tightly regulated biosynthesis allows generating two levels of molecular diversity (see below) and encoding protein-specific sequences in the HS chains depending on cell type or activation.



Controlled disruption of one or several GAG/protein interaction(s) represents a promising field that could advantageously complement therapeutic antibodies or aptamers if adapted drug design technologies were available, which is currently not the case. To push forward toward this frontier, we merged advanced synthetic organic chemistry with molecular modeling aided rational design, combinatorial and fragment based design or supramolecular approaches to design: i. glycoconjugates binding multiple sites of the target (hybrid HS/peptide or topologic mimetics of HS long fragments); ii. a differential screening based technology for the systematic optimization of HS type glycoligands (6TMATIC); iii. self-assembled nano-objects coated with combinatorial bioactive surfaces to trap HS binding proteins (NanoGAG); iv. probes to address the specificity/mechanism/structure or inhibit enzymes involved in GAG biosynthesis or catabolism (Sulf@AS). These programs are developed within interdisciplinary networks and funded by different organizations (ANR, LERMIT, Paris Saclay University). Our expertise in the total synthesis of fully defined HS fragments or mimetics, including the development of innovative, reliable and scalable methodologies, played a key role in these projects. In order to meet the challenge of synchronizing tasks within such collaborative projects, by being able to deliver the designed compounds within predictable time frames and requested quantities (up to hundreds of milligrams), we identified and calibrated all critical parameters for each steps of the syntheses. Optimized procedures were compiled into a reference manual that is maintained up to date. Moreover, to answer the unmet need of precise HS fragment/mimetic concentration knowledge for biological evaluations, we validated a NMR based quantification of final compounds. Carrying on these standardization was time consuming and present a low publication potential, nevertheless it represents a decisive investment for internal use, outsourcing of advanced synthetic intermediates preparations (Roowin CRO) and in view of potential transfer to a start-up or the industry. It can be anticipated that the professionalism of our overall approach was decisive for Sanofi decision makers to collaborate with us in the field of synthetic vaccines. In brief and as exemplified below, our activities span from basic research in organic synthesis and glycosciences to innovation (6TMATIC project awarded through the 2016 Paris-Saclay Prematuration program, a PCT patent on HIV entry inhibitors published in 2016 and a 2012 patent licensed by Aryballe Technologies in 2014), including biological activity determinations ranging from physicochemical quantification of interactions to therapeutic activity validation in animal models.

Methodological developments selection illustrating our progress toward our general objectives:

1-Sustainable development concerns prompted us to give priority to biosourced starting material and regioselective reactions when conceiving new syntheses. In this context, regio and stereoselective aqueous anomeric allylation of unprotected sugars emerged as key step to prepare self assemblable building blocks for the NanoGAG program, while an oligomerizable maltotrioside unit was prepared in 46% global yield (9 steps, 10 g scale) from biosourced maltotriose.

2-High yielding and stereoselective 1,2-*cis*-glycosylation conditions were optimized for both 2-azido-2-deoxy-D-*gluco*syl and maltotriosyl donors and shown to display excellent reproducibility in oligomerization process up to dp$_{12}$. We also identified additives improving dramatically both yields and stereoselectivities of glycosylations at *O*-4 of D-glucuronic acid moiety.

3-Palladium-catalyzed decarboxylative coupling was established as unique tool for efficient *O*-allylation of acid/base sensitive saccharides, such as HS fragments, and further used as key step to functionalize the non-reducing end of HS fragments. This strategy was designed to complement our "repairing conditions" thiol-ene based reducing end functionalization and opens the way to highly divergent aqueous click-reaction based preparation of libraries of HS long fragments topologic mimetics.

4-Dual fluorous taggings of glycosyl donors and acceptors were implemented for fluorous assisted split/mix/demix combinatorial syntheses of HS fragments. An efficient microwave-assisted Heck cross-coupling between unreactive perfluoro-olefins ($C_6H_3F_9$ to $C_{14}H_3F_{25}$) and aryl bromides was developed as key step in the preparation of reducing end tagged acceptors.

5-A strategy designed for the preparation of putative inhibitors of the human endosulfatase H-Sulf-2 was fully validated at the dp$_3$ level and currently extended to the preparation of dp$_{5,7,9}$.

Selection of completed syntheses and biological activities:

1-The validation of the 6TMATIC technology is ongoing within a LERMIT consortium, taking the CXCL12 chemokine as first example, with two endpoints: i. demonstrate the therapeutic potential of targeting CXCL12 by a HS type glycoligand in a murine model of the human WHIM syndrome; ii. perform the 6TMATIC optimization of the lead selectivity for CXCL12. The 6TMATIC protocol implementation relies on two libraries whose syntheses have been completed. The first one (10 members) contains repeating region fragments ranging from tetra to dodecasaccharides ([IdoA2S-GlcNS6S]$_m$, m = 2,3,4,5,6) and either hydrophilic (HOdp$_n$: deprotected) or hydrophobic (BnOdp$_n$: benzylated). It was designed for lead selection, *ie.* select between hydrophilic or hydrophobic categories and determine the lead optimal length. In the CXCL12 case, following SPR-based and functional assays, the library members were screened for their *in vivo* ability to mobilize leukocytes and delocalize CXCL12 from bone marrow, using AMD3100 as positive control. Gratifyingly, BnOdp$_{8 \text{ and } 12}$ showed similar potency to AMD3100, while BnOdp$_6$ and HOdp$_{8,12}$ were inactive. The second library (26 members), designed to drive "Lead Optimization", contains HO and BnOdp$_8$ in which selectivity elements are frame shifted along a repeating region continuum. Surface Plasmon Resonance based differential screening allowed identifying selectivity determinants for CXCL12.

2.Late stage aqueous "repairing conditions" thiol-ene reaction was used to introduce a reactive amino group on each BnOdp$_{4\text{-}12}$ library member for further conjugation to a CD4 mimetic. The resulting glycoconjugates were tested for their ability to inhibit cell infection by X4 or R5 tropic HIV strains (clades B and C) revealing a critical clade/tropism dependence on the optimal HS fragment length. The tropism/clade molecular determinants driving HIV-gp120/polyanion interactions were identified and found to correlate well with the one used in algorithms for V3 sequence based tropism prediction.

3.In collaboration with Sanofi, we completed the total synthesis of dimeric and octameric fragments of a bacterial capsular polysaccharide.

4.NanoGAG: a collection of gold or lipid core nanoscale objects with combinatorial surfaces was built by self-assembling of sulfated or non-sulfated disaccharide-based building blocks. Complementary techniques were implemented to investigate their structures and their interactions with HS binding proteins. The results clearly demonstrate a nanoparticle surface composition dependence of protein recruitments. In-depth exploration of the CXCL12/nanoparticle interactions revealed an original mode of action with intellectual property potential.

Collaborations: H. Lortat-Jacob, R. Vivès (IBS, Grenoble); F. Baleux (Institut Pasteur, Paris); R. Daniel (LAMBE, Univ. Evry); K. Balabanian, F. Bachelerie (Inserm UMR-996, Clamart, Univ. Paris Sud); S. Lesieur (Institut Galien, Châtenay-Malabry, Univ. Paris Sud), C. Sizun (ICSN, Gif sur Yvette), S. Cohen-Kaminsky (Inserm UMR-S 999, Plessis-Robinson, Univ. Paris Sud), N. Giraud (LCBPT, Univ. Paris Descartes), P. Trouilleux (Sanofi Montpellier), P-A. Driguez (Sanofi Chilly-Mazarin).

Funding: ANR Emergence 2011-2013 (Hépaclamp, **17** k€ with F. Baleux, R. Legrand, Coord: H. Lortat-Jacob); ANR PIRI-Bio 2010-1014 (Hépaféron, **306** k€ with H. Lortat-Jacob, R. Daniel, Coord: H. Lortat-Jacob); Industrial contract with Sanofi 2013-2016 (**200** k€ with P. Trouilleux, P-A. Driguez, Sanofi, Coord. D. Bonnaffe,); LabEx LERMIT 2012-2014 (Lermit T2, **132** k€ with S. Lesieur, C. Sizun, F. Bachelerie, Coord: D. Bonnaffe and K. Balabanian); LabEx LERMIT 2015-2017 (Lermit T2, **129** k€ with S. Lesieur, C. Sizun, F. Bachelerie, Coord: D. Bonnaffe and K. Balabanian); Prématuration IdEx Paris-Saclay 2016-2017 (6TMATIC, **42** k€ ,Coord. D. Bonnaffé); IdEx Paris-Saclay (Départements SdV et Chimie) 2017 (5 k€ with S. Lesieur, C. Sizun, Coord: S. Lesieur); ANR PRC 2018-2022 (Sulf@as, **30** k€ with I. Vilgrain, R. Daniel, Coord: R. Vivès); LabEx LERMIT 2018-2019 (Lermit T2, **10** k€ with S. Lesieur, C. Sizun, F. Bachelerie, Coord: D. Bonnaffe and K. Balabanian); Labex LERMIT Emergence 2018-2019 (Sulf@mark, 15 k€ with S. Cohen-Kaminsky, R. Daniel, Coord: C. Le Narvor); China Scholarship Council (2 PhD 2012-2015 et 2015-2019), Labex LERMIT (1 PhD grant), MESRI (1 PhD grant).

Highlights

1. G. Vincent and N. Rabasso have been involved in the creation and the management of the ICMMO chemical library («Chimiothèque de l'ICMMO») that is registered to the National Library network; it offers ICMMO member the opportunity to perform biological evaluation on new synthetic compounds, thus providing a new potential for valorization of fundamental research. This library is managed under the supervision of G. Vincent with temporary help from technicians.

2. Patent WO2013124810 (A1) "*Capteurs de nez ou de langue électroniques*" published 29/08/2013 was licenced by Aryballe Technologies (08/**2014**) that further raised 6 M€ to develop the first universal and portable odor sensor that mimics the human olfactory receptors.

3. D. Bonnaffé and C. Le Narvor have been awarded with the «Prematuration IdEx Paris-Saclay 2016» grant for the 6TMATIC project "*Proof of concept for a rational and systematic combinatorial technology in order to optimize the selectivity of interactions between a glycol-ligand and a therapeutic target".*

4. C. Kouklovsky secretary (2013-2015), then President (2015-2018) of the Organic Chemistry Division of the French Chemical Society. D. Bonnaffé President, C. Le Narvor secretary of the French Glycoscience Group (2013-2014).

5. G. Vincent has completed the total synthesis of bipleiophylline, one of the most structurally complex alkaloids. This work, funded by the ANR was accomplished via a collaboration with a team in the faculty of pharmacy, and has been published in *Nature Chemistry.*

2 Organisation and life of the research team

Management, organisation and scientific animation

The team is organized in four thematic groups, with an identified group leader for each theme. As the team is located in two separated buildings, the resources are allocated for each location. CNRS and University funding is distributed according to the number of permanent people. Other grants (ANR or Industrial) are managed by the project holder, with a contribution to the common expenses.

The team organizes research seminars every two weeks with participation from all the team members (one team member is in charge with organizing these seminars); moreover, bibliographic seminars for students and postdocs are organized on a regular basis, with participation from some students from other ICMMO teams.

3 SWOT analysis

Strengths

- ✓ Dynamism of the team:
- ✓ High impact factor for the publications
- ✓ Numerous fruitful national and international collaborations.
- ✓ High involvement for grant applications (ANR, LabEX, Europe, etc.).
- ✓ High involvement in collective actions and responsibilities within the Institute, University, Scientific Societies, research networks and in teaching.
- ✓ High number of communications in international symposia.
- ✓ Scientific activities from fundamental research to technology transfer: interdisciplinary and interaction with companies.

Weaknesses

- ✓ Need to sustain partnerships with the industry
- ✓ Increase the attractiveness to students
- ✓ Improve the “timing” for the writing of publications

Opportunities

- ✓ Integration in the IDEX and LabEx policies.
- ✓ New opportunities for interdisciplinary collaborations with the BPC (Biology Pharmacy Chemistry) project
- ✓ Involvement in the future Paris-Saclay "Institut Santé et Innovation Thérapeutique" federating several research teams from both Paris-Saclay Chemistry and Life Sciences departments.

Threats

- ✓ High uncertainties concerning the funding for research resulting in a lack of continuity in driving the projects
- ✓ Non-renewal of technical staff for assistance to research
- ✓ Impact of the relocation of ICMMO (BPC project) on research activities
- ✓ Shortage of PhD grants in organic chemistry

4 Scientific strategy and projects

The MSMT team was created in 2013 by the gathering of several groups that shared the same interest in modern aspects of organic synthesis and natural products chemistry. The main topics for our scientific activities were as listed below:

-Modern methods for selective synthetic transformations
-Stereoselective synthesis
-Synthesis of natural products and biomolecules
-Access to molecular diversity
-Chemoenzymatic synthesis

These methodological studies were applied to the chemistry of alkaloids, amino acids and peptides, glycosylated derivatives, etc.

For the 2020-2024 period, the team wishes to continue these studies with the same goals and strategies. However, there will be some changes in the group members:

-A. Fadel is retiring in fall 2018
-V. Alezra will leave the ICMMO in late 2018.
-A CNRS researcher (A. de la Torre) has been recruited for fall 2018.

Consequently, the team will be reorganized into two main axes:

Modern Methods for Natural Product Synthesis	Glycosylaminoglycan and Molecular Diversity
Group Leader: C. Kouklovsky	Group Leader: D. Bonnaffé
Members:	Members :
C. Kouklovsky, PR	D. Bonnaffé, PR
N. Rabasso, MCF	A. Alix, MCF
G. Vincent, CR CNRS	C. le Narvor, CR CNRS
A. de la Torre, CR CNRS	Jérôme Hénault, AI CNRS
Philippe Pigeon, MCF (teaching staff ; not involved in research activities)	

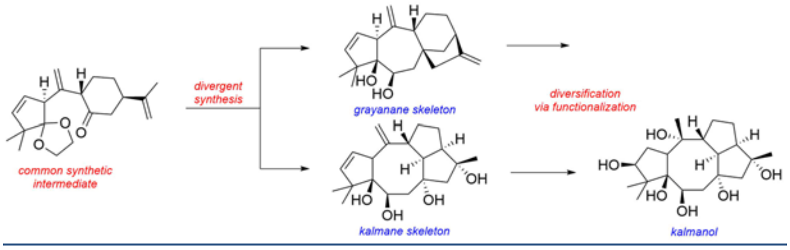
It should be also noted that the relocation of the ICMMO with the BPC project will also impact the scientific activities of the team (as for all ICMMO teams).

1. Modern Methods for Natural Product Synthesis

This topic contains 4 projects including a new one.

Collective Synthesis of Complex Terpenic Natural Products (NEW PROJECT). (C. Kouklovsky, A. de la Torre)

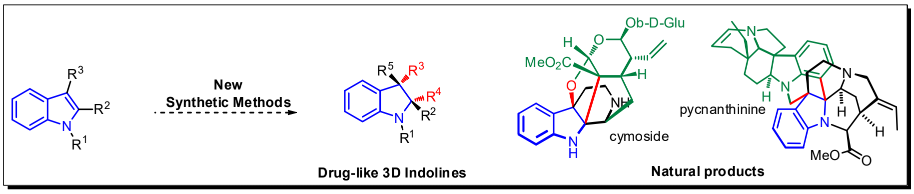
This project is linked to the recruitment of A. de la Torre. It involves the collective synthesis of two families of complex natural terpenes. Collective synthesis means the development of common synthetic strategies for a wide family of compounds, differentiation occurring at the very last stage of the synthesis.



It requires highly selective methods for the regioselective functionalization of complex molecules. This concept will be applied for the synthesis of grayanane and kalmane families of terpenes. Grayanane and kalmane derivatives are biogenetically related some terpenes of these families possess very promising biological properties. Therefore, the project consists in the rapid synthesis of a common synthetic precursor followed by access to both grayanane and kalmane frameworks using ring contraction or extension reactions, then diversification by functionalization to the natural products. The synthetic strategy will need the development of original reactions, and will be applied to the synthesis of kalmanol.

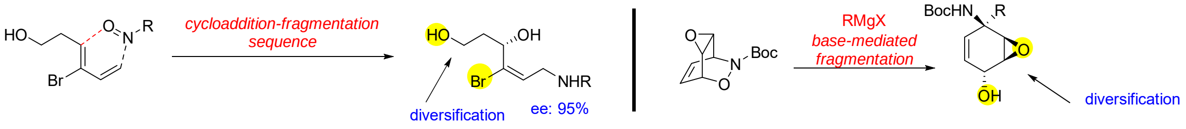
Dearomatisation of Indoles for the Total Synthesis of Complex Indole Alkaloids (G. Vincent)

The main goal is the discovery of *unusual modes of reactivity of the indole nucleus* in order to achieve *stereoselective dearomative difunctionalization of indoles.* We will mainly rely on the reversal of polarity of the indole nucleus for the generation of electrophilic indoles and of indolyl free-radical species. Indeed, we intend to implement these concepts into enantioselective catalytic reactions. These new synthetic methods will deliver original *three dimensional drug-like molecular architectures* ("escape from flatland") from flat starting material and will allow us to achieve the *total synthesis of several indole alkaloids* such as cymoside and pycnanthinine.



Synthetic Applications of Heterocycloaddition Reactions (C. Kouklovsky)

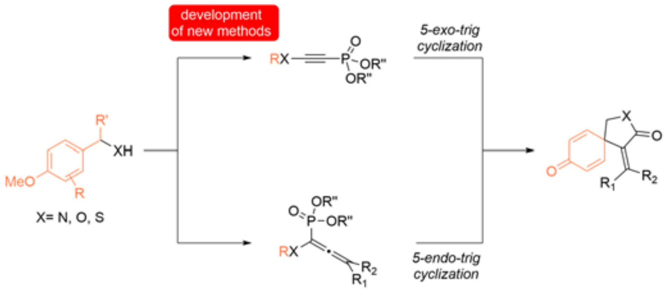
In the recent years, we have extensively studied heterocycloaddition reactions, especially the nitroso Diels-Alder reaction. We have thus introduced new selective synthetic sequences enabling the rapid access to highly functionalized building blocks by a cycloaddition-fragmentation sequence of steps.



The project will consist in exploring the scope and applications of these new sequences, in view of access to molecular diversity in the field of lipid metabolite and cyclitol derivatives, respectively. A particular attention will be driven towards the selectivities of the transformations: regio- and stereoselectivities.

Chemistry of Phosphorous-Containing Biomolecules

Over the past few years, from unsaturated aminophosphonates, we have developed few methodologies for the synthesis of spirodienone lactams for which the potential in the synthesis of natural products is important. We wish to continue in this field and further investigate the reactivity of both alkynyl and allenylphosphonates. Furthermore, we wish to prepare new allenylphosphonates byreplacing the nitrogen atom with other heteroatoms such as oxygen or sulfur. This requires the development of new strategies to access these unknown structures. We will then study the reactivity of these new species with respect to oxidation reactions in order to prepare new spirocyclic structures whose potential for the synthesis of natural molecules will be studied. In addition, the development of alternative methods, respecting the principles of green chemistry, will be considered.



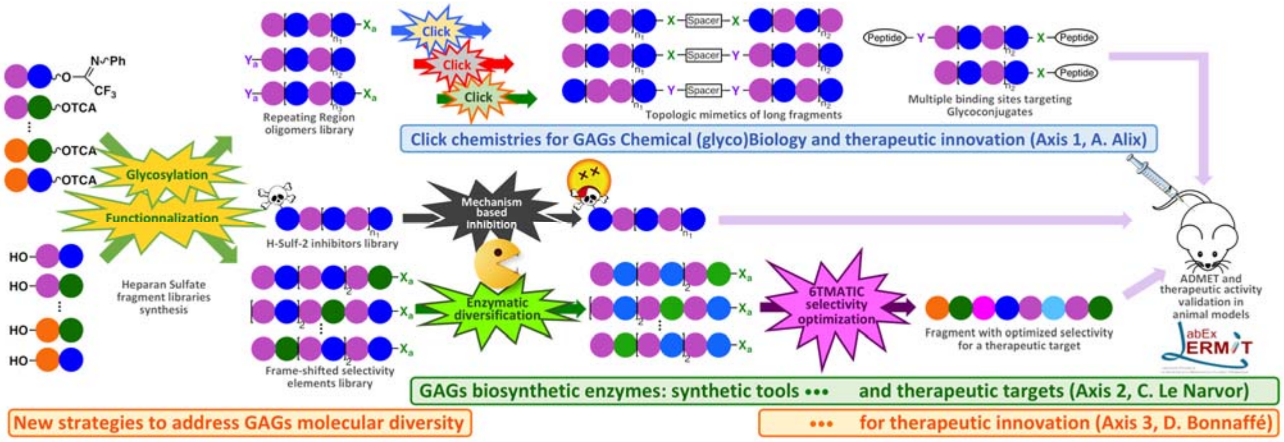
2. Glycosaminoglycans and Molecular Diversity

Our goal for the next five years will be to expend and integrate the different approaches previously developed into a global toolbox allowing the rational design and systematic optimization of glycoligands able to selectively disrupt a physiologically relevant interaction between a protein of therapeutic interest and HS chains. The toolbox's instruments are complementary and capitalize on the two levels of molecular diversity found in HS to bring innovative solutions to decipher protein-HS interactions and overcome the current limitations in the field (see scheme below): i. hydrophilic (OH) or hydrophobic (OBn) repeating region oligomer libraries (dp_4 to dp_{12}) and topologic mimetics of long fragments library (lead selection); ii. frame shifted selectivity elements library (dp_8) and multiple binding site targeting glycoconjugate (lead optimization).

To expend the scope and efficiency of the existing toolbox's instruments, we will capitalize on: i. both our recently optimized dual reducing end/non-reducing end functionalization strategy and new breakthrough in (bio)orthogonal click chemistry based ligation protocols to set up a highly divergent and parallel aqueous click-reactions based preparation of topologic mimetics of HS long fragments and expend the existing one (axis 1); ii our frame shifted selectivity elements dp_8 library and collaborations on HS chains biosynthetic machinery (granted by the ANR and LERMIT) to both optimize the selectivity of Mechanism Based Inhibitors towards H-Sulf2 or 1 and perform the enzymatic diversification of the frame shifted library (axis 2). iii. our ability to implement new stereoselective glycosylation strategies to expend the coverage of the HS chain molecular diversity within our libraries, with the objective to increase the potency of the 6TMATIC optimization protocol (axis 3).

Based on established collaborations and programs within the LERMIT LabEx, we will: i. perform the ADMET studies in mice of our CXCL12-glycoligand lead; ii. determine the active dose; iii. evaluate its therapeutic potential in a murine model of the human WHIM syndrome; iv. Optimize its selectivity for CXCL12 using the

6TMATIC protocol. We are confident to be able to demonstrate, within the next five years and using CXCL12 as an example, the suitability of our systematic approach for the rational design and optimization of an HS-type glycoligands targeting a protein of therapeutic interest. We then plan to apply to the Paris-Saclay SATT maturation program for further technology transfer.
Most importantly, we do not restrict ourselves to GAGs: Negotiations are currently on-going with Sanofi to pursue the collaborative program on the design, synthesis and evaluation of a new synthetic glycovaccine candidate, while we are waiting for the final answer from the ANR for a project aiming to develop glycoderivatives as early diagnostic tool for pancreatic cancers.



For the beginning of the 2020-2024 period, the team will be located in two separate buildings. In 2022 following the BPC project, the relocation of ICMMO in a new building will enable the gathering of all team members in a same location. The team is organized in a way to provide consistency and synergy for all team members:

-*Team seminars every two weeks*: Research seminars for permanent or non-permanent members (research and bibliographic seminars). These seminars allow the complementary expertizes from all team members to discuss about current research project and provide solutions for improvement.

-*Regular meetings for permanent members*: These meetings are for all administrative and financial aspects of the team work: recruitment, research funds, team organization, equipment.

-*Common financial and staff* resources: The financial resources will be distributed according to the ratio of permanent team members. However, a pooling of a part of these resources will allow to pay for the general expenses (administration and technical support, chemicals and solvents, small equipment, congresses for students). Contract management (ANR, Europe, Industry) will be carried by the contract holder, with an amount being used for the pooling of resources.

Efforts to achieve the scientific goals requires important human and financial involvement. The current size of the team staff is however diminishing with several members leaving the team for various reasons. It is crucial to maintain a minimal number of permanent researchers; this goal is partially achieved with the recruitment of a CNRS researcher in late 2018.

Our scientific activities are largely supported by the technical support team of ICMMO (NMR, MS, XRD) ; Furthermore, the team arranges many technical means (HPLC, CPG, automatic flash chromatography, capillary electrophoresis, solvent purification apparatus, cell and yeast culture, molecular modelling). These facilities should not be jeopardized by the non-replacement of technical support staff. Furthermore, although the team members have always been very dynamic the search for proper funds, one should question the impact of the writing of grant proposal on the time allowed for research.

Self-assessment document

Team 3 - ECM

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Catalyse Moléculaire**
Acronym:	**ECM**
Director's name (current contract):	**Emmanuelle SCHULZ**
Director's name (future contract):	**Giang VO-THANH**

SELF-ASSESSMENT DOCUMENT

1 Research products and activities

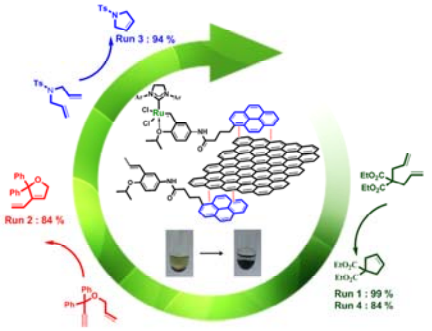
Scientific output

The Equipe Catalyse Moléculaire is made up of 36 people as of June 30, 2018; 15 permanent members (1 Emeritus professor, 9 teacher-researchers, 4 researchers and 1 ITA, 8,36 ETPC), 5 postdoctoral fellows, 11 doctoral students and 5 students (M2, L3, L2 ...). Our research is organized around 4 themes: Homogeneous and heterogeneous asymmetric catalysis (animation E. Schulz and team direction), Ionic liquids and catalysis (G. Vo-Thanh), catalytic polycyclizations (V. Gandon), Lanthanides (R. Gil). David Leboeuf joined the team in October 2013, appointed CR at the CNRS, on a joint project with the groups of E. Schulz and V. Gandon and there has been no movement of staff since this arrival. The objectives of the Molecular Catalysis team concern the development of new chemical reactions for the synthesis of chiral organic molecules (enantioenriched), with potential biological properties, by selective catalytic processes. The chiral catalysts targeted are essentially metal complexes, but also organic catalysts. Particular attention is paid to the design of new methods for the recovery and recycling of catalysts and the use of ionic liquids, new media (chiral or achiral) for synthesis and catalysis in the context of a chemistry aimed at meeting the current requirements of atom economy and sustainable development. To achieve these objectives, we are interested in the understanding of reaction mechanisms, particularly through kinetic studies, characterizations of intermediates, or molecular modeling. This research is conducted not only according to the aforementioned thematic organization, but also supplemented by interactions between the different members of the groups, in a matrix arrangement that allows an optimal alliance of different know-how. The Catalyse Moléculaire team published 123 articles in international peer-reviewed journals with an average impact factor of 5.32. This corresponds to a number of 2.68 publications/ETPC/year.

Catalyse asymétrique homogène et hétérogène

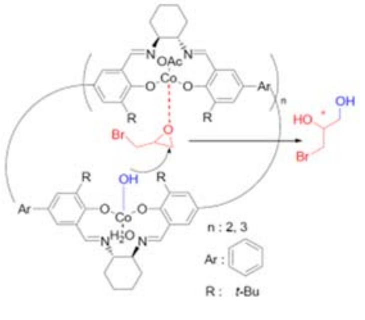
In line with the work carried out during the previous quinquennial and taking into account the issues of eco-compatible chemistry, we continued our research towards optimal methods for reuse of chiral organometallic complexes and the development of efficient metal-based catalysts for selective alkene hydroamination of unprotected primary amines. The use of electrochemistry has been also developed as an efficient tool for performing electrocatalysis.

Heterogenization of (asymmetric) catalysts by formation of non-covalent bonds (E. Schulz, DR CNRS, C. Bouvier, IE CNRS, H. Nasrallah, PhD student)

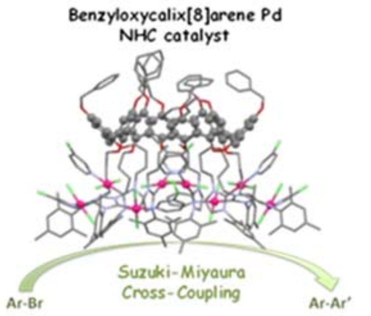


Having previously demonstrated the efficient reuse of chiral bis(oxazoline)-based organometallic complexes in various asymmetric reactions through formation of non-covalent interactions with different supports, we have adapted this methodology to the recovery of ruthenium complexes, active catalysts to promote metathesis reactions. This project has been supported by the ANR program CD2I CFlow-OM (PI M. Mauduit, Rennes, 2012-2015) which aimed at developing a process for the industrial processing of vegetable oils. In this context, we studied the immobilization of Ru complexes by reversible π-π or charge-transfer complex interactions, on silica supports modified with trinitrofluorenone or on carbon supports. We have evaluated the performances (activity, selectivity, recycling) of these new supported catalysts in the metathesis reaction of benchmark substrates and also unsaturated esters.

Heterogeneization of chiral derivatives of Salen type (E. Schulz, DR CNRS, M. Mellah, MCF, F. Ibrahim, H. Dandachi, N. Zidelmal, PhD students, E. Zaborova, I. Abdellah, Postdocs)



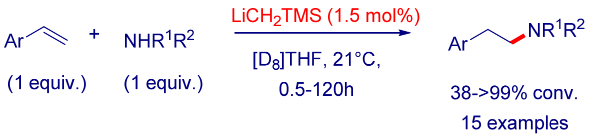
In accordance with the principles of green chemistry, we have studied the possibility of recycling chiral organometallic complexes by using them in the form of polymers. Based on our expertise obtained in the field of organic conducting polymers from salen derivatives and their evaluation in catalysis, we have explored heterobimetallic dual catalysis to perform the hydrolytic kinetic resolution (HKR) of different epoxides. In this context, and to favor cooperative activation, we have prepared and tested cobalt-containing Calix-salen complexes, as macromolecular cyclic structures, easily obtained through condensation of appropriate disalicylaldehyde derivatives with enantiopure diamines. Enhanced



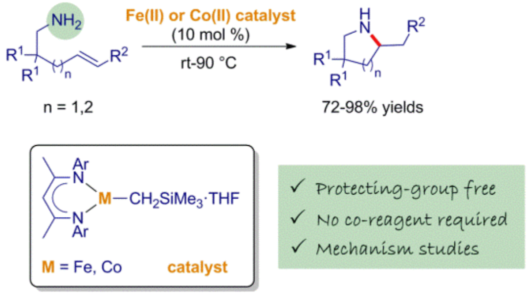
activity and enantioselectivity have been obtained with these catalysts for the transformation of difficult substrates, such as *meso*-epoxides, for instance and they have been easily recovered and reused by simple filtration. This last theme is carried out in collaboration with colleagues from the Lebanese University in Beirut thanks to one co-supervised these in the period. It was also supported by the LabEx Charm3At for collaboration with Dr. O. David (ILV, Versailles). The LabEx also allowed starting two new collaborations, one of them with the polymer group of the SM2B Team (Pr. P. Roger) and Ecole Polytechnique (Dr. A.-C. Gouget) for the synthesis of salen-containing polymers by atom transfer radical polymerization, their characterization and their catalytic properties in HKR. Furthermore, with the group of Dr. V. Huc (ECI), new platforms, based on Calix[8]arenes, have been dedicated to synthesize well defined heterogeneous catalysts that already proved to be efficient for C-C couplings (NHC-Pd complexes) or HKR reactions (Co-Salen complexes).

Hydroamination reactions With alkali bases, lanthanides or group IV elements (E. Schulz, DR CNRS, J. Hannedouche, CR CNRS, S. Germain, PhD student)

During the preceding five-year period, we have amply developed the enantioselective intramolecular hydroamination reaction with chiral lanthanide complexes. This work led us to have many invitations to write reviews in this field. In recent years, we have been keen to discover the reactivity of our complexes to promote the intermolecular version of the reaction. Binaphthylamido alkyl yttrium complexes have thus been proven to promote the anti-Markovnikov addition between various styrene derivatives and secondary amines efficiently. Moreover, we were also able to prepare various β-arylethylamine derivatives by lithium-catalysed anti-Markovnikov selective intermolecular hydroamination reactions of secondary aliphatic amines and vinylarenes. Use of as little as 1.5 mol % $LiCH_2TMS$ as solid base in THF proved to be an efficient room-temperature protocol for delivering the targeted products in up to complete conversion. In collaboration with Pr. G. Giambastiani (Florence, Italy), we have shown that cationic complexes of zirconium and hafnium have very competitive catalytic activities with respect to the best zirconium cationic catalysts of the state of the art. Another collaboration in Italy, (Pr. F. Ragaini, Milan) led to the preparation of new biamidoalkyl ytium complexes from bis-arylaminoacenaphthylenes, which proved also to be efficient in the intramolecular hydroamination reaction, specifically for substrates normally reluctant in undergoing cyclization such as those featuring an internal non-activated C=C.



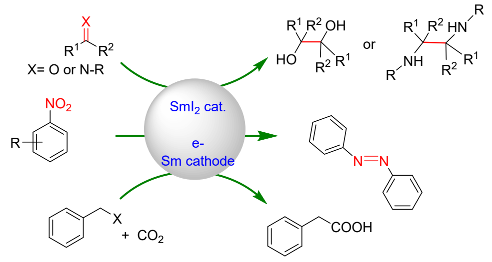
Hydroamination reactions With iron or cobalt complexes (J. Hannedouche, CR CNRS, E. Bernoud, Postdoc, C. Lepori PhD Student)



As part of a research program devoted to the development of well-defined and low-coordinate first-row transition metal complexes for atom-economical catalytic applications, we have synthesized and characterized a novel family of structurally-defined β-diketiminato-iron(II) and -cobalt(II) alkyl complexes. These complexes represent first examples of the Fe(II)- and Co(II)-mediated hydroamination of electronically unbiased primary amines by displaying unique catalytic abilities of promoting the selective *exo*-cyclohydroamination of primary aliphatic alkenylamines. For both catalytic reactions, we have undertaken comprehensive mechanistic investigations by means of complementary experimental (deuterium-labelling, kinetic and stoichiometric experiments) and computational studies. The computational investigations for iron and cobalt systems have been done in collaboration with Dr S. Tobisch (University of St Andrews) and Pr A. Llédos/Dr. G. Ujaque (Universitat Autònoma de Barcelona) respectively. On the basis of these collaborative studies, the reaction catalyzed by β-diketiminatoiron(II) complexes favours a stepwise-σ-insertive mechanism over a proton-assisted concerted N–C/C–H bond-forming non-insertive pathway while that catalyzed by β-diketiminatocobalt(II) complexes operates through a stepwise non-insertive mechanism as original alternative to the classically reported hydroamination mechanisms. The deeper knowledge of mechanistic intricacies was exploited further to improve the selectivity and catalytic efficiency of our iron-based systems. This work led us to have 4 invitations to write reviews in this field.

Electrosynthesis and electrocatalysis with Sm (II) (M. Mellah, MCF, Linhao Sun, Yufeng Zhang and Sakna Bazzi PhD student, Gaëtan Le Duc Postdoc)

In agreement with the history of our laboratory in the field of lanthanides, we recently developed electrocatalytic procedure based on Sm (II) derivatives as a reducing agent for C-C and C-heteroatom bond forming transformations. The guiding principle of this electrochemical process is based on the facile regeneration of the active low oxidation state catalytic species using a bare samarium electrode as a cathode. We also found that the electrolytic media plays a crucial role in the catalysis and significantly enhanced the reactivity of the Sm^{II} species. These results have urged us to evaluate the potential of our catalytic approach to reduce efficiently and selectively other functional groups. Thus, we have recently developed a facile, efficient alternative for synthesizing a wide variety of symmetrical and asymmetrical azobenzenes. Catalytic selective reductions of sulfoxide and phthalimide were demonstrated. Also, in collaboration with Dr C. Gosmini (Ecole Polytechnique) work is ongoing to reduce catalytically CO_2 as building block for the synthesis of valuable molecules.

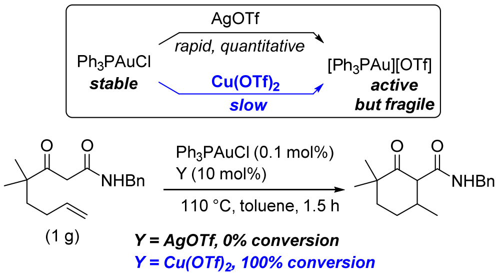


Polycyclisations catalytiques

Over the past 5 years, our group has remained focused on the development of original homogeneous catalytic methods towards the synthesis of cyclic compounds. One aspect of our work aims at circumventing the limitations of late transition metal catalysis by devising new activation protocols that allow to control the decomposition of the complex and therefore significantly diminish its loading. The second aspect is to replace noble metals by more abundant elements from the first row transition metal series, or by main group metals. All these projects have been supported by computational studies to rationalize the reaction mechanisms. Computational chemistry, especially DFT calculations, still occupies a prominent position in the group and constitutes on its own the third aspect of our investigations.

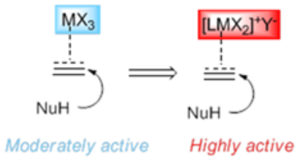
Gold catalysis (V. Gandon, PR; C. Bour, MCF; S. Bezzenine-Lafollée, MCF; Weizhen Fang, PhD student; M. Vayer, PhD student; Amandine Guérinot; Postdoc, Marc Presset; Postdoc, M. Sircoglou, Postdoc).

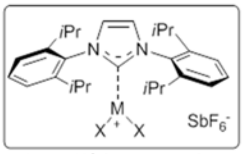
In order to improve the overall efficiency of gold-catalyzed transformations, we have discovered that Cu(I) and Cu(II) salts could activate LAuCl precatalysts, while lowering their decay into inactive nanoparticles. This decomposition phenomenon is typically observed with Ag(I) activators, which are commonly used to generate the active cationic gold complex. On the other hand, the Au/Cu catalytic system proved versatile and allowed to carry out a variety of reactions with very low loadings of the gold precatalyst and without requiring tedious ligand design. Indeed, simple phosphines could be used successfully on gram-scale reactions.



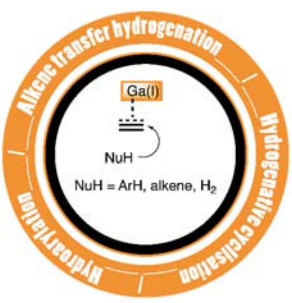
Gallium and indium catalysis (V. Gandon, PR; C. Bour, MCF; Zhilong Li, PhD student; B. Michelet, PhD student; M. Vayer, PhD student; A. El-Hellani, PhD student; S. Tang, PhD student; J. Monot, ATER; M. Presset, Postdoc).

We have developed new families of cationic Ga(I), Ga(III), In(I) and In(III) catalysts able to imitate the behavior of noble transition metal complexes in π-acid catalysis or transfer hydrogenation. These species exhibit either NHC or fluorobenzene ligands. They behave as soft Lewis acids able to trigger the formation of highly delocalized non-classical carbocations from alkynes and alkenes. They are especially useful in skeletal reorganization reactions leading to polycyclic compounds after C-C or C-H bond formation.

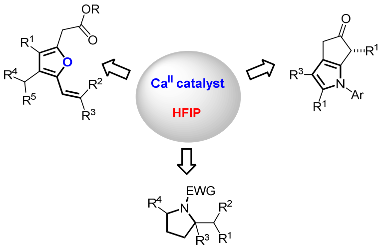




$[IPrMX_2]^+[SbF_6]^-$, M = Ga, In, X = Cl, Br, I



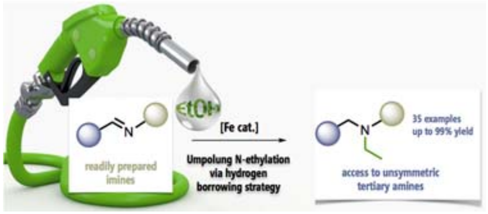
Calcium catalysis (V. Gandon, PR; C. Bour, MCF; D. Leboeuf, CR CNRS; S. Bezzenine-Lafollée, MCF; E. Schulz, DR CNRS; B. Michelet, PhD student; C. Qi, PhD student; L. Marin, PhD student; S. Morcillo, Postdoc; M. Presset, Postdoc).



We have exploited the exceptional σ-Lewis acidity of Ca(II) complex, sometimes exacerbated by the use of hexafluoroisopropanol as solvent (HFIP), to activate electron-poor C=C bonds in hydroamination reactions, or to activate C*sp*^{3}-O bonds for the synthesis of carbocycles or oxygen- or nitrogen-containing heterocycles. In particular, the low-tech air-stable calcium pre-catalyst $Ca(NTf_2)_2$ showed an exceptional versatility in reactions leading to furans, pyrroles or pyrrolidines.

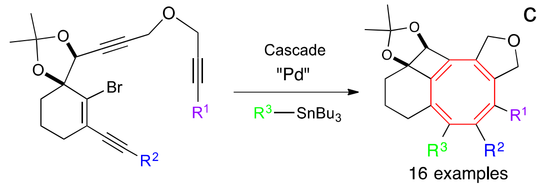
Iron catalysis (V. Gandon, PR, C. Bour, MCF, M. Vayer, PhD student).

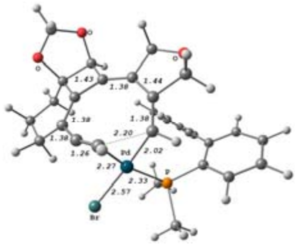
The borrowing hydrogen strategy has been applied to the ethylation of imines, using an air-stable iron complex as precatalyst. This approach has opened new perspectives in this area, as it allowed the synthesis of unsymmetric tertiary amines from readily available substrates and ethanol as C2-building block. A variety of imines bearing electron-rich aromatic or alkyl groups at the nitrogen atom could be efficiently reductively alkylated, without requiring the use of molecular hydrogen.



DFT computations (V. Gandon, PR; G. Grelier, PhD student).

In addition to providing a mechanistic insight into the aforementioned and other in-house projects, DFT computations have been carried out on various collaborative projects on Au-, Rh-, Fe-, Pd-catalyzed reactions and other catalytic processes leading to polycyclic compounds. Among recent achievements, we have deciphered the intriguing Pd-catalyzed carbocyclization leading to polycyclic cyclooctatetraenes in collaboration with J. Suffert and G. Blond from Unistra.

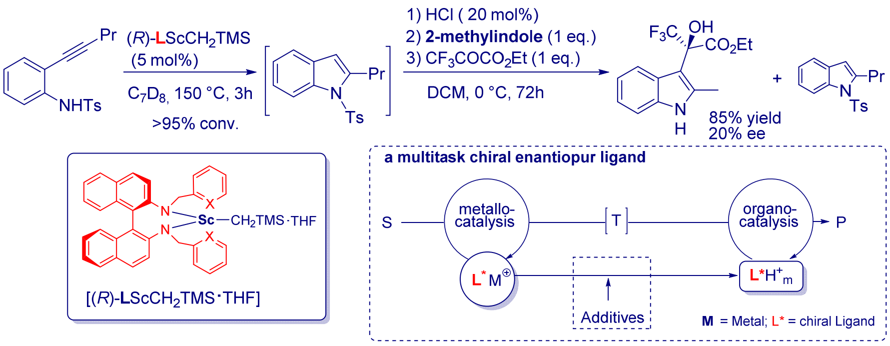




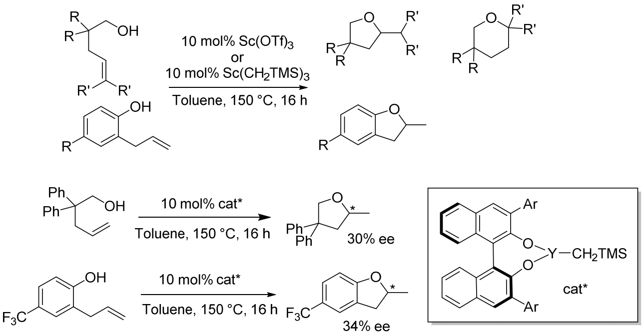
Lanthanides

Asymmetric assisted tandem catalysis (J. Hannedouche, CR CNRS, R. Gil, MCF, S. Bezzenine, MCF, R. Carlino, PhD Student, A. Aillerie, V. Rodriguez-Ruiz, S. Perato, Postdocs)

As part of a research program devoted to the development of asymmetric applications of assisted tandem catalysis, we have recently reported the first use of a multitask chiral ligand in asymmetric metallo-organo assisted tandem catalysis. In this protocol, the chiral ligand of the newly designed rare-earth catalyst of the first reaction was converted into a novel organocatalyst (R)-HL·HCl for the second transformation in a tandem sequence alkyne hydroamination / enantio-selective Friedel–Crafts alkylation. The transformation of the organometallic catalyst into the organic catalyst was simply triggered by the addition of HCl and was undoubtedly confirms by heteronuclear ^1H–^{15}N NMR correlations through a series of HMBC experiments. Additionally, the observation of some enantioinduction in the tandem sequence confirms the relay of the chiral tetradentate ligand between the two catalysts. More recently, we focus our attention to extend our relay concept of the chiral-inducing agent in asymmetric assisted tandem catalysis to the chiral anion-mediated chemistry in which the enantiopure noncovalently-bounded anion from a metallocatalyst will subsequently be converted into a chiral organocatalyst. This project is done in collaboration with Pr D. Prim (ILV, Université de Versailles).



Intramolecular hydroalkoxylation of unactivated alkenols catalyzed by rare earths complexes. (R. Gil, MCF, S. Bezzenine, MCF, R. Carlino, PhD Student)

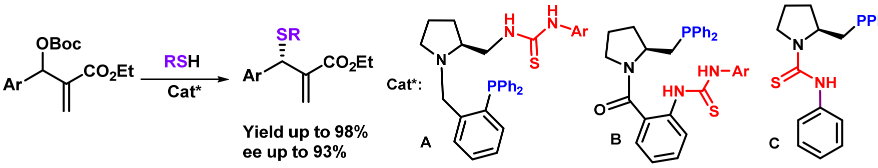


Cyclisation of unactivated alkenols by hydroalkoxylation is one way to produce in one step various cyclic ethers In order to activate the substrates; this transformation requires very efficient catalysts. Rare earths triflates were tested because of their strong Lewis acid property. These complexes were compared in hydroalkoxylation with alkyl rare earths which possess also basic properties. Among various rare earths triflates, it was found that the more reactive is the scandium triflate. The hydrogen atom of the alcohol function would be made more acidic and the mechanism would go through a cationic intermediary. The product is then obtained according a Markovnikov selectivity. Trialky scandium or yttrium, prepared from LiCH2TMS and RECl3, can be also employed in hydroalkoxylation; in this case the catalyst is transformed with the alkenol into rare earth trialkenolates. In a second step, this insertion of the C=C bond into the O-metal bond can occurred leading also to a Markovnikov product. Both kinds of catalyst are efficient with some differences of activities according the starting materials. Moreover, one chiral complex of alkyl yttrium bearing a binaphtholate derivative gave encouraging results since enantioselectivities up to 34 %ee were obtained.

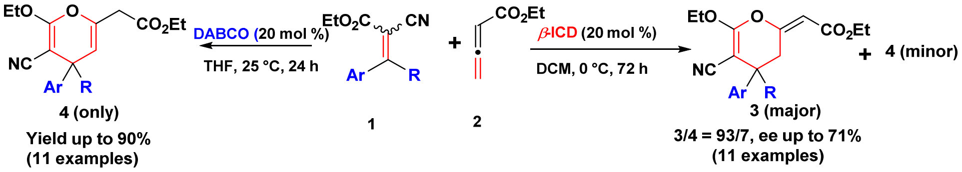
Liquides ioniques et Catalyse

The main part of our research activities is based on the valorization of easily accessible and inexpensive biomass compounds (isosorbide, isomannide, natural amino acids such as L-proline, *(S)*-pyroglutamic acid, ...). The transformation of these compounds under 'Green Chemistry' conditions, namely, solvent-free synthesis under microwaves activation method, allowed us to prepare (reversible) functionalized chiral ionic liquids, multi-dentate ligands (amino-alcohols, diamines, phosphines,...), chiral *N*-heterocyclic carbenes and functionalized chiral organocatalysts. These compounds have shown excellent activities in asymmetric metal or organic catalysis. Part of the group's research activities concerns the synthesis of therapeutic products (natural or unnatural) and their derivatives for QSAR studies. Some application examples are presented below. It should be noted that during this five-year period, many international and national collaborations have been established.

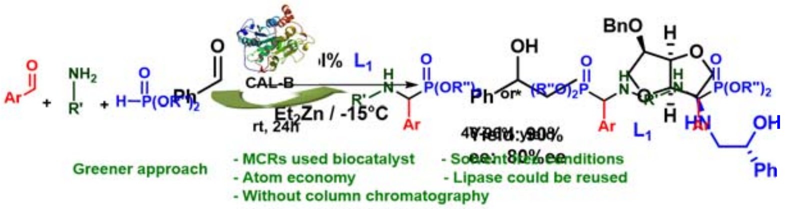
Asymmetric organocatalysis (G. Vo-Thanh, Prof; M. Toffano, CR CNRS; C. Bournaud, MCF; T.-T.-D. Ngo, T.-H. Nguyen, PhD students, Vietnamese Government Scholarships-Program 332 and 911).



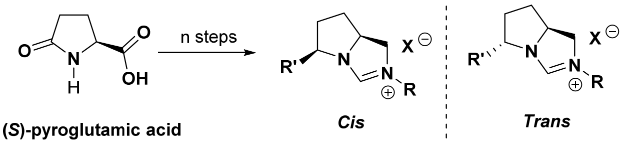
Having previously reported the synthesis of new bifunctional chiral phosphine-thiourea organocatalysts **A**, **B** and **C**, derived from L-proline, and their applications in asymmetric [3+2] cyclisation between ethyl-butan-2,3-dienoate and *N*-benzylidene-*p*-toluenesulfonamide; we have demonstrated, in this project, that these compounds catalyzed efficiently asymmetric allylic substitution of *tert*-butoxycarbonyloxy-MBH adduct with phthalimide. Good yields and enantioselectivities were observed. We have also described the first example of phosphine-thiourea organocatalyzed C–S bond formation affording enantioenrichied α-methylene-β-mercapto esters in good yields and with enantiomeric excess up to 93%. In collaboration with the Prof. Sasai's group (Osaka University), and supported by Sakura and Core-to-Core Programs (Japan-European Program), we have reported the first [4+2] annulation of allenoate and all-carbon tetrasubstituted alkenes catalyzed by an amine catalyst for the synthesis of highly functionalized *2H*-and *4H*-pyran derivatives. These results will open opportunities in synthesis of bioactive heterocyclic products and other pharmaceutical products.



Chiral ligands and NHCs: Design, synthesis and applications in asymmetric catalysis (G. Vo-Thanh, Prof; C. Bournaud, MCF; M. Toffano, CR CNRS; A. Thomasset, L. Bouchardy, PhD students).

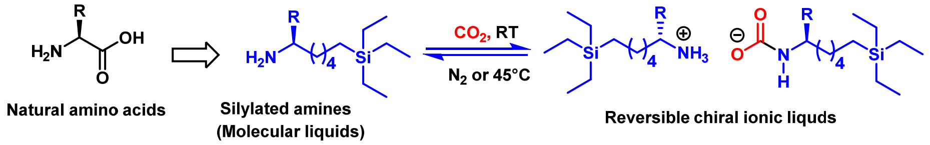


During the past five years, some new families of ligands (amino alcohols, diamines, phosphines, ...) were designed and synthesized from isosorbide and isomannide as optically pure, inexpensive biomass starting materials. The transition metal complexes formed with these ligands are evaluated for catalytic activity in asymmetric carbon-carbon, carbon-heteroatom bond formation reactions. An example of β-amino alcohol ligand in ethylation of benzaldehyde is presented. In continuation of our research on the design and synthesis of new chiral ligands for asymmetric catalysis, a new and flexible procedure for the preparation of *cis*- and *trans*-bicyclic functionalized chiral azolinium salts, precursors to *N*-heterocyclic carbenes, derived from L-proline and (*S*)-pyroglutamic acid has been developed. The efficiency of these NHC ligands has been evaluated in asymmetric allylic substitution and in conjugate addition of Grignard reagent to α,β-unsaturated ketones. This work is currently underway in our group.



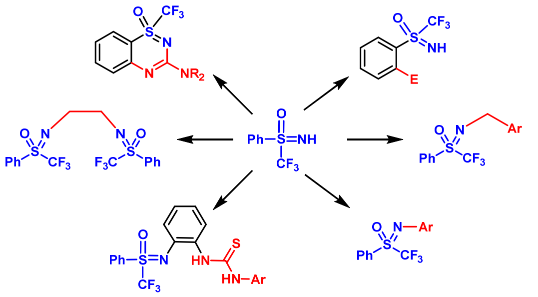
Reversible (chiral) ionic liquids: Design, synthesis and applications in (asymmetric) organic synthesis (G. Vo-Thanh, Prof; C. Bournaud, MCF; M. Toffano, CR CNRS; V. Rodriguez-Ruiz, Post-doc, L. Bouchardy PhD student).

In continuation of our research on the synthesis and applications of chiral ionic liquids as new chiral reaction media for asymmetric synthesis and catalysis, of which G. Vo-Thanh is one of the pioneers in this research field, we have managed to synthesize and formulate, in collaboration with Dr. F.-D. Boyer (ICSN-Gif sur Yvette), a novel class of reversible chiral ammonium carbamate-based ionic liquids derived from natural amino acids. Silylamines reacted reversibly with CO_2 to form ammonium carbamates referring to as RevCILs. Some physical properties of these chiral ammonium carbamate salts were measured, especially their reversibility temperature and their stability which were determined thanks to DSC and TGA analyses. The properties of reversibility, chirality, and ease of preparation should make these silylamine-ionic liquid phases as promising solvents and/or catalysts for several applications, especially in asymmetric catalysis fields. It should be noted that for the first time, single-component RevCILS derived from natural amino acids have been reported. This work is currently underway in our group.



Fluorinated compounds chemistry (G. Vo-Thanh, Prof; C. Bournaud, MCF; M. Toffano, CR CNRS; T.–N. Le, PhD student, Vietnamese Government Scholarships-Program 'Chimie Pharmaceutique)

This work focuses on the preparation of a new family of (chiral) perfluorinated sulfoximines and sulfinimines. Different transformations and functionalizations of fluorinated sulfoximines have been developed in collaboration with Dr. E. Magnier's group in Versailles. These new compounds are used as organocatalysts or (chiral) ligands for transition metal catalyzed reactions. This methodology is applied to the synthesis of therapeutic products, eg Prazosin analogues.



Synthesis of Bio-based polymers for antibacterial surface applications. Structure-Antibacterial Activity Relationships (SAAR) studies (G. Vo-Thanh, Prof; C. Bournaud, MCF; M. Toffano, CR CNRS; N. Marets, Post-doctoral researcher)

Preparation of new polymers and polymeric surfaces with antibacterial properties would be of great interest in different areas such as household, industry, hospital. These polymers could be used respectively as disinfection solution or to manufacture sheets and clothes for protection against nosocomial infections. They could be obtained by a polymerization process using monomers which are obtained in some steps starting from isosorbide. This project, in collaboration with Prof. P. Roger (ICMMO), is funded by the Roquette Company and will not be detailed for confidentiality reasons.

Enzymatic promiscuity (M. Toffano, CR CNRS).

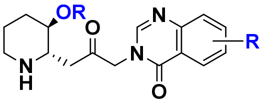
Recently, M. Toffano, in collaboration with Prof. L. Zouioueche (Annaba University), have developed a simple and eco-friendly preparation of α-aminophosphonates and Bis(α-aminophosphonates) *via* a multicomponent *Kabachnik-Fields* reaction in the presence of an immobilized *Candida Antarctica* lipase as catalyst under solvent-free conditions.

Structure-Activity Relationship studies of Febrifugine, antimalarial activity, and Gambogic Acid (GA), antitumor activity (G. Vo-Thanh, Prof.)

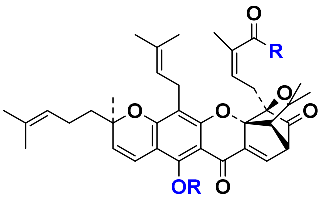
As part of an agreement signed between Paris-Sud University and VAST (Vietnam Academy of Science and Technology), G. Vo-Thanh, in collaboration with researchers at the Institute of Chemistry of Natural Substances in Hanoi, has developed the synthesis of Febrifugine and GA derivatives. Thus, 10 Febrigugine and 25 GA derivatives were synthesized. In vitro, antimalarial activity evaluation, for Febrifugine derivatives, indicated that all synthesized compounds had strong antimalarial activity against both chloroquine-sensitive and -resistant strains of P. falciparum. The cytotoxicity of GA derivatives was tested on the cancerous cell lines Lu1, HepG2, RD and showed very promising results. SAR studies are currently underway on new synthesized analogs.

Highlights

The ECM team increased its total number of publications (123) and the average impact factor (5.32) during the last quiquennial. Notably, the team published its work in 11 papers with impact factors over 9, and was invited to write 9 reviews in high impacting journals, including a "News and Views" article published in Nature by E. Schulz. We wish to highlight the activities of Pr. V. Gandon who received special recognition form our community (2012-2017, IUF junior member, 2015, SCF distinguished junior member and 2017, recipient of the Jean-Marie Lehn Price from the SCF-DCO). His expertise has resulted in the establishment of much new fruitful collaboration and many invitations in France and abroad.



Febrifugine derivatives



GA derivatives

The ECM team is now recognized for its ability to effectively replace noble metals or rare-earths by more abundant elements from the first row transition metal series or by main group metals to perform atom-economic reactions such as cyclohydroamination of unbiased primary amines or polycyclisations. These results were supported by DFT calculations providing mechanistic insight into these transformations. The team is also attentive to the transformation of biomass into ionic liquids or organocatalysts, and original applications were published in the recent years. The use of rare-earth metals remains an activity that persists in the team with promising results in new hydroelementation reactions, and successes in SmI_2 electrogeneration and subsequent use to promote substrates functionalization. The expertise in catalysts heterogeneization sparked new collaborations and development of new immobilization processes. All our research is done in collaboration with many French teams but we want to highlight our efforts towards international partnership and in particular with Vietnam, Japan, China, Algeria, Argentina and Lebanon. This is reflected in our active participation in COST, GDR and GDRI networks, Core-to-Core Program…

LCM members have been invited to deliver 34 invited conferences, 81 seminars and 78 oral talks in national and international congresses. The research of the team is financed as a whole by a common pot, filled by recurring money but also 7 ANR funding and 17 LabEx Charm3At supports (mainly for one year postdoc), either as PI or partner. We also worked in close interaction with industrial partners for research collaborations (Roquette and EDF). Worth mentioning is our recent involvement in the valorization of our work, which was mainly until now the result of fundamental research (funding for prematuration projects, involvement in a start-up creation, 2 patents). We also tried to better highlight our results with outreach efforts (echo-CNRS). Team members and their doctoral students are very committed to participating in the organization of many scientific events (SECO, GECO, GECOM, Lanthanide days, International Vietnamese-French School). The team is very present for training through research: 19 PhD students have defended their thesis during this contract and 11 more are in progress.

All members of the team are significantly involved in the collective life of the team, the unit, but also the University and the research support agencies/authorities during this five year period. Locally, about three members of the team participate in the institute's council and its committees. We are also involved in the life of the university (M. Mellah, member of the CS, president of the Cephyten, S. Bezzenine VP-enseignement of the chemistry department). All the members of the group participate in numerous expertises, taking part in recruitment commissions or the assignment of lecturer or professor positions throughout the national territory (participation in 14 juries over the period); we are also present to many thesis (94) and HDR (13) defenses. We are or have been present in HCERES and ANR committees, in the CNU 32, at the SCF-idf and DCO…. At the international level, G. Vo-Thanh is Scientific Advisor of the Ministry of Science and Technology (MOST) of Viet Nam since 2012.

2Organisation and life of the research team

Management, organisation and scientific animation

The ECM team has a staff that varies between 30 and 40 people, depending on the time of year, because we receive many students in training. The team is very present for training through research: 19 PhD students have defended their thesis during this contract and 11 more are in progress. More than two-thirds of our doctors have a fixed position (for 75 % of them in the private sector and for others in the public sector). The other doctors are currently in post-doctorate and 4 of them still looking for a job. We participated in the orientation and training of 24 M2 students and 25 other students (M1, L3, L2, Magister, Erasmus…). We further welcomed 21 postdocs and ATER, 7 of them are still in progress. Among the postdocs who participated in our research 3 of them are now lecturer, 4 obtained a position in the private or public sector, and 4 continued with new post-doctoral research.

Our scientific organization, as described above, is based on thematic groups to carry out our research. In addition to informal exchanges within and between groups, the team organizes weekly internal scientific seminars with all members. Permanent or students are invited to present very recent scientific articles they have chosen, and the seminar is completed by the intervention of a student who summarizes the progress of his current research work or presents a theme of his choice, out of his direct expertise. About our practical organization, the permanent staff meets 5-6 times a year, during which scientific projects, recruitments and material acquisitions are discussed and prioritized. The financial resources are in their entirety put in a common pot. The practical tasks of daily life are distributed among all the members of the team.

3SWOT analysis

Strengths	**Weaknesses**
Clear and varied expertise in the team National and international recognition New themes	Number of publications to be strengthened Fundamental research
Opportunities	**Threats**
ANR and LabEx Calls Collaborations	Financial dependence on calls Administrative tasks

4Scientific strategy and projects

In the next quinquennial, the main objectives of the Molecular Catalysis team will remain focused on the finding of selective (asymmetric) catalytic processes on the one hand, and on the development of new chiral ligands or organocatalysts on the other hand. Our research will always be in line with the theme of sustainable chemistry, which is more than ever a crucial societal challenge to take. All the team members have been dynamic and active in responding to calls for funding (ANR, Labex, etc) and developing international collaborations (Asia, Europe and the Americas). This aspect will be further encouraged, notably at the European level. In order to address the identified weaknesses of this quinquennial (see SWOT), our goal for the next one will be to improve our visibility by increasing the dissemination of our scientific results. We will also care for broadening our fundamental work to applied research. For this purpose, industrial collaborations will be developed and strengthened.

Catalyse Moléculaire, ECM
G. Vo-Thanh, Pr, UPSud

Catalyse supportée et électrocatalyse
E. Schulz DR, CNRS
M. Mellah MC, UPSud

Liquides ioniques et catalyse
G. Vo-Thanh Pr, UPSud
C. Bournaud MC, UPSud
M. Toffano CR, CNRS

Polycyclisations catalytiques
V. Gandon Pr, UPSud
C. Bour MC, UPSud

Catalyse organométallique homogène
J. Hannedouche CR, CNRS
R. Gil MC, UPSud
S. Bezzenine MC, UPSud

Chiralité
H. Kagan Pr Emérite, UPSud

Soutien technique
E. Kolodziej, AI-CNRS

Administratively, there are 5 research groups within the ECM team. However, these entities are not compartmentalized, since all team members have been collaborating with each other for many years. These internal collaborations will be galvanized, not only within the ECM team, but also at the ICMMO level. National and international collaborations are always a strong point of the team, and this will obviously be strengthened and developed for the coming years. The team leader will change, but the management system, including daily activities and budget aspects, will remain virtually identical for the next period, as it is already appreciated by the laboratory members for its efficiency.

The permanent staff members of the ECM remain practically unchanged,[2] but there are some re-organizations between research groups compared to the last 5-year period. Among the permanent members of the laboratory, two assistant professors, Dr. Jean-Yves Legros and Dr. Florence Hélion, are still actively involved in teaching responsibilities and currently wish to fully devote their time to pedagogical tasks and collective responsibilities within our team and at the Chemistry Department level.

Below, the main research topics that researchers of ECM team wish to develop for the next five-year period are briefly presented.

Groupe 'Liquides ioniques et Catalyse'

In the next five-year period, our research activities will remain on the development and the valorization of natural and/or biomass products for applications in asymmetric catalysis. The project focuses on the design and synthesis of a new class of multifunctional chiral organocatalysts in which a Brønsted (or Lewis) acid function and a Lewis Base moiety will be connected by a chiral linker. These new molecules will be obtained in some steps from commercially available reagents or from chiral natural molecules derived from biomass.

Another part of catalysis project concerns the development of phosphorous chemistry. Our objective aims at designing and synthesizing chiral phosphinic acids derived from phospholane structure which has never been reported in literature. These chiral phosphinic acids will be used as new Brønsted acid catalysts and will open new applications to organocatalyzed asymmetric transformations.

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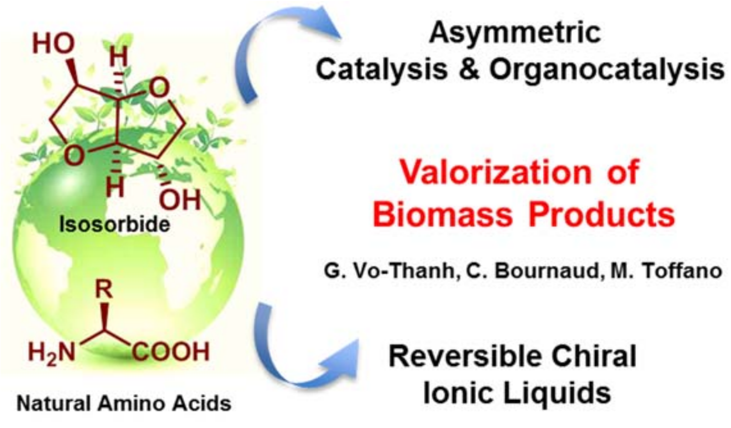
[2] Except Dr. David Leboeuf, CNRS researcher, who will leave the ECM team in the late 2019 to benefit, at his request, an availability to follow his spouse abroad.

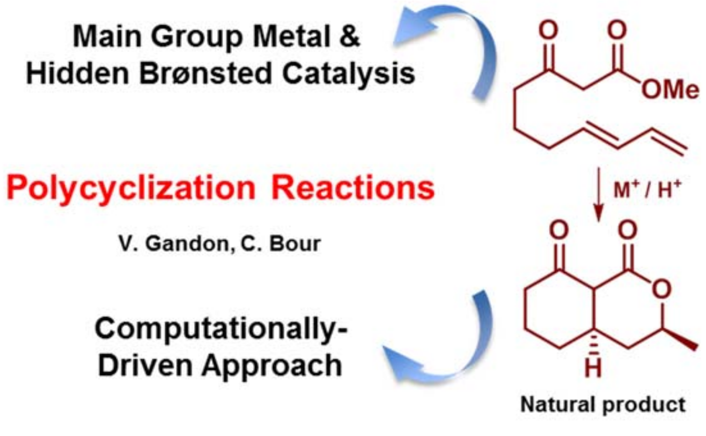


Thanks to our expertise in the ionic liquid chemistry field, we wish to develop a new methodology for selective protection (and deprotection) of functional groups in organic synthesis by using reversible ionic liquid as a temporary protecting group of diol or amino alcohol. An amino (or a hydroxyl) function of these substrates can react reversibly with CO_2 to form an ammonium carbamate (or carbonate) referring to as RevILs. After performing chemical transformations on these compounds, the protecting group could be easily removed by bubbling a displacing gas (N_2 or Argon) through the ionic liquids or by heating them at 45°-50°C. On the same principle, a new concept of organocatalyst recycling by CO_2 reversible reaction will be studied.

Part of our research will deal with the synthesis of natural or unnatural products of biological and therapeutic interest. In this topic, Tagitinin C and its derivatives, possessing anti-inflammatory, anti-cancerous properties will be designed and synthesized for QSAR studies. This project is in collaboration with researchers at the Vietnam Academy of Science and Technology.

Groupe 'Polycyclisations catalytiques'

We wish to capitalize on our past 5 years findings regarding the use of abundant main group and first row transition metals in selective catalytic processes. The development of Ga-, In-, Ca-, Fe- and other eco-compatible metal-catalyzed reactions has opened new perspectives in the synthesis of heterocycles, natural products, bio-sourced industrially relevant compounds, etc. In a maturing strategic approach, we have started to exploit these new processes, focusing on flavonoid-derived colorants and tertiary amines of biological interest. We have also started research programs aimed at the use of our strong Lewis acids in lignin depolymerization. In addition to these applied chemistry projects, fundamental research will still occupy a prominent position in our group, by pursuing three main goals:



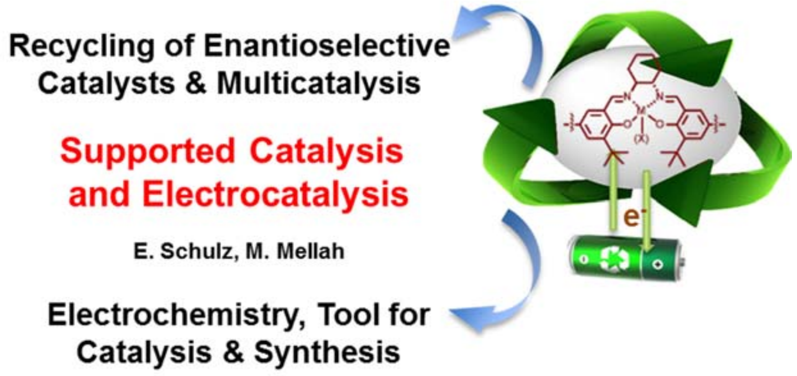
i) The development of ***new main group metal-catalyzed cyclizations*** involving transfer hydrogenations, cross-couplings, metathesis, CH-activations or other reactions that are believed to belong to the territory of noble metals catalysis.

ii) ***Mechanistic studies focused on the role of protons in metal catalysis***. Organic synthesis greatly relies on strong Lewis acid-catalyzed processes and the use of such compounds raises questions about the nature of the active species. Strong Lewis acids have indeed the potential to mediate the formation of protons in various ways in the reaction medium (hidden proton catalysis) or decompose into Lewis acids that can outcompete the initial Lewis acid as the true catalyst (hidden Lewis acid catalysis). Besides, metals and protons can actually cooperate during the catalytic event. This part of our project is a quest for the real active species in catalytic processes involving strong Lewis acids.

iii) ***Computational studies directed towards metal-catalyzed cyclizations***. In line with point ii above, we have noticed that the part of the catalyst than activates the substrate in our reactions is not necessarily the metal ion itself, but it can be a ligated solvent molecule. So-called innocent counterions can also play a dramatic influence of the selectivity. DFT computations have led us in the past to gain insight into these processes and to delineate new concepts such as the metal-templated bifunctional organocatalytic activation. We have still many reactions to investigate in the future, in main group and transition metal catalysis, which should reveal unsuspected mechanisms with iconoclastic activation modes.

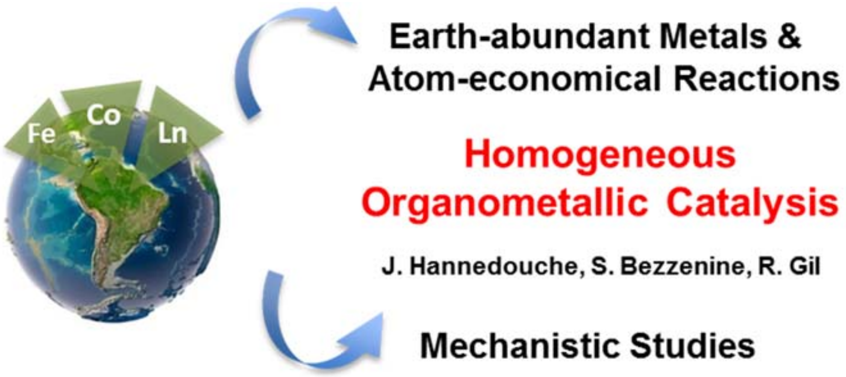
Groupe 'Catalyse supportée et électrocatalyse'

In line with our objectives to perform efficient, atom-economic (asymmetric) transformations, our work will be continued with our collaborators. Immobilization of (asymmetric) organometallic complexes on macrocycles such as tailor-made calixarene structures proved already successful to promote catalytic transformations of major interest with formation of high yield product, high selectivity, high recyclability and especially with almost no metallic contamination. Being a stakeholder with V. Huc (ECI) of the Novecal Company created by C. Martini last spring, we will continue our efforts to widen the scope of calixarenes, as a suitable support combining an electron-rich backbone with confinement, in various heterogeneous catalytic reactions implying different ligands and metallic salts. We wish also to explore asymmetric tandem catalysis by taking advantage of the heterogenization of the catalysts not only for their recycling but also for their targeted positioning towards multicatalysis, whether it is cooperative or orthogonal. The heterogeneization methods explored will concern the co-electropolymerization of different metallic salen complexes, the controlled co-polymerization of dedicated salen species (ATRP, RAFT with P. Roger, ESM2B) but also the co-immobilization of pyrene-tagged salen derivatives by non-covalent π-π interactions on carbon surfaces (rGO, CNT, graphite… with N. Jaber, Lebanese University). Furthermore, the same procedure will be applied to the co-immobilization of both salen complexes and (chiral) organocatalysts (with O. David, ILV) to widen the scope of the explored tandem catalytic reactions. Concerning our activity in electrocatalysis, we will pursue our investigations for the development of catalysis based on samarium complexes as reducing reagent. In this context, we will focus our research principally on the catalytic reduction of CO_2 as widely available and cheap C1 building block. Finally, we wish to develop new asymmetric catalytic methodologies promoted by photocatalysis, through the covalent assembly of a photosensitizer and the Jacobsen catalyst to better understand the various photophysical events in the activation of the enantioselective catalyst for oxidation catalysis (with A. Aukauloo, ECI).



Groupe 'Catalyse organométallique homogène'

In the next period, our group that merge some of the long-term and more recent expertise of our laboratory in rare-earth and base metal chemistry respectively, will focus on the development of **structurally-defined organometallic complexes from earth-abundant metals** (Ln, Mn, Fe, Co…) for **atom-economical catalytic applications** (hydro- and di-functionalisation, dehydrocoupling…) targeting key and useful synthetic building blocks. Our recent findings with well-defined low-coordinate first-row late transitions metal (Fe, Co) and rare-earth (Sc, Y, Sm, Yb) offer opportunities to explore and develop novel and efficient catalytic reactivities for the (stereo)selective formation of carbon-carbon, carbon-heteroatom bonds or other types of bonds from ubiquitous starting materials. To do so, we will focus our efforts towards a better understanding of the parameters affecting the reactivity and the selectivity of our designed complexes, at different metal oxidation states, in **elemental reactions of organometallic chemistry** as key steps in many catalytic cycles. In parallel to these studies on atom-economical reactions, part of research will also be devoted to the development of asymmetric step-economical catalytic protocols based on one-pot catalysis with a particular focus on **asymmetric metallo-organo assisted tandem catalysis**. Our group will have **a mechanistically-driven approach based on the complementarity between experimental and computational studies**. This approach will be at the core of our research and will be carried out in close collaboration



with in-house and external (French and international) research teams, mainly for theoretical studies. Such fruitful partnerships on our ongoing projects have been set-up during the past five-years period and will be pursued and strengthened.

Groupe 'Chiralité'

Although the presence of Prof. Henri Kagan in the team is less frequent, his contribution to the scientific community and particularly to the outreach of the ECM team is exemplary. His exchanges with us and his scientific advice during our discussions are always very important and a source of inspiration for our young researchers. Prof. Kagan maintains a strong scientific communication at the international level and receives many solicitations, which makes his group a true entity of the ECM team.

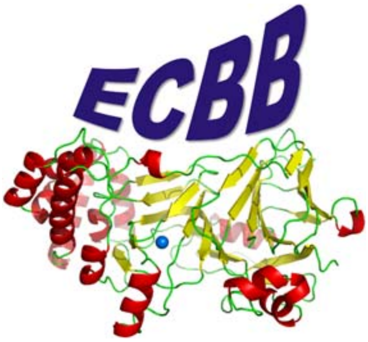
Self-assessment document

Team 4 - ECBB

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

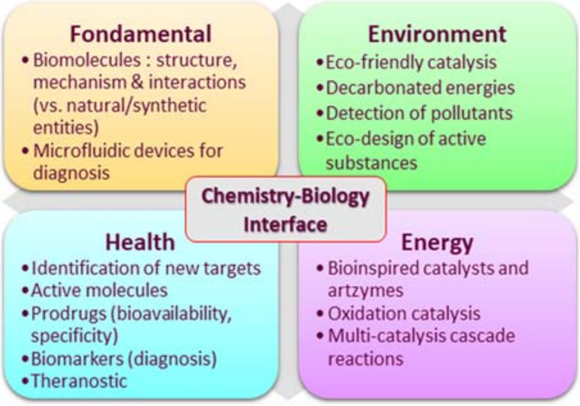
Team name:	**Chimie Bioorganique et Bioinorganique**
Acronym:	**ECBB**
Director's name (current contract):	**Laurent SALMON**
Director's name (future contract):	**Laurent SALMON**



1 Research products and activities

Scientific output

The **Team of Bioorganic and Bioinorganic Chemistry** (ECBB) develops its research at the **chemistry-biology** interface and combines the areas of **bioorganic chemistry** and **bioinorganic chemistry**, first, to the fundamental study of **biological processes** at the molecular level, of secondly, the design of molecules or devices to meet the current major societal challenges relating to fields of **health**, **energy** and the **environment**. The research includes: i) understanding the **mechanisms of action of biomolecules** (enzymes, metallo-enzymes...) and their **interactions** with natural or synthetic entities (substrates, inhibitors, metal complexes, electrochemical bioreceptors...), ii) identifying original **therapeutic targets** for developing new types of **drugs**, including eco-design of molecules with therapeutic interest and the synthesis of **prodrugs** of the active ingredients in controlled release in space and time, iii) the development of **artificial enzymes (artzymes)** or **bio-inspired catalysts** for oxidation catalysis, enzymatic multicatalysis in cascade, oxidation of water, or enzymatic catalysis of new reactions, and iv) the development of **electrochemical biosensors** and microfluidic devices for ultra sensitive and specific detection of **biological biomarkers** in body fluids or **contaminants** in food or environmental matrices.



Global domains of research developped by ECBB.

These scientific objectives are grouped under 3 main themes developped by 12 permanents (9 permanents on June 2018) and 32 PhD and postdoctoral researchers. The skills specific to each of these themes are in fact complementary and allow a broad study of various fondamental and societal issues at the interface of chemistry and biology, as described hereafter. Indeed, ECBB is attached to the two LabEx LERMIT (Theme 1) and CHARMMMAT (Themes 2 & 3). Scientific balance sheet is given in Table 1 below.

Table 1. Scientific balance sheet of ECBB team (January 1st. 2013-May 31st. 2018)

ACL publications (article + review)	55	*Publications average IF*	5.377	*Posters*	54
Book chapter	4	*ACL/ETPC/yr (ETPC = 4.87)*	2.05	*Proceedings*	5
Patents	2	*PhD defences*	13	*Congress organization*	8
Plenary-Invited lectures/keynotes	21	*PhD publications*	41	*Editorial board*	2
Oral communications	40	*Publications/PhD*	3.15	*Post-docs*	11
Invited research seminars	7	*PhD publication average IF*	4.95	*Research grants*	23

Theme 1 - Results

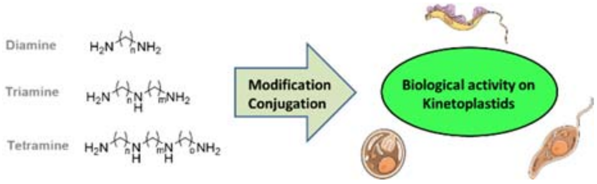
SYNTHESIS AND EVALUATION OF ENZYME INHIBITORS FOR THERAPEUTIC PURPOSES

R. Labruère[1] (MCF), S. Pethe (MCF), M. Therisod[2] (Prof.), C. Blonski[3] (DR), F. Ramiandrasoa[4] (IR), L. Salmon (Prof)

[1]Recruited Sept 1st. 2013, [2]retired April 1st. 2015, [3]leaved May 19th. 2016, [4]retired July 1st. 2018.

Theme 1 is mainly devoted to the synthesis and evaluation of enzyme inhibitors for therapeutic purposes including antiparasitic, antifungal, antibacterial and anticancer agents. Besides therapeutic interests, inhibitor are also used as valuable tools for structural and mechanistic studies of enzymes, as well as for diagnostic purposes of protein biomarkers. Specificity, bioavailability, and environmental issues are further adressed by designing self-immolating pro-drugs and by adressing specific carriers or properties of pathogenic cells.

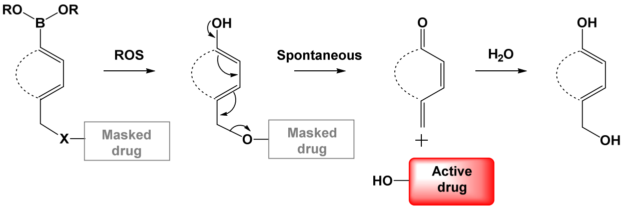
1- Polyamine-based anti-kinetoplastid agents.



Targeting polyamine transport in Kinetoplastids.

The protozoan parasites are the causative agents of severe diseases such as African trypanosomiasis, Chagas disease or Leishmaniasis. These are devastating infections that carry a considerable health burden on poor population. Treatments rely on a small number of drugs which mostly have a limited efficacy and high level of toxicity. In recent years, it has been shown that the metabolism and transport of polyamines were essential in parasites. Indeed, these are therapeutic targets of interest against the Kinetoplastids. Inspired by literature data and previous work from our laboratory, we elaborated new synthetic compounds as potential antikinetoplastids. Fifty-four compounds, divided into three chemical series, have been synthesized and evaluated. Many have shown a micromolar activity in vitro against parasite. In vivo evaluation on mice models was carried out for the most promising derivative (*Bioorg. Med. Chem. Lett.* **2015**, *Bioorg. Med. Chem.* **2017**, *Eur. J. Med. Chem.* **2018**).

2- Antitumor prodrugs activated by reactive oxygen species



Activation of antitumor prodrugs by reactive oxygen species.

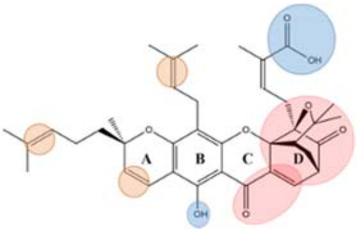
Cancer is the second leading cause of death globally, and was responsible for 8.8 million deaths in 2015. The drugs available in clinic often present similar toxicity towards both cancer and normal cells. Therefore, there is an urgent requirement for alternative chemotherapies. A relevant strategy relies on the development of prodrugs, masked forms of active drugs that are designed to be activated after an enzymatic or a chemical reaction (*Angew. Chem. Intern. Ed.* **2015**). In this project, prodrugs are prepared for the specific activation by the tumor environment. A targeting moiety is added to the prodrugs in order to increase the molecular uptake into cancer cells. Among the different metabolic pathways, the activation of antitumor prodrugs by reactive oxygen species (ROS) is particularly promising and has been developed in our laboratory. As tumor cells generate high amounts of ROS, such as H_2O_2, we have designed H_2O_2-activable prodrugs of doxorubicin. These derivative are tested against eight cancer cell lines and will be further evaluated using the Chick Chorioallantoic Membrane (CAM) assay.

3- Inhibitors against pan-drug resistant carbapenemase-producing Gram-negative bacteria

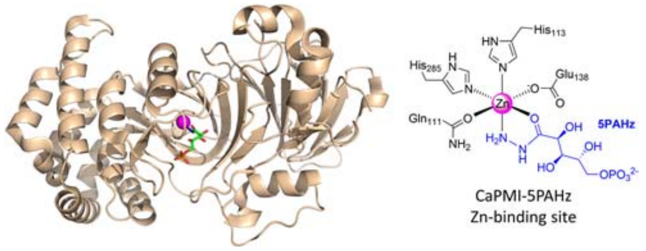
Fighting pan-drug resistant carbapenemase-producing Gram-negative bacteria is one of the most serious health concern of these last years. In 2015, we joined the JPIAMR (Joint Programming Initiative on Antimicrobial Resistance european project DesInMBL (coord. T. Naas, APHP, Univ. Paris-Sud) and synthesized new inhibitors of the pandemic NDM-1 metallo-β-lactamase (patent in preparation).

4- Derivatives of Gambogic acid & Tagitinin C as anticancer agents

Since 2016, a new project has been set up on the development of anti-cancer agents by pharmacomodulation of natural substances, Gambogic acid and Tagitinin C, in partnership with Prof. G. Vo-Thanh (ICMMO, ECM) and two teams of biologists from Vietnam and Korea. Gambogic acid, extracted from resin of *Garcinia* species, was modified via peptidic coupling on the carboxylic acid and modification of the phenol functions. We also undertook the synthesis of Tagitinin C derivatives in order to increase its biological activities.

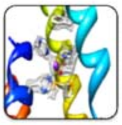


5- Aldose-ketose isomerase inhibitors: structural, mechanistic, therapeutic & diagnostic aspects



3D crystal structure of CaPMI-5PAHz complex (PDB 5NW7).

Phosphoglucose isomerase (PGI) and phosphomannose isomerase (PMI) are promising targets for the design of anti-metastatic and antifungal agents, respectively. The glycolytic enzyme PGI is also known as the cytokine AMF (autocrine motility factor) involved in proliferation of cancer cells. With Dr. Korri-Youssoufi (Theme 3), we designed highly efficient carbohydrate-based electrochemical biosensors for the detection of the cancer biomarker AMF in human plasma (*Biosens. Bioelectron.* **2017**). PMI from *Candida albicans* (CaPMI) is a zinc-dependent monofunctional enzyme which is essential for the vialability of the pathogenic fungus. CaPMI is thus considered as a potential target against fungal infections. Because PMIs from *C. albicans* and *H. sapiens* have a high level of sequence identity, detailed structural information of these enzymes is needed for the development of species-specific inhibitor. We obtained the 3D crystal structure of CaPMI in complex with a strong competitive inhibitor, 5-phospho-D-arabinonhydrazide (5PAHz) at 1.85 Å (PDB 5NW7, collab. H. van Tilbeurgh, I2BC, Univ. Paris-Sud). This structure allowed us to identify all of the active site residues and to elucidate the isomeration mechanism of Type I PMIs (*FEBS Lett.* **2018**).



Theme 2 - Results

DESIGN AND SYNTHESIS OF NEW METAL COMPLEXES AND STUDY OF THEIR INTERACTIONS WITH BIOMOLECULES

F. Avenier (MCF), R. Ricoux (IR), W. Ghattas[1] (CR), J.-P. Mahy (Prof)

[1] Recruited Oct 1st, 2016.

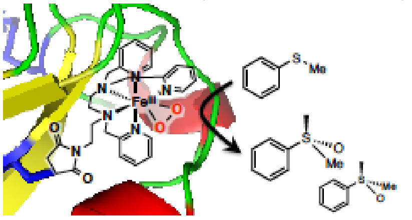
Activities developed in theme 2 are built on the Group's internationally recognized know-how in Bioinorganic Chemistry for the development of biomimetic systems of heme- (cytochromes P450, peroxidases...) and non-heme metalloenzymes (mono- and bi-nuclear iron hydroxylases) from transition metal complexes including metalloporphyrins or non-porphyrinic mono- or bi-metallic complexes, and for the design of artificial metalloenzymes by insertion of metal complexes in various proteins. The main objectives of the subjects developed are the elaboration and mechanistic study of new selective and effective (bio)-catalysts that can be used under eco-compatible conditions and which have potential industrial applications.

1- Catalysis of selective oxidation reactions by artificial metalloenzymes (Artzymes) and iron-binuclear complexes.

The development of new catalysts for selective oxidation reactions is of major interest for industrial applications, such as the enantio-selective oxidation of substrates usable in fine chemistry (sulfides, aromatics, alkenes…) and in pharmaceutical chemistry (production of metabolites), in fuel chemistry (oxidation of hydrocarbons) and in depollution (oxidation of toxic dyes, oil pollutants, and poly-halogenated aromatics). In a global context of sustainable growth, the generation of such catalysts that can operate under eco-compatible conditions (water, T_{amb} and P_{atm}), using clean oxidants such as O_2 or H_2O_2, is a real challenge that must be addressed. In vivo, such reactions are carried out by either hemoproteins (peroxydases, cytochrome P450 monoxoxygenases), or by non-heme iron monooxygenases (methane monooxygenase, MMO), that catalyze the oxidation by O_2 of many substrates, even as little reactive as n-alkanes, in the presence of electrons from NADPH delivered to the iron by a flavin-reductase. A double strategy was then developed in the last 5 years. First, following the results obtained for about 15 years in the field of artificial hemoproteins, new artzymes were constructed by incorporation of heme or non-heme metal complexes into protein scaffolds following the host-guest, Trojan Horse or covalent attachment strategies, and, second, biomimetic complexes were prepared by association of metal ions into ligands that mimic the first coordination sphere of natural metalloenzymes.

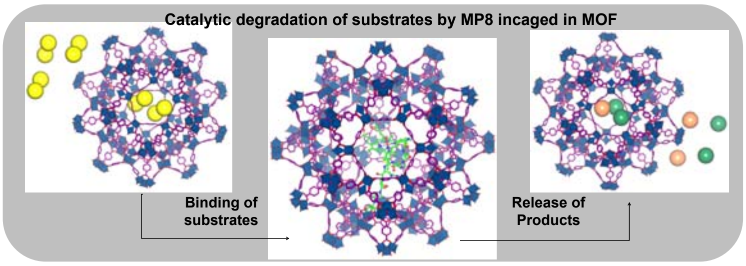
⇨ **First, hydrogen peroxide, that is the equivalent of the 2 electrons reduction product of O_2 (H_2O_2 ⇔ O_2 + 2 H^+ + 2 e^-) was used as an oxidant.**

1-1. *Enantioselective oxidation reactions catalyzed by Artzymes* (in collaboration with F. Banse, ICMMO, D. Mandon, Brest et B. Schöllorn, Paris 7, **ANR CATHYMETOXY**).



New artificial metalloenzyme were generated by the non-covalent insertion of an anionic Fe(III)-porphyrin–testosterone conjugate into a neocarzinostatin variant, NCS-3.24, following the so-called 'Trojan Horse' strategy (*Dalton trans.* **2014**) or by covalent grafting of a Fe(II)-TPA complex into □-Lactoglobulin (*Chem. Eur. J.* **2015**). In both hybrid biocatalysts, the protein protected the metal complex from oxidative degradation and induced the chemoselective and slightly enantioselective sulfoxidation of thioanisole by H_2O_2 with respective ees of 13% and 20%. In the later case, a high-spin (S = 5/2) Fe(II) □(η_2-O_2) intermediate was identified as the active species responsible for the oxygen atom transfer.

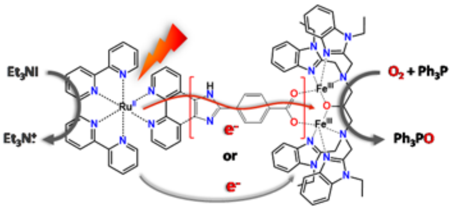
1-2. *Insertion of metalloenzymes into "Metal Organic Frameworks" (MOF)* (in collaboration with Inst. Lavoisier Versailles, PhD thesis E. Gkaniatsou, **LabEx CHARM3AT**)



Microperoxidase (MP8), a very useful and exceptionally active micro-enzyme that performs two distinct catalytic functions (peroxidase and monoxygenase) was immobilized into a highly porous and robust MOF, MIL-101(Cr) (*Mater. Horiz.* **2017**). The data show that, after immobilization, MP8 shows an enhanced catalytic activity in the selective oxidation of dyes by H_2O_2.

1-3. *Iron complexes as biomimetic systems for non-heme iron enzymes* (PhD thesis A. Tréhoux)

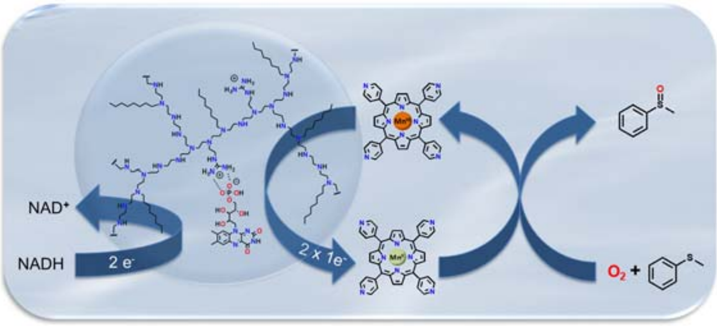
Two kinds of such complexes were synthetized: First, diiron complexes (Coord. Chem. Rev. **2016**), inspired by methane monooxygenase, were synthesized with a particular emphasis on studying the influence of the second coordination sphere during oxidation catalysis. Such complexes were found to be able to catalyze the oxidation of various substrates by H_2O_2 (*J. Mol. Catal. A* **2015**). Second, [Fe(BPMEN)ACC]SbF_6 was synthetized and characterized as a structural and functional mimic of ACC-oxidase, an iron enzyme responsible for the oxidation of 1-aminocyclopropane carboxylic acid (ACC) into ethylene involved as growth hormone in plants (Coll. with J. Simaan, ISM2 Marseille) (*Dalton Trans.* **2015**).



⇨ **A second generation of systems that were able to use O_2 as an oxidant were developped:**

Dinuclear Fe(III) complexes coupled with a photoactivable ruthenium complex catalyzed the photoassisted activation of O_2 to generate of a peroxo species and the oxygen-atom transfer to phosphine derivatives (*Angew. Chem. Int. Ed.* **2013**). Time-resolved X-ray absorption spectroscopy studies confirmed the involvement of such peroxo intermediates in the mechanism of these reactions (*Chem. Commun.* **2017**).

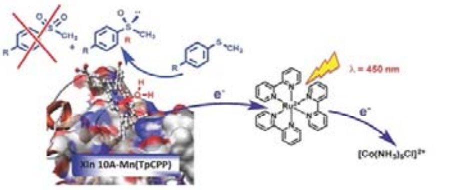
1-4. Bio-inspired oxidation catalysts for environmentally friendly chemistry (**ANR BIOXICAT, LabEx CHARM$_3$AT**, PhD thesis Y. Roux)



An artificial flavoreductase was prepared by incorporation of a flavin mononucleotide (FMN) in a water-soluble polyethyleneimine polymer, bearing a locally hydrophobic microenvironment. This supra-molecular entity allowed the efficient reduction of FMN by NADH and was able to catalyze a very fast single-electron reduction of Mn(III)-porphyrin (*Nature Commun.* **2015**) and of a Tris(picolyl)amine Cu(II) Complex (*Dalton Trans.* **2016**) by splitting the electron pair issued from NADH. This was fully reminiscent of the activity of natural reductases such as the P450 reductases with kinetic parameters, which were 3 orders of magnitude faster compared with other artificial systems. The reduced manganese porphyrin activated O_2 and catalyzed the oxidation of organic substrates in water. Replacing manganese porphyrins by polyoxometallates (POM) also gave interesting results.

⇨ **A third generation of systems that catalyzed the photoassisted oxidation of H_2O was developed:**

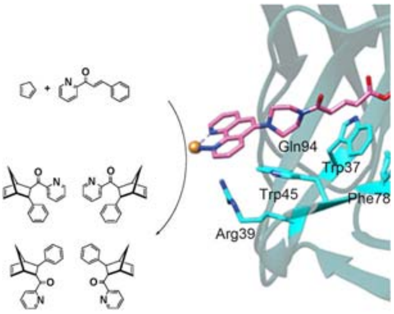
1-5. Photo-catalytic oxidations by artificial Ru-metalloenzymes



Association of a $[Ru(bpy)_3]^{2+}$ chromophore with artificial metalloenzymes such as BSA-Mn(III)-corrole (*Dalton Trans.* **2016**) and Xylanase A-Mn(III)-porphyrin (*Catalyst* **2016**) allowed the visible-light water activation, leading to Mn-oxo species that performed the photoassisted stereoselective oxidation of sulfides.

2- Catalysis of selective reactions of synthetic interest by artificial metalloenzymes (Artzymes) (Coll. A. Urvoas, I2BC, J-D. Maréchal, Barcelone).

The main objective **was there to** develop new biomimetic systems and artificial metalloenzymes to catalyze enantioselective reactions of interest for synthetic organic chemistry such as, for example, catalytic C–H amination (*Angew. Chem. Int. Ed.* **2014**), ester hydrolysis, reductions or C-C bond creation.



Following the Trojan horse strategy, associating a Neocarzinostatin variant (NCS 3-24) with testosterone-Zn(II)-dipyridylamine and –Cu(II)-phenanthroline conjugates, afforded new artificial metalloenzymes that catalyzed resp. the hydrolysis of phosphodiesters (RNase like activity, *Bioorg. Med. Chem.* **2014**), and the stereo-selective Diels-Alder cyclization of cyclopentadiene with azachalcone (*ChemBioChem* **2016**). The later reaction could also be catalyzed by artificial metalloenzymes that were obtained by covalent attachment of a Cu(II)-phenanthroline complex into mutants of alpha-repeat protein, □-rep A3, that constitute a new versatile artificial scaffold for metalloenzyme design (*Chem. Eur. J.* **2017**).

Finally**, the same reaction was also catalyzed "in cellulo"** by artificial metalloenzymes based on the A2A adenosine receptor embedded in the cytoplasmic membranes of living human cells (**ANR REBAR**). The metalloenzymes were assembled at the surface of the cells by inserting into the receptor binding site conjugates of strong antagonists that were covalently bound to copper(II) catalysts.

Theme 3 - Results

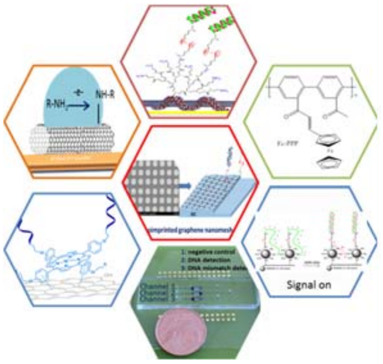
DESIGN OF ELECTROCHEMICAL BIOSENSORS AND BIOCHIPS FOR DIAGNOSIS AND ANALYSIS

Hélène Dorizon (MCF), Hafsa Korri-Youssoufi (DR)

The approach developed in Theme 3 consists on designing biosensors generating an electrochemical signal sensitive to biological reactions. We are interested in conducting materials which can act as platform to assembly different groups and then could be enough sensitive to various chemical or biological reactions that performed on their surface. The objective is to obtain direct electrochemical response without any amplification step. This could be obtained by measuring the electron transfer ability of redox marker attached to the surface or by measuring electrical properties of the membrane layer through the electrochemical impedance spectroscopy. The activities of the team since 2013 have been focused on four objectives:

1. **Engineering of conducting materials and nanomaterials** as transducers and the study of new approaches to amplify the transducer signal response through the modulation of electronic and ionic transfer.
2. **Study of functionalization and association modes** of molecules and/or biomolecules to these materials.
3. **Design of various biosensors** which investigated various biological recognition reactions through guest/host interaction.
4. **Integration of biosensors into microfluidic system** and multiplexing systems.

These activities have been investigated during the PhD program of **7 students** and have been supported by collaboration with various institutes with complementary skills to the team (biology, physician, nanotechnology…). The activities of the team have lead to the production of **24 publications** and **1 international patent**.



General activities of Theme 3.

Thus, the engineering of materials as transducers to generate sensitive platform system has been one of the main objective and various organic materials have been studied, including organic conducting polymers (polypyrrole, poly(para-phenylene) and derivatives), carbon nanomaterials consisting of carbon nanotubes and graphene sheets as well as organic macromolecules such as dendrimers and porphyrins. The functionalization has been investigated, in the objectives of obtaining high density of biomolecules on the surface and maintaining the electronic properties of these transducers. Biosensors have been developed within various molecular biological reactions. Thus, the effects of various reactions on the electrochemical biosensors properties have been studied, such as, immuno-reactions, effects of the structuration of the aptamers after various interactions (aptamer/protein and aptamer/small organic molecules), the effects of carbohydrate/ protein interactions and the DNA hybridization in complex sample such as PCR sample or reel sample and the ability of identification of single polymorphism mutation in the case of drug resistance. The team has also studied the integration of these biosensors into microfluidic systems in order to improve the kinetics of host-guest interaction and to decrease the detection limit. These systems have been used for the development of different types of biosensors as analytical tools that have an interest in food safety (mycotoxins) and health care (tuberculosis, prion protein, influenza virus, cancer diagnosis). The results obtained could be resuming in fundamental aspect firstly by analyzing the various parameters in the design of conducting transducers and their modifications that influenced the electron transfer ability and the sensitivity of the biosensors, secondly the effect of biological system and the host/guest interactions in the biosensors response and finally the influence of introduction of such system into microfluidic systems. Finaly these new concepts of detection lead to patent and technology transfer through spin off creation. Our many activities allowed us to demonstrate that:

- The high density of immobilized biomolecules on the surface has a large effect on the sensitivity of biosensors. This has been demonstrated by the functionalization of polypyrrole and carbon nanotubes with dendrimers PAMAM which allowed the immobilization on the surface of a large number of amino groups, and then biomolecules, that influenced biosensors performances.
- The soft approach of functionalization of various conducting materials through electrochemically oxidation of amines allows the incorporation of functional groups without any modifications of electron transfer ability.
- The modification of carbon nanomaterials, such as graphene, could be obtained through strong interactions with aromatic macrocycles such as porphyrins or oligomers based on poly(p-phenylene). These hybrid materials brought some interesting properties in term of electron transfer ability and sensitivity.
- The nano-structuration of graphene improves performances of DNA sensing leading to detection of sub-attomolar level. This was explained by high surface of immobilization obtained through artificial edge where the attachment process as well as the electron transfer sensitivity are enhanced.
- Direct detection without amplification of genomic DNA is possible for the multi-target diagnosis of biomarkers in real samples. This was demonstrated with a fluidic chip integrating three fluidic channels equipped with electrochemical bioreceptors based on carbon nanotubes and incorporating a redox marker.
- Structured materials and their chemical properties such as the presence of charges on the surface could have a large effect in the biological reaction (*ie*. hybridization reaction) or aptamer association. This was demonstrated in the case of positively charged nanomaterials modified with DNA probes. The negatively charge DNA interact with the positively surface and lie on it and then block electron transfer ability. When recognition reaction is achieved with the target such as complementary DNA, the biological complex leads to less interactions with the surface and then the electron transfer ability of attached redox marker increases. This approach leads to a signal on of redox response after detection process. Patent has been deposit and maturation project within SATT Paris-Saclay for technology transfer to spin off is under process.

Highlights

- **23 research contracts** were obtained for the considered period (6 ANR, 3 international grants, 1 SATT maturation grant, grants from 2 LabEx, IRS and foundations…), highlighting *team dynamism and research adequation to actual scientific issues of societal interest* (cancer research, antibiotic resistance, ecodesign of drugs, design of artzymes, eco-friendly catalysis, detection of pathogenic biomarkers and pollutants, design of new generations of biosensors and microfluidic devices…).
- **Recruitment of 2 permanent members**: 1 as assistant professor (R. Labruère, 2013) in bioorganic chemistry (self-immolating based prodrugs) and 1 as CNRS researcher (W. Ghattas, 2016) in bioinorganic chemistry (multicatalysis in cascade, artzymes), *highlighting novelty and originality of the scientific research themes of ECBB*. Meanwhile, 1 prof (M. Thérisod, 2015) and 1 CNRS research engineer (F. Ramiandrasoa, 2018) retired, and 1 CNRS research director (C. Blonski, 2016) left the team for health reasons.
- **International Patent and technology transfer through 570 k€ grant support from SATT Paris-Saclay for maturation project PATTOX** ("Analytical devices for the detection of pathogens and toxins", H. Korri-Youssoufi, N. Mejri-Omrani, S. Chebil, 2017-2018), which highlights strong dynamism of ECBB Theme 3 group towards *industrial valorization of academic research discoveries*.
- **31 non-permanent researchers** (18 PhD + 11 post-docs + 2 SATT engineers) strongly contributed to the development of team's research subjects. PhD defences led to 41 publications (average IF = 4.95), highlighting good management of PhD students and quality of their scientific researches.
- **Average IF = 5.377** for ECBB publications, showing high quality of team researches.
- **Participation of ECBB team in 2 LabEx**: CHARM3AT (*Chemistry of Multifunctional Molecular Architectures and Materials*), **with J.-P. Mahy (ECBB) as director** and LERMIT (*LabEx in Research on Medication and Innovative Therapeutics*), and in *BioMedical Engineering* (BME) **IRS** project, showing strong involvement of ECBB at interfaces between chemistry, physico-chemistry and biology.

2 Organisation and life of the team

Management, organisation and scientific animation

The scientific objectives of ECBB team for the considered period (Table 2) were grouped under 3 main themes and developped by 12 permanents (9 permanents on June 2018) and 32 PhD and postdoctoral researchers. ECBB team was managed by Dr. Casimir Blonski (Jan 1st. 2013-Jun 30th.2015), followed by Prof. Laurent Salmon since Jul 1st. 2015. For health reasons, Dr. Blonski left the team on May 19th. 2016. Dr. Hafsa Korri-Youssoufi assists the team manager when he is not available.

Table 2. ECBB organizational chart (black: present; grey: past): [1]recruited Sept 1st. 2013, [2]retired April 1st. 2015, [3]left May 19th. 2016, [4]Retired July 1st. 2018, [5]Recruited Oct 1st. 2016, [6]team security manager.

	L. Salmon: team manager - S. Latimier (50%): team assistance					
	Theme 1 **Synthesis and evaluation of enzyme inhibitors for therapeutic purposes**		**Theme 2** **Design and synthesis of new metal complexes & study of their interactions with biomolecules**		**Theme 3** **Design of electrochemical biosensors and biochips for diagnosis and analysis**	
Permanent	L. Salmon	Prof. UPSud	J.-P. Mahy	Prof. UPSud	H. Korri-Youssoufi	DR CNRS
	R. Labruère [1]	MCF UPSud	F. Avenier	MCF UPSud	H. Dorizon [6]	MCF UPSud
	S. Pethe	MCF UPSud	R. Ricoux	IR CNRS		
	M. Thérisod [2]	Prof. UPSud	W. Ghattas [5]	CR CNRS		
	C. Blonski [3]	DR CNRS				
	F. Ramiandrasoa [4]	IR CNRS				
Non-permanent	S. Courtiol-Legourd	PhD	A. Trehoux	PhD	A. Miodek	PhD
	M. Devillers (50%)	PhD	Y. Roux	PhD	B. Zribi	PhD
	E. Jagu	PhD	T. Di Méo	PhD	M. Devillers (50%)	PhD
	L. Ahmad	PhD	Y. Chevalier	PhD	N. Mejri-Omrani	PhD
	T.-H. Au	PhD	K. Kariyawasam	PhD	S. Bizid	PhD
	M. Gayral	Postdoctoral	F. Gkaniatsou	PhD	Y. Wang	PhD
	A. Diez Martinez	Postdoctoral	W. Ghattas	Postdoctoral	R. Khoder	PhD
	S. Serra	Postdoctoral	F. Hammerer	Postdoctoral	M. Hamami	PhD
	E. Rascol	Postdoctoral	K. Cheaib	Postdoctoral	N. Mejri-Omrani	IT-CDD
	M. Abellan Flos	Postdoctoral	V. DuboscIard	Postdoctoral	S. Chebil	IT-CDD
	C. Skarbek	Postdoctoral	A. Naim	Postdoctoral		

Funds managing and administrative tasks are managed by the team manager and Stéphanie Latimier (ATRF P2, 50%) based on monthly lab councils. Scientific animation is managed by the team manager, as well as by the Themes managers: Prof. L. Salmon, Prof. J.-P. Mahy, and Dr. H. Korri-Youssoufi for themes 1,2, and 3, respectively. Scientific animation is based on weekly lab seminars organized by Dr. Raphaël Labruère, then by Dr. Wadih Ghattas. Health and security issues are managed by Dr. Hélène Dorizon for the team.

3 SWOT analysis

Strengths

- Strong involvement of research axes towards *societal issues* including environment, energy, and health, as well as towards *fundamental issues* like understanding mechanims of action of biomolecules and their interactions with natural or synthetic entites.
- Numerous *research contracts* including 2 LabEx and 1 maturation project grant highlight team strength.
- Large spectrum of *skills*, including synthetic chemistry, physico-chemistry, electrochemistry, surface sciences and biology, allows the team to address successfully, at the molecular level, complex issues at the chemistry-biology interface.

Weaknesses

- Team organization into three rather different research domains might be considered as a weakness, with only 2 to 4 permanent members attached to each theme. However, not only many PhD and post-doctoral students reinforce each of these themes making them viable independently, but inter-theme research subjects also allow the team to increase sharing of competences.
- A relatively low number of peer-reviewed and WoS indexed publications (55) however compensated by a good average IF of 5.377.
- Only 2 patents and no industrial collaboration: the team should increase interaction with industrial partners in the near future.

Opportunities

- Involvement in the future Paris-Saclay Institute of Therapeutic Innovation rassembling seveal research teams from both Paris-Saclay Chemistry and Life Sciences departments.
- Close location in BPC to other ICMMO teams interested by chemical-biology interface.
- Participation to an increasingly number of public and private calls in domains including environment, materials and drug discovery.

Threats

- Coherence of the ECBB team might be challenged by:
  - team organization in 3 themes,
  - involvement in 2 LabEx,
  - teams coming from the faculty of pharmacy in the future BPC structure.

4 Scientific strategy and projects

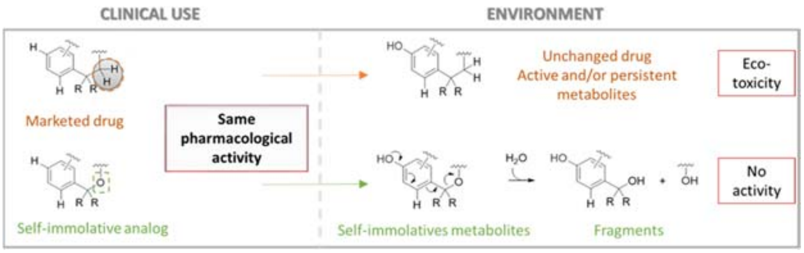
The future organization of ECBB team will likely remain unchanged. However, inter-theme researches will be further encouraged, as well as partnerships within ICMMO itself and with teams in the perimeter of University Paris-Saclay. Resources for achieving the scientific objectives will include international and national public grants, as well as local, PIA, and foundation grants.

Theme 1 - Projects

SYNTHESIS AND EVALUATION OF ENZYME INHIBITORS FOR THERAPEUTIC PURPOSES

Raphaël Labruère (MCF), Stéphanie Pethe (MCF), Laurent Salmon (Prof)

1. Eco-design of drugs incorporating a self-immolative structure

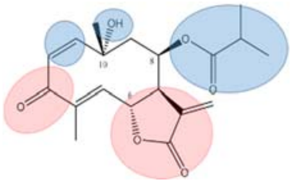


Self-immolative prodrug strategy.

Active pharmaceutical ingredients (APIs) and their metabolites (mAPIs) are commonly found in the environment since wastewater treatment plants are not generally prepared to deal with all of them. The toxic effects of APIs/mAPIs on organisms caused by their intrinsic properties, wide variety, presence as a mixture, and chronic exposure urges the scientific community to consider the entire life cycle of drugs and their environmental impact. Our project is based on the structural modification of already marketed drugs for programming them towards self-immolation after having fulfilled their therapeutic purpose. Indeed, once excreted, our rationally designed eco-drugs will undergo particular modifications in the biomass by predictable metabolism, which will trigger their self-disassembly, consequently losing their original activity and toxicity.

2. Derivatives of Gambogic acid and Tagitinin C as new anticancer agents

Following the synthesis of Gambogic acid derivatives, pharmacomodulation of Tagitinin C, isolated from *Tithonia diversifolia* leaves, will be undergo. Tagitinine is a sesquiterpene lactone known to possess anti-inflammatory, anti-proliferative and anti-cancer activities. Different modification strategies are imagined by Michael reaction, Heck reaction and 3 + 2 cycloaddition from the natural molecule extracted and purified in Vietnam. Biological assays will initially be carried out in ECBB on various cancer cell lines and then in Vietnam and Korea to elucidate the mechanism(s) of action of Tagitinin C, Gambogic acid and their newly synthesized derivatives.



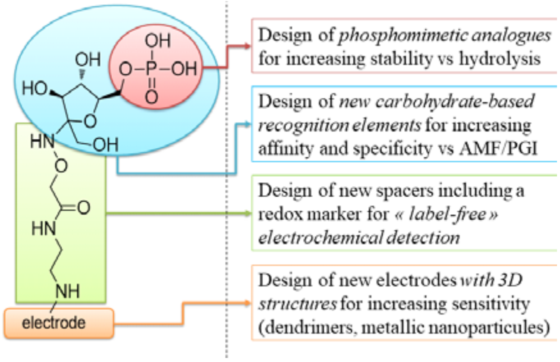
Structure of Tagitinin C

3. Design of species-specific inhibitors of PMI from *C. albicans* as new antifungal agents

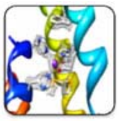
Using polarizable molecular modelling (collab. Dr. N. Gresh, UPMC, Paris) and protein crystallography (Prof. H. van Tilbeurgh, I2BC, Univ. Paris-Sud), new species-specific inhibitors of PMI from *C. albicans*, not inhibiting human PMI and PGI, will be designed, synthesized and evaluated as therapeutic agents for the treatment of fungal infections in immunodeficient patients.

4. Carbohydrate-based electrochemical biosensors for quantification of autocrine motility factor in human fluids (collab. Theme 3, Dr. H. Korri-Youssoufi)

The intracellular glycolytic enzyme phosphoglucose isomerase (PGI) is also known as an extracellular tumor-secreted cytokine named autocrine motility factor (AMF) which stimulates active migration of tumor cells. Elevated levels of AMF are found in the serum and/or urine of patients in several types of cancer and thus can be used as a biomarker of cancer progression. Known analytical methods for the determination of AMF concentration in human fluids are difficult to adapt for rapid and systematic analyses. The project aims to design new electrochemical biosensors that would allow early detection of an on-going metastatic process in cancer patients through the quantification of AMF as biomarker in human fluids. The project includes: i) the design of new phosphomimetic-carbohydrate-based bioreceptors, ii) the integration of the redox marker into the biosensors for "label-free" electrochemical detection, iii) the integration of biosensors in 3D structures, iv) the evaluation of biosensors on real human fluids (plasma and urine) from healthy patients and from patients with different types of cancer (collab. Prof. F. André, IGF, Villejuif).



Design of electrochemical biosensors for AMF diagnosis in human fluids.



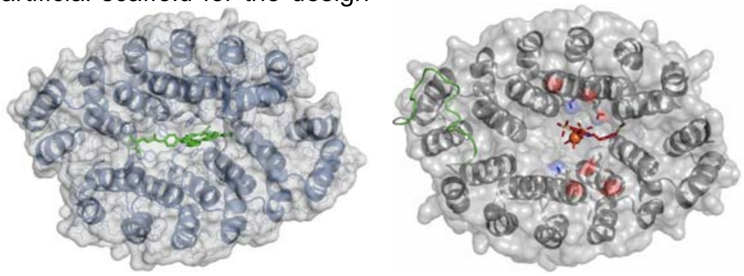
Theme 2 - Projects

DESIGN AND SYNTHESIS OF NEW METAL COMPLEXES AND STUDY OF THEIR INTERACTIONS WITH BIOMOLECULES

Frédéric Avenier (MCF), Rémy Ricoux (IR), Wadih Ghattas (CR), Jean-Pierre Mahy (Prof)

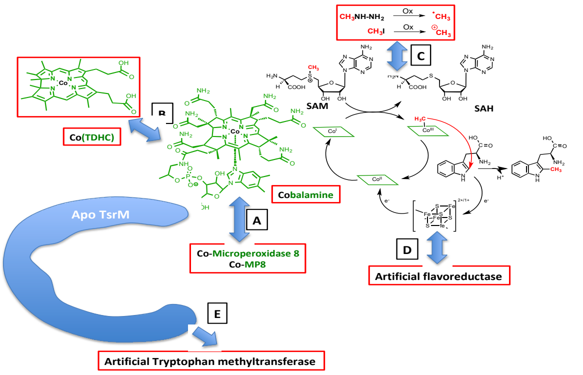
1. Catalysis of selective reactions by artificial metalloenzymes (Artzymes) (Coll. A. Urvoas, I2BC, J-L Renaud, COBRA Caen, J-D. Maréchal, Barcelone, N. Doucet, Laval, Canada).

We will keep on taking profit of Xylanases, and of alpha-repeat protein (α-Rep A3) mutants as new versatile artificial scaffold for the design of artificial metalloenzymes by covalent attachment of: (i) Fe-, Mn- and Ru-porphyrins, for selective oxidation and cyclopropanation reactions, (ii) Knölker complex for the selective reduction of ketones (by ATH) and (iii) copper-dpa complexes for enantioselective photoredox C-C bond forming reactions (PhD thesis K. Kariyawasam, **projet ANR 2018 AMPHOR**).

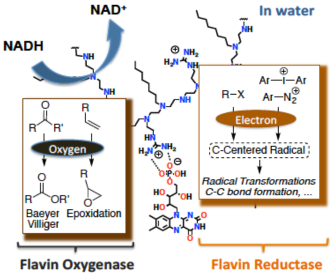


2. Creation of C-C bonds by artificial radical SAM enzymes and biomimetic systems (ANR Carb2zyme) (Coll. O. Bertault, Micalis, INRA Jouy en Josas).

Biomimetic systems for B12 radical SAM enzymes will be developed with two objectives; first, to help elucidating the mechanism of the methyl transfer reaction catalyzed by B12 radical SAM enzymes and, second, to develop MP8 based biomimetic systems and new artificial metalloenzymes that would be able to catalyze the selective methylation of organic compounds such as tryptophane, just like B12 radical SAM enzymes do, using methylhydrazine or methyl iodide as methyl radical donating agents.



3. Bio-inspired oxidation catalysis for a more environmentally friendly chemistry (PhD thesis Y. Chevalier, ANR ARTENOSYN, LabEx CHARM3AT, Coll. J.-P. Goddard, Mulhouse).



The ability of the artificial reductase, previously prepared by incorporation of flavin cofactors (FMN) into a modified water soluble polyethyleneimine polymer, to collect and split electron pairs from NADH to deliver, under anaerobic conditions, single electrons to organic molecules into a locally hydrophobic micro-environment will be used to initiate radical reaction by single electron transfer (SET). With J.-P. Goddard as an expert, a large scope of radical reactions will be evaluated. Alternatively, under aerobic conditions, the reduced flavin ($FMNH_2$) will react with dioxygen to form organo-peroxo intermediates, which is known to perform oxidation reactions such as Beyer-Villiger, epoxydation or sulfoxidation reactions.

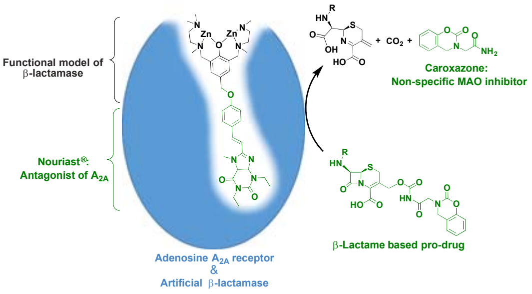
4. Insertion of metalloenzymes into "Metal Organic Frameworks" (MOF) (In collaboration with C. Sicard & N. Steunou, Inst. Lavoisier Versailles and J. Ouazzani, ICSN Gif/Yvette)

The encagement of enzymes into Metal Organic Frameworks MOF will be extended to other enzymes of interest such as nitro-reductase and to bienzymatic systems associating, for example, a reductase, that will regenerate NADH necessary to provide electrons to activate O_2 that will then be used by a second enzyme, microperoxidase 8, to catalyze selective oxidation reactions.

5. Reactions for therapy and diagnosis

4-1. Theranostics oriented by receptor-based Artzymes (Projet ANR 2018 THOR).

The design of artificial enzymes anchored at the surface of living cells will be adapted to the development artificial metalloenzymes for theranostics that can be used to catalyze in vivo the activation of pro-drugs (therapy) and / or pro-sensors (imaging, diagnosis). The A_{2A} receptor will be transformed *"in vivo"* into an artificial metallo-β-lactamase *via* the covalent attachment of one of its antagonists (**Drug 1**) to a dinuclear zinc(**II**) complex known to be able to catalyze the hydrolysis of β-lactams, which will cause the release of either a **drug 2** or a fluorescent probe.

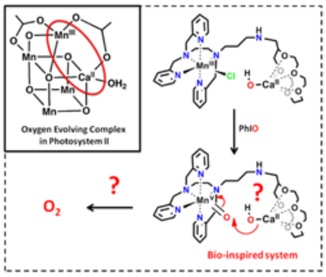


4-2. Development of multifunctional peptide probes for medical imaging and radiotherapy for the treatment of breast cancer (Coll. S. Bourgault, D. Chatenet, projet France-Canada research Fund 2018)

This project aims to develop neuropeptide Y (NPY) Y1 receptor-specific theranostic agents that can be used as diagnostic and / or therapeutic tools for malignant breast tumors. For this, new tools will be developed, that combine the advantages of (metallo)porphyrins (MRI, fluorescence detection, phototherapy) that will be conjugated with peptide antagonists of the NPY1(selectivity, solubility, imaging, radiotherapy) to facilitate the detection, surgery and / or eradication of tumors by photo. /radiotherapy.

6. Photosystem II mimics : studying the O-O bond making mechanism

Mimicking the activity of the oxygen evolving complex (OEC) for water oxidation is of prime importance for the future production of decarbonated energies (H_2 fuel). In this context, we are synthesizing hetero-binuclar Mn/Ca (or Fe/Ca) complexes in order to study/evaluate the role of the calcium ion in the O-O bond making mechanism. These research should contribute to the development of future bio-inspired catalysts capable of replacing noble metals for such processes.

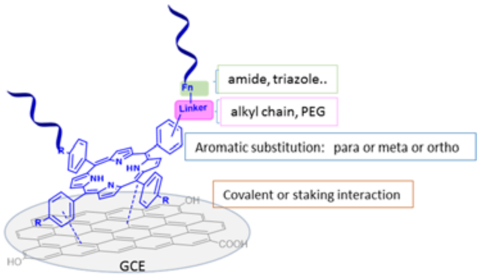


Theme 3 - Projects

DESIGN OF ELECTROCHEMICAL BIOSENSORS AND BIOCHIPS FOR DIAGNOSIS AND ANALYSIS

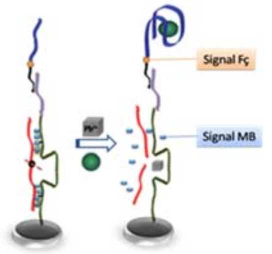
Hélène Dorizon (MCF), Hafsa Korri-Youssoufi (DR)

The main objectives of the current research project is the design of nanomaterials and nanostructured materials and the study of their structural and electrical properties for understanding their properties. This will allow a rational design of the transducers. Two kind nanomaterials will be studied:

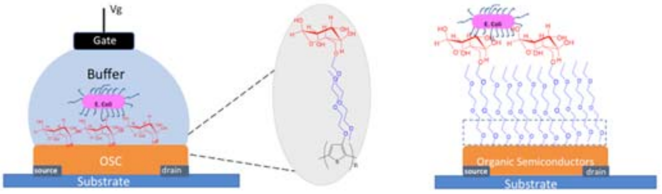


- Hybrid nanomaterials based on metalloporphyrins conjugated to graphene nanosheet developed previously as transducers for DNA biosensors will be studied. Such nanomaterials have demonstrated an improvement of electron transfer ability and high sensitivity to DNA hybridization (PhD Y. Wang 2017). We want to study electronic and structural properties of this hybrid materials based on graphene and tetra-phenylporphyrins derivatives functionalized in meso position with various functional groups such as carboxylic amines. We would like to underline the mechanism of such association and their effect on the structural properties of such complex as well as electronic properties of graphene. The electronic properties of such hybrid could affect the properties of graphene such as the gap. Improvement of electrical properties of graphene may depend on functional group and its position on aromatic ring. To address these issues, we want to perform, at the TEMPO beamline, absorption (XAS), and photoemission (XPS and ARPES) experiments in synchrotron Soleil. The results obtained will help in the design and synthesis of new organic macromolecules to improve graphene properties and their applications in various biotechnological area such as biosensors devices.
- Nanomaterials based on polypyrrole with various dimensional structures such as nanowires and nano-spheres have been developed through electrodeposition process with free template. These nanomaterials showed a very high detection performance for DNA biosensors in term of sensitivity which reach attomolar range (PhD R. Khoder 2018). Structural and electrical properties of such nanostructures will be studied and compared to others process of fabrication of nanostructured polypyrrole such as nano-impression.

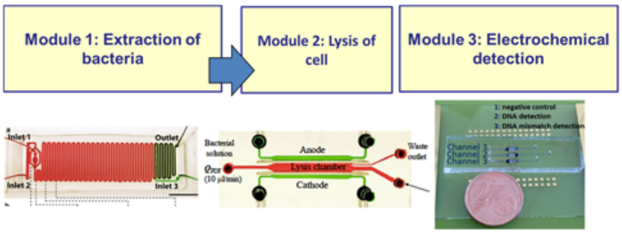
New concepts and approaches for design of direct detection systems based on electrical measurement will be studied. Two aspects will be explored: the bio-receptor design and detection approach.



- The first concerns biological design of immobilized bioreceptors and their ability for detection of multi-target analysis. This will be explored by multimodal biosensors designed for targeting different molecules of interest present in the same sample. This will be demonstrated by using bioreceptors based on oligonucleotide where various properties could be obtained. Aptamer could be associated to biosensors for targeting small molecule and DNAzyme could be immobilized for targeting metal ions present in the same sample. This project will be applied for detection of pollutant in waste water (PhD M. Hamami, 2018).
- Novel bio-electronic devices for bacteria detection will be based on hetero-structure formed with bi-layer stacks of Organic SemiConductors (OSCs) materials as transducers, and PEG-carbohydrate as sensing layer which specifically interacts with pathogenic bacteria. The goal is to present a proof-of-concept of label-free detection of bacteria using Electrolyte-Gated Organic Field-Effect Transistors (EGOFETs). The aim is to develop improved materials for EGOFET, which can operate in aqueous solution with high stability and selectivity. These new OSC materials are expected to facilitate ions and electrons transport and improve antifouling adhesion with non-specific target and facilitate association with bioreceptor through simple chemical process based on amphiphilic interaction using orthogonal solvants for deposition.



- Integration of biosensors and all the chemical process before detection in microfluidic platform for direct analysis of sample will be developed for genomic detection of bacteria and resistance to antibiotic. The microfluidic platform will integrate 3 modules allowing: 1/ extraction of pathogens directly from the whole blood sample, 2/ lysis of these pathogens, and 3/ direct detection without PCR amplification.



Self-assessment document

Team 5 – SM2B

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Synthèse de Molécules et Macromolécules Bioactives**
Acronym:	**SM2B**
Director's name (current contract):	**Philippe ROGER**
Director's name (future contract):	**Philippe ROGER**

SELF-ASSESSMENT DOCUMENT

1 Research products and activities

Scientific output

The SM$_2$B (Synthèse de Molécules et de Macromolécules Bioactives) team was created on January 1, 2014. It is the result of the recomposition of the G2M (Glycochimie Moléculaire et Macromoléculaire) team, which as of 1 January 2013, consisted of 15 permanent members (8 lecturer-researchers, 3 CNRS researchers and 4 ITA / BIATTS) divided into 4 thematic areas. The team SM$_2$B was formed on the basis of 3 of the 4 G2M themes : "Synthèse de biomolécules, stratégies et applications", "Glycomimes, reconnaissance et systèmes photoactifs" et "Polymères et surfaces". The 9 permanent members of these 3 themes included 5 lecturers-researchers, 2 CNRS researchers and 2 BIATTS. During the five-year period 2013-2018, three departures occurred: the retirements of A. Malleron (IE) and JM Beau (PRU) who have an ongoing activity in the team as emeritus researcher and the mutation for Caen University of B. Lepoittevin. Our efforts, our attractiveness and the joint support of the ICMMO and of our guardianship UPSud allowed us to recruit one new PRU and two MCU, what increased the size of the team (10 permanents). All this information is summarized in Table 1 below. Since 2013, the team has welcomed 22 students including 15 M2 students; 6 PhD students, 1 Post-doctoral fellows and 18 trainees at the L2 to M1 educational level. To make our priority objectives more readable and to structure the human resources affected, at the beginning of the five-year period we reduced the number of our themes to two: **"Synthesis of biomolecules"** and **"Polymers and surfaces"** located in two different buildings (420 and 430).

Table 1 : Composition of the SM$_2$B team with the current members (in black) and the members who retired or left for a mutation (in red) during the period.

Name	First Name	Status	Employer	HDR	Comment
« Synthèse de Biomolécules » theme					
BEAU	Jean-Marie	PUEM	UPSUD	X	*emeritus since September 1, 2017*
BOURDREUX	Yann	MCU	UPSUD		
DOISNEAU	Gilles	MCU	UPSUD	X	
GUIANVARC'H	Dominique	PU	UPSUD	X	*arrived on September 1, 2017*
URBAN	Dominique	CR	CNRS	X	
VAUZEILLES	Boris	DR	CNRS	X	
« Polymères et Surfaces » theme					
AUBRY-BARROCA	Nadine	MCU	UPSUD		*arrived on July 1, 2014*
AYMES-CHODUR	Caroline	MCU	UPSUD	X	*arrived on November 1, 2016*
LEPOITTEVIN	Bénédicte	MCU	UPSUD	X	*left on September 1, 2015*
ROGER	Philippe	PU	UPSUD	X	
SALMI-MANI	Hanène	MCU	UPSUD		*arrived on September 1, 2015*
Technical support					
COSTA	Ludovic	ADT	UPSUD		
MALLERON	Annie	IE	UPSUD		*retired on December 31, 2013*

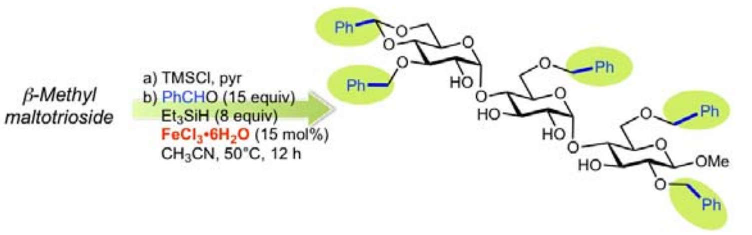
The research activity for the period (2013-2018) has mainly concerned the study of novel synthetic methods in molecular and macromolecular chemistry and polymer surface functionalization. These methods have been exploited in the construction of chemical tools useful in fundamental and applied glycobiology for human health (bacterial and viral infections, metabolic labeling) and plant health (plant growth stimulants for a sustainable agriculture). Research projects were based on the use of renewable resources from the biomass as starting materials in the preparation of bioactive compounds of high added value.

This activity results in **47 articles** in peer-reviewed journals, with an **average impact factor of 4.7**, corresponding to 1.62 articles / full-time equivalent researcher, **8 patents**, **84 oral communications** (invited or selected) in scientific meetings and **53 posters**.

The **"Synthesis of biomolecules"** theme is involved, through synthetic organic chemistry, in a better understanding at the molecular level of the function of complex biological systems. Part of our research focuses on molecular events controlled by carbohydrates and glycoconjugates. Our objective is to develop simple or complex molecular tools (natural structures, mimic constructs, etc.) that can be used in diverse applications. The chemistry of carbohydrates is a dominant feature of our activities with an emphasis on reducing drastically the number of synthetic steps from abundant natural products. Our expertise falls into the following themes.

Atom-economical transformations and glycoprobes

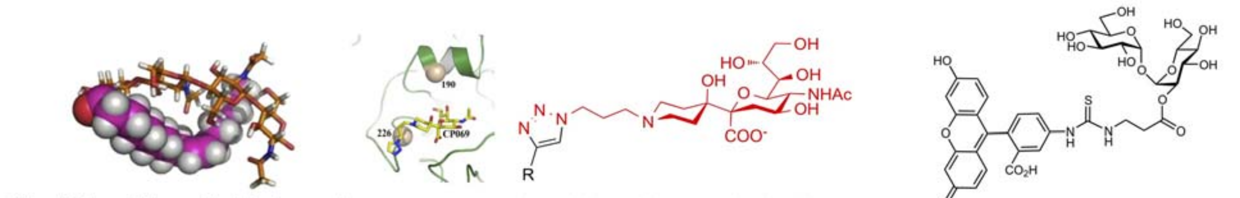
- The discovery of **atom-economical, catalytic one-pot multi-step processes** for the chemo- and regioselective transformations of carbohydrates and polyols ("one catalyst in a single reaction vessel"). These transformations, avoiding time-consuming protection/deprotection steps and the isolation of intermediates, are catalyzed by copper(II) triflate or the environmentally friendly and inexpensive iron(III) chloride hexahydrate. This last catalyst was very efficient on disaccharides and one trisaccharide (*Eur. J. Org. Chem*. **2017**, 3355). Catalysis by triflic acid associated with powdered molecular sieves is a better option with the important the NHCO-containing functionalities on carbohydrates (e.g. derivatives of D-glucosamine) (*Chem. Comm*. **2014**, *50*, 1067). In addition, we demonstrated that chitin, source of the α-pentaacetate of *N*-acetyl glucosamine (GlcNAc) in one step, is the "bio-precursor" of simple GlcNAc α-glycosides by direct activation with catalytic amounts of copper(II) triflate in a heated sealed-vessel reactor. This methodological work also includes new developments in radical chemistry, such as the first evidence of a 1,7-hydride shift in a regioselective deprotection reaction on polyfunctional substrates (*Angew. Chem., Int. Ed. Engl.* **2013**, 52, 9572).



- The development of a novel **direct and chemoselective umpolung process** on the carbohydrate glycals without relying on the preparation of intermediary pi-allyl transition metal complexes, with samarium diiodide as a simple reducing system. This proceeds with a high stereochemical outcome in the carbon-carbon bond forming step. It provided a new approach to the α-*C*-glycosides of the *N*-acetyl neuraminic acid (*Angew. Chem. Int. Ed.* **2014**, 53, 6184). This single electron reductive metallation procedure was applied to the discovery of new selective hemagglutinin (HA) ligands and neuraminidase (NA) inhibitors targeting the binding or the catalytic site, respectively. Both glycoproteins are crucial for the viral infection by *Influenza* of type A virus (flu virus).

- The deconstruction of chitin, one of the most abundant renewable biopolymers, and reconstruction from fragments to highly bioactive glycoconjugates and glycoprobes. It has been used in the **total synthesis of the Nodulation and Mycorrhizal Factors** and some mimetic structures for open-field tests (in collaboration with Bayer CropScience). The elaboration of photoactivatable glycolipid probes has also been very useful for the first identification of the long-elusive nodulation factor receptor (*Angew. Chem. Int. Ed.* **2014**, 53, 11912).

- the catalytic one-pot multi-step processes using the iron catalyst was extended to the trehalose disaccharide for the **synthesis of novel highly antigenic sulfoglycolipids** (*J. Org. Chem*. **2013**, 78, 7648). Increasing the length of the chiral 1,3-methyl branch fatty acid of mycobacterial diacylated sulfoglycolipid analogues induces a dramatic improvement in their antigenic properties, giving products more potent than the natural antigens. These constructs should make excellent candidates as components of sub-unit vaccines. This project also involves the preparation of imaging probes based on trehalose and mycolic acids for the study of the mycomembrane biogenesis in mycobacterium and related organisms.



Glycolipids which are Nodulation and Mychorrizal symbiotic factors

A monovalent alpha-sialyl mimic that binds to the H3 HA site (good model of the H1 HA)

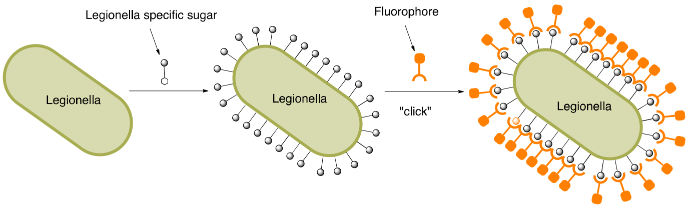
A new FITC-trehalose probe (unpublished)

Illustrations of glycoprobe constructs relying on the above atom-economical methods

Metabolic Glycan labeling

Our group pioneered the use of specific carbohydrate analogues for the **quick detection of living bacteria**, using metabolic glycan labeling. The use of a carbohydrate modified by a chemical reporter group deceives bacterial metabolism, leading to the incorporation of this carbohydrate into surface glycans. The reporter (e.g. azido) group can then be detected by conjugation with a fluorophore, therefore labeling the bacterial surface. For example, the detection and numeration of Gram-negative bacteria can be performed via the assimilation of a 3-deoxy-d-manno-octulosonic acid (Kdo) derivative (Kdo-N_3), since Kdo is an essential component of lipopolysaccharides (LPS), glycolipids which are present only at the surface of Gram-negative bacteria. This approach allows for rapid detection of the presence of living Gram-negative bacteria, and finds applications in different domains including microbiological quality control. Beyond labeling and imaging, when used in combination with streptavidin-coated magnetic beads, this strategy allows the **concentration of a target**, biotin-labeled **bacterium** from a mixture or complex medium.

Another development of this strategy uses a carbohydrate (Legionaminic acid), which is specifically present at the surface of *Legionella pneumophila*, a bacterium responsible for most cases of legionellosis. Legionellosis is a serious disease presenting a relatively high fatality rate, and leading to epidemic events attracting high media attention. The main prevention strategy is based on regular control of installations, which are susceptible to allow development of the bacterium. The classical detection method relies on bacterial culture and requires more than ten days. The new method should significantly shorten this delay, since different strains of *Legionella pneumophila* have been labeled in the lab in **less than 24 hours**. This was the first time that metabolic glycan labeling could be used for direct species identification (*Angew. Chem. Int. Ed.* **2014**, 53, 1275).



A strategy to specifically label Legionella pneumophila

A company named Click4Tag has been created at the end of 2014 to exploit this work on bacterial labeling.

More recent applications of this strategy resulted in specific labeling of plant cell wall by incorporation of Kdo-N_3 within rhamnogalacturonan II, a Kdo-containing parietal polysaccharide (*Plant J.* **2016**, 85, 437). Further applications to tumor cell labeling are also under study.

The main activity of the **"Polymers and surfaces" theme** consists in preparing new polymers, mainly from biobased products, using original and innovative synthesis methodologies. The anti-adhesive or coordinating properties of those synthesized polymers make it possible to envisage various fields of application ranging from antibacterial textiles to catalysis and purification of radioactive effluents. The originality of our activity is based on the synthesis of new monomers and on the study of their polymerization by using the classical tools of macromolecular engineering such as controlled radical polymerization (mainly ATRP: Radical Polymerization by Atom Transfer) in order to control the molecular weight, the composition and the architecture of polymers synthesized in solution or grafted onto different types of surfaces (fibers, film sheets or polymer sheets). In surface chemistry, we have continued to develop our skills in the initial activation step required of our surfaces either by UV irradiation (*Eur. Polym. J.*, **2018**, *103*, 51), by plasma treatment (*J. Polym. Sci. Pol. Chem.*, **2015**, *53*, 1975) or by chemical treatment such as aminolysis (*J. Polym. Sci. Pol. Chem.*, **2016**, *54*, 2689 and *J. Colloid Interface Sci.*, **2017**, *500*, 69). Thus, new materials functionalized with different types of molecular chains have been prepared according to the desired application.

From our 11 ACLs, half of them concern a public health application with the aim of offering new antibacterial surfaces to effectively fight against pathogenic bacteria, for example in the case of nosocomial infections encountered in the medical / hospital field. This objective was supported from 2010 to 2015 by the ANR with the SANBACT project ("Chimie Durable Industries Innovations" program). Sophie Bedel has benefited of a thesis grant financed by this contract (thesis defended in 2014). She functionalized PET (poly(ethylene terephthalate)) surfaces by introducing amine functions by NH_3 plasma treatment. The graft density optimized for amine function (of the order of 2 functions per nm^2) made it possible to obtain polymer brushes on the surface following the covalent attachment of an ATRP polymerization fragment. Among the many monomers synthesized in the laboratory by Sophie Bedel, tests carried out on several pathogenic strains demonstrated that the most promising monomer was thymyl methacrylate (*J. Polym. Sci. Pol. Chem.,* ***2015****, 53, 1975*). During this project, a new grafting from methodology using an intermediate layer of polydopamine (*Prog. Org. Coat.*, **2015**, *82*, 17) was also carried out on steel, giving the possibility of treatment of steel tools and instruments infected in the agro-food industries or in a hospital setting. As part of a project funded by the Triangle of Physics in 2014-2015 (collaboration with E. Raspaud (Laboratoire de Physique des Solides, UPSud) and C. Regeard (Institut de Génétique Moléculaire, UPSud), we studied the mechanical properties of bacterial biofilms during their detachment from a surface (*J. Phys. Chem. B*, **2016**, *120*, 6080). Thanks to funding from LabEx Charmmmat, we were able to invite Professor B. Gupta for a month in 2016. This enabled us to publish in the new journal "Global Challenges" in 2018, a joint review, about modification strategies for the development of antimicrobial catheters (*Global Challenges*, **2018**, *2*, 1700068).

During this five-year period, our expertise in surface chemistry was enhanced by two projects carried out under the LabEx Charmmmat. The first project entitled "Silipolysalen", aimed at the **synthesis and controlled polymerization on silicon of monomers with chelating functions (salen)** of transition metals for asymmetric synthesis in a heterogeneous medium. This project was carried out in collaboration with the Molecular Catalysis Team (ECM) of ICMMO (E. Schulz, M. Mellah) and the group "Electrochimie et and Thin Films" of the Laboratory of Condensed Matter Physics of Ecole Polytechnique (A.-C. Gouget and F. Ozanam) as part of N. Zidelmal's thesis (2015-2018). A first publication resulting from this work has demonstrated the catalytic activity and the possibility of easy recycling of polymers synthesized by ATRP in solution (*Polymer*, **2018**, *135*, 261). The proof of concept of the silicon grafting of model monomers and the essential contribution of FTIR-ATR spectroscopy to obtain quantitative information on the graft density and the length of the grafted chains were also demonstrated during this work. An effort has to be made in the future to graft catalysts on silicon. The second Charmmmat project realized in 2016 in collaboration with the team of P. Mialane (ILV Versailles) allowed us, within the framework of I. Bazan post-doctoral's position (1 year), to develop new polymer materials based on hybrid polyoxometallates with promising photochromic and luminescent properties (*J. Mater. Chem. C*, **2017**, *5*, 6343). In a study carried out in collaboration with B. Keita (LCP, UPSud) new hybrid materials based on graphene and a cyclic polyoxometalate, were shown, with or without the addition of ionic liquid polymer, to remarkably improve the electrochemical properties with respect to those observed with vitreous carbon (*Eur. J. Inorg. Chem.*). In collaboration with the Institute of Surfaces of Mulhouse (T. Elzein, M. Brogly) we did self-assemblies of thioalkyl-functional chains on gold surfaces in order to study, by PM-IRRAS spectroscopy, the influence of the terminal functionality on the final orientation of the chains (*J. Adhes.*, **2013**, *89*, 416).
in 2015 an international collaboration with the Lebanese Atomic Energy Commission (LAEC) was initiated by the beginning of the thesis of M. Maaz (financed by the two partners' own funds), allowed us to develop a new and very promising subject thanks to the synthesis of **new polymers, derivatives of 4-vinylpyridine (4VP), having exceptional coordination properties of lanthanides and actinides** (*J. Colloid Interface Sci.*, **2017**, *500*, 69 and 2 patents filed in 2017). The potential applications of these new polymers are under study and concern not only **the nuclear industry** but also the fight against counterfeiting, biomedical imaging, etc.

The year 2017 marked the beginning of the GASP project "Biobased High Gas and Vapor Barrier Polymers for Packaging" supported by ANR as part of a Collaborative Research Project Company / Public PCRE involving 6 academic partners, 2 start-ups and 2 industrials. In this context, Manon Le Gars started her thesis under the co-supervision of Ph. Roger and J. Bras (LGP2, PAGORA, INP Grenoble). **The thesis objectives are to improve the barrier properties to gases and vapors of a biodegradable and biobased polymer PLA** (polylactide).

Finally, an international collaboration with the National Chiao Tung University (NCTU) of Taiwan was initiated in October 2017 thanks to the co-tutelary thesis of Shu-han Chang who will spend 2 years in France from October 2018 to work on the **development of a new sensor based of imprinted polymers for the detection of pollutants**.

During this period, we also had interactions with the socio-economic world with two collaboration contracts with the start-up Ethera in 2013-2014 and 2016-2017 on the synthesis of fractions of amylose for sensor application. We are also partners in two other research collaborations carried out 1) by V. Huc (ECI, ICMMO) with the Vernet Company (6-month contract in 2017) on a confidential subject and 2) carried by G. Vo-Thanh (ECM, ICMMO) with the Roquette Company (one-year post-doctoral position started in October 2017) also on a confidential subject.

To conclude, during this five-year period, we have maintained a high level of scientific production, despite the renewal of our members. Our research activity has evolved and diversified in terms of applications that are no longer essentially medical-public health but also concern catalysis, nuclear and packaging industry. At the national level, we started in 2017 a large-scale ANR collaboration on a topic related to the preparation of biobased polymers with high barriers to gases and vapors for packaging. We also improved our international visibility through established collaborations with Lebanon, India and Taiwan.

Highlights

- Departures of J.-M. Beau (emeritus) and B. Lepoittevin and arrivals of D. Guianvarc'h, N. Aubry-Barroca, C. Aymes-Chodur and H. Salmi-Mani.
- The discovery of atom-economical, catalytic one-pot multi-step processes on carbohydrates including the chitin polymer for the construction of highly bioactive glycoconjugates and glycoprobes.
- The use of specific carbohydrate analogues for the quick detection of living bacteria, using metabolic glycan labeling.
- The discovery of a new polymer derived from 4-vinylpyridine highly efficient for radiodecontamination purposes.
- Promising antibacterial properties of polymer surfaces grafted with thymyl and vanillin-derived biobased monomer.

2 Organisation and life of the research team

Management, organisation and scientific animation

The team is organized in two research themes (see Table 1) that are located in two different buildings. The group leader is the representative of the team members during the various laboratory meetings. He relays the scientific, administrative and daily informations transmitted by the director of the institute in order to ensure the proper functioning of the team.

Each theme is managed by a scientific supervisor. The team leader relies on the two scientific supervisors to form an animation committee. This animation committee discuss regularly to optimize the team's progress, in terms of scientific policy, organizational and financial aspects, as well as human resource issues and any other points requiring decision-making. Team meetings of whole staff are organized 3-4 times per year in order to discuss all the above listed points. As far as scientific steering is concerned, projects are carried out autonomously by the project leaders in close collaboration between the various researchers of the team. Joint meetings will be held regularly during which interns, PhDs and post-doctoral fellows are especially invited to rehearse their oral presentations before scientific meetings or presentations at the end of the internship. They promote exchanges between the various actors and ensure good overall cohesion. Group meetings are held regularly during which 1 person (permanent or non-permanent researcher) present ongoing work or a bibliographical study on a topic of interest to the thematic in order to federate the group on new projects.

The team benefits from recurring credits from its two guardianships, which enable it to ensure the basic operation (maintenance costs, purchase of consumables, internal invoicing, etc.) and own financing obtained in calls for proposal essential to develop projects. Members of the team are regularly invited and encouraged to respond to the various calls for tenders (local, national and international) that they are concerned with.

3 SWOT analysis

Strengths	**Weaknesses**
Strong valorization of the results (patents, startup); success in obtaining grant funding; strong involvement in transmission of knowledge; ability to recruit new researchers; multidisciplinary research; affiliation with the Labex Chamrmmat; recent arrival of a new Professor and 2 Lecturers with highly complementary expertise.	Lack of CNRS researchers; lack of PhD students (less than 1/HDR); difficulties in recruiting PhD students on a regular basis; location on two different buildings ; departure of the group leader (JMB) of SB theme.

Opportunities	Threats
CNRS recruitment; development of new projects in the team; application of some members of the team to the Labex Lermit; strong dynamics in Chemical Biology and potential creation of a Chemistry-Biology pole in the Institute.	Cost of multidisciplinary research; Strong international competition; Limited number of grants for fundamental research.

4 Scientific strategy and projects

• Scientific orientation

In order to take into account the evolution of the team, its name will be slightly modified to Synthèse de Molécules et de Macromolécules pour le Vivant et l'Environnement (SM$_2$ViE). The « Synthèses de biomolecules » theme will also change its name to « Synthèse et Réactivité de Molécules pour le Vivant ».

The SM$_2$ViE Team will be positioned mainly at the interface between Synthetic Chemistry and Biology. Its staffs possess highly complementary skills in organic synthesis (synthesis of bioactive molecules, glycochemistry, organometallic chemistry), in chemistry and physical-chemistry of polymers (controlled polymerizations, surface functionalization), and more recently in biochemistry (enzymology, protein study and nucleic acids) and will work in collaboration with biologists.

The work will focus on the development of new synthesis methods to develop chemical tools for the study or regulation of biological processes and environmental issues.

Research priorities will focus on:

1. The organic synthesis of molecules dedicated to the study of fundamental or applied biological issues. Two aspects will be studied in a complementary way: (*i*) the development of new and efficient synthesis methods to obtain these chemical tools and (*ii*) the setting up of optimal experimental conditions for the use of these chemical tools on biomolecules (enzymes, proteins, peptides, nucleic acids, lipids ...) and living cells before their implementation in more complex systems in collaboration with biologists.

2. The study of methodologies for synthesizing polymers and/or surfaces from molecules or macromolecules that are mainly biobased with the objective of obtaining new functionalities useful in the field of public health (e.g. materials for bacterial anticontamination, for nuclear waste water treatment, as biosensors, …) or in the field of catalysis or for the improvement of biobased polymers technological properties. This work will be realized in collaboration with chemists, biologists and physicists.

The team will be structured around these two main themes, each requiring their own collaborations, but the interactions between these two themes will also be strongly encouraged. Thus, the team recently started a project involving skills of both groups in glycoconjugate synthesis and in polymeric materials with antimicrobial properties.

« Synthèse et Réactivité de Molécules pour le Vivant » theme

Due to the recruitment of a PU with skills in biochemistry and chemical biology in the field of post-translational modifications and epigenetics, new research projects will be introduced in the team while maintaining several current projects relying on the expertise in glycochemistry in which the group has acquired an international recognition. In the next contract, our projects will be focused on two objectives: we will develop chemical probes to understand at the molecular level and to modulate different biological events; furthermore, we will pursue the development of new methods for the synthesis of carbohydrate-containing bioactive molecules. These two aspects are highly complementary and closely related: the projects in the field of chemical biology will require the development of new and efficient synthesis of the different chemical tools; conversely, the methodology developments in glycochemistry will be applied to new biological issues. Some of the projects are detailed below.

- **Glycochemistry: methodology development**

The synthesis of biologically active glycoconjugates or analogues is a challenging task in organic chemistry, which usually requires selective and lengthy multi-step sequence of transformations. In order to access such structures, the laboratory will maintain its interest in the development of efficient and selective methodologies. For this purpose, we will continue to develop new synthetic methods for the activation of the anomeric position of sugars, involving radical and/or organometallic species. Because of their great biological importance, special efforts will be made for the selective anomeric formation of carbon-carbon bonds using samarium-mediated Reformatsky-coupling reactions in the sialic acid series Kdo, Kdn and Neu5Ac. We will also pursue efforts in the field of "Lewis acid-catalyzed tandem catalysis", processes in which glycosidic units are orthogonally protected in a one-pot procedure. The development of these eco-friendly synthetic procedures will help in the rational design of important tools useful in fundamental biology (cellular recognition, oxidative stress), in human health (new *C*-sialylated structures as a model in anti-flu strategy, rapid synthesis of mycobacterial probes) and in the agro-biochemical field (valorization of biomass as a renewable resource for the synthesis of biologically active chitooligosaccharides).

- **Metabolic Glycan labeling**

Our efforts in the field of Metabolic Glycan Labeling will be pursued in several new directions. We will explore dual labeling of bacteria for high-resolution imaging of their envelope, visual localization of different regions of their lipopolysaccharides, and potential quantification of the level of incorporation of modified monosaccharides (in collaboration with S. Lévêque Fort, ISMO, and J.-L. Pernodet, I2BC, *CNRS Mission Interdisciplinarité*). Further applications to *in vivo* imaging of bacterial infections using PET radiotracers will also be studied (with B. Kuhnast, IMIV, *France Life Imaging*).

The production of high-added-value molecules from biological resources often involves the chemical transformation of the bio-sourced material to allow its conjugation to a molecular platform, a drug or a carrier. The advent of bioorthogonal conjugation techniques together with metabolic glycan engineering offers new opportunities for the elaboration of bio-sourced polysaccharides for various industrial applications. We aim at establishing a proof of concept, via the adaptation of metabolic lipopolysaccharide engineering. This methodology will be exploited as a straightforward and efficient strategy to produce new, well-defined glycoconjugate vaccines targeted against cholera, a diarrheal disease remaining a major public health concern and later extended to other bacterial pathogens like *Klebsiella* or *Pseudomonas* (IngeniOse Project, with C. Grandjean, UFIP Nantes, and ICSN, *Agence Nationale de la Recherche*).

Sialic acids are major players in many biological functions such as host-pathogen recognition. Whereas the biosynthesis pathways of sialic acids and the associated enzymes are quite well described in eukaryotes, this is not the case in bacteria. We will develop new labeling tools and study incorporation of sialic acids using metabolic glycan labeling, in pathogenic bacteria in comparison with human cells, as well as in cellular infection models, in order to detect key differences and characterize phenotypic variations that will be used to screen chemical libraries. While the majority of published articles focus on cell-level bioimaging using a fluorescent probe, we will additionally attempt to gain in sensibility and resolution by using metal probes detectable by modern electronic microscopy methods.

- ***Detection of Reactive Oxygen Species***

Elaboration of molecular probes for *in cellulo*, or *in vivo*, detection of enzymatic activities (peptidases, esterases, glycosidases, …) or chemical species (ions, chemical messengers, pollutants, reactive species, …) represents one of the major challenges addressed by Chemical Biology. In this context, Reactive Oxygen Species (ROS) are, for example, species produced when our cells are subject to oxidative stress conditions, and lead to molecular lesions within living organisms. This universal process is associated with aging, as well as cancer and several neuro-degenerative diseases such as Alzheimer's or Parkinson's.

Our project targets the elaboration of efficient synthetic strategies, physicochemical characterization, and biological studies of new specific and sensitive probes. The tools that we will develop will find diverse applications in biology, such as *in cellulo* or *in vivo* surveillance of the production of ROS, including hydrogen peroxide, which is potentially linked to certain pathologies. Probes based on boronic acids or esters have previously been described for the detection of hydrogen peroxide, but they proved poorly reactive/sensitive, and require high H_2O_2 concentrations and long reaction times to be activated. In preliminary studies, we have developed a new, borinic acid-based probe prototype which proved very reactive. We will further consolidate these studies by the development of new synthetic strategies, as well as new probes, better suited for biological applications (with ICSN, Gif-sur-Yvette, M. Pucheault, ISM Bordeaux, L. Jullien, PASTEUR Paris, *IDEX Paris Saclay*)

- **Trehalose and Mycolic Acid-Based Probes for the Study of Mycomembrane Biogenesis**

Recently, chemical-biology-based strategies have emerged for the study of bacterial pathogens, giving biologists the opportunity to have powerful new tools for probing bacteria. Actually, probes for the study of mycobacterial envelope remains challenging since Mycobacteria and Corynebacteria have an atypical organization being composed of complex glycolipids (mycolic acids esterified to α,α-D-trehalose). They form a very impermeable and rigid barrier that might contribute to the exceptional resistance of mycobacteria towards chemotherapeutic molecules. The biosynthesis of these cell wall mycolate esters has been studied during the last decade but the mechanisms of their assembly in the bacterial envelope is largely unknown.

In this context, we will pursue a work that emerged in the team during the previous contract in the field of chemical biology. In particular, the expertise acquired in trehalose chemistry including the synthesis of complex fatty acids and selective modifications of trehalose will be applied to determine the specificity and the interplay between several enzymes named mycoloytransferases in the biogenesis of the envelope of these mycobacteria. New bioorthogonal trehalose-based probes will be synthesized to elucidate the precise role of these enzymes in a physiological context (collaboration with Prof. Nicolas Bayan, Institut de Biologie Intégrative de la Cellule Université Paris Sud). The study of physical properties of the mycomembrane will be carried out in collaboration Prof. Federica Migliardo (University of Messina).

- **Chemical tools for the study of epigenetic modifications**

Epigenetics defines the changes in gene expression that are not coded by the DNA sequence and are inheritable. The main epigenetic factors are chemical modification of histones (methylation and acetylation) and DNA methylation, but new modifications have recently expanded the epigenetic landscape. Considering the potential of "druggability" of proteins involved in epigenetics, the precise characterization of their activity might offer new opportunity for therapeutic intervention. In recent years, the study of chromatin biology has greatly benefited from chemical biology tools and biologists are becoming aware of the importance of these strategies to address fundamental structure/function problems in epigenetics. We recently developed both chemical tools and proteomic approaches based on photolabeling or bioorthogonal labeling coupled to mass spectrometry to study several epigenetic modifications and we will continue these projects in the future contract in collaboration with biologists.

In particular, we will continue a recently initiated project aiming at defining the methylome of a key histone lysine methyltransferase in order to extend our knowledge of non-histone lysine methylation. Enzymes that catalyze this modification act by transferring the methyl group from the cofactor S-adenosyl-L-methionine (SAM) to the ε–amino group of a lysine. A chemical-biology-based strategy in which artificial cofactor S-adenosyl-L-methionine (SAM) molecules and modified enzymes are engineered to label substrates gave interesting results on different enzymes and will be implemented on our enzyme of interest. First encouraging results allowed us to obtain a grant from ANR in 2017 (AMetHist project, collaboration with Raphaël Margueron, Curie Institute in the department of Genetic and Developmental Biology) and new cofactor analogues with functionalizable methyl surrogates will be developed and characterized in vitro. We will consider extending this strategy to other methyltransferases and to another important post-translational modification, ie *O*-GlcNAcylation, by designing new GlcNAc analogues for the labeling of substrate proteins with tag allowing an efficient detection by mass spectrometry which still remains challenging.

Furthermore, we will pursue the development of chemical probes to gain insight into the biological function of unusual epigenetic DNA modifications. We have recently developed a photolabelling approach to characterize protein-DNA complexes in proteomic studies by trapping binding proteins of specific DNA sequences containing epigenetic modifications. We now will use it for the study of modified nucleobases such as β-D-glucosyl-5-hydroxymethyluracil (base J), a hyper-modified base discovered in parasites responsible for tropical diseases (collaboration with Prof. Philippe Grellier, Unité Molécules de Communication et Adaptation des Micro-organismes, Museum National d'Histoire Naturelle (Paris).

« Polymères et Surfaces » theme

In the continuity of the previous contracts, the research thematic areas associated to the Polymers and Surfaces theme will be devoted to the development of new methodologies involving eco-compatible syntheses (by photochemical, plasma or chemical treatment) in order to prepare new Polymeric Materials (PM) from molecules or macromolecules in particular from biobased components with the objectives to elaborate polymers and/or functional surfaces.

Depending on the nature of the grafted functionality (anti-adhesive, coordinating metals, gas barrier, etc.), these new materials will be useful in several areas such as the fight against surface bioburden in medical-hospital and food industry, the nuclear industry, etc. Thus, interactions with the socio-economic world will be favored (companies and start-up's partners of ANR GASP, valuation of our two recent patents, etc.).

- ***« PM for antibiocontamination »***

Research efforts currently focused on the development of "antibacterial polymers or/and surfaces" based on biosourced molecules will be pursued with a view to obtaining biocidal, bacteriostatic, anti-adhesive or anti-biofilm properties. This topic was recently confirmed via the assignment in October 2016 of a MESRI allocation for Thu N'Guyen PhD student. The aim of the present thesis consists on the development of new grafting methodology allowing to the development of new surfaces presenting a highly performant antibacterial activity. In order to do this, the considered strategy consists in the grafting by a controlled polymerization methodology of a chain possessing one or more leaving groups, by followed by a chemical post-modification allowing to the incorporation of antibacterial species on demand functions. Regarding the development of antimicrobial materials research axis, the recently integrated lecturers, are conducting their research in the improvement of silicone rubber and PET based surfaces by means of photochemistry and plasma treatment. In addition, an inter-thematic axis involving 5 members of the team was set up in 2017. The research objectives consist to increase aqueous solubility of natural antibacterial molecules. Thereby, glycosyl fragments were incorporated on their stuctur and thus a library of 27 glycoconjugates was constituted, some of them presents promising antibacterial activity. Water-soluble, one-dimensional polymers will be then synthesized from the most active glyconconjugates to study the antibacterial activity of the polymer solutions in planktonic media, and to possibly consider their grafting on surfaces. These types of unifying and multidisciplinary projects ensure the expanding of the numerous of collaborations with chemists, physicists and microbiologists from different organizations (ITT New Delhi, Université Paris Sud: LPS, ISMO et I2BC, Université de Versailles, INRA, AgroParisTech, Ecole Polytechnique). Thus, most of these collaborations will be pursued or even reinforced.

- ***« PM for catalysis »***

In order to continue to develop this axis, a promising subject dealing with the preparation of different kind of catalysts grafted onto PET fibers for the supported catalysis, a call proposal has been deposited and selected for the second selection phase in the framework of the ANR (in collaboration with E. Schulz, ECM-ICMMO and O. David, ILV). It is hoped that the LabEx "Charmmmat" will continue to support in the future, our collaborative research (ECM and École Polytechnique) devoted on salen grafting on amorphous silicon, in the continuity of the Silipolysalen (2015-2018) contract.

- ***« PM for the nuclear industry »***

In collaboration with the Lebanese Atomic Commission, the promising results obtained in the context of the Mohamad Maaz's thesis explain the interest of the Polymer and Surface group to continue in this line of research. In order to finance a new thesis, in the continuity of the Mohamad Maaz works, an allocation from the Lebanon is currently under discussion.

- ***« Biobased PM »***

As a part of the GASP project "Biobased High Gas and Vapor Barrier Polymers for **Packaging**" supported by ANR. The work in this field will consist in improving the barrier properties to gases and vapors of PLA. The involved strategy consists in incorporating cellulose nanocrystals and calixarenes. On the other hand, to enhance the dispersion of cellulose nanocrystals in PLA polymeric matrix, these later are functionalized with hydrophobic polymer layers.

Thanks to the established collaboration with NCTU of Taiwan, Shu-han Chang will work on the development of new biobased polymer sensors for the detection of aromatic pollutants.

• Priority needs

Due to the recruitment of a new PU who will reorient a part of the projects toward chemical biology approaches and the recruitment of two new lecturers in the polymer group, we do plan thus to recruit permanent positions within the next five-year contract. For CNRS, we are prospecting for 2 candidates (CR), one in Chemical-Biology and the other in Polymer Chemistry in the near future.

Self-assessment document

Team 6 - RMN

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**RMN en Milieu Orienté**
Acronym:	**RMN**
Director's name (current contract):	**Denis MERLET**
Director's name (future contract):	**Denis MERLET**

LRMN
Laboratoire de RMN
en milieu orienté

SELF-ASSESSMENT DOCUMENT

1 Research products and activities

Scientific output

The main research themes of the "RMN en milieu orienté" team focus on the development and analytical promotion of NMR in liquid media and oriented environments. The common to all of the research activities is the use of NMR in liquids and in oriented media, either for the physicochemical study of materials, or for new structural and stereochemical information which can be used by the (bio) chemists. Nuclear Magnetic Resonance is an extremely powerful analytical tool for structural analysis for instance, nowadays used as a routine technique with the well-known limitation. Due to the Brownian motion in the isotropic solvent, residual dipolar couplings (RDC), residual quadrupolar couplings (RQC), residual anisotropic part of the chemical shift (RCSA) are null but these anisotropic interactions have intrinsically structural, conformational and orientational information. This is the aim to use oriented solvent to have access to new informations/measurements. In addition, the use of chiral liquid crystal solvent led to a new method of enantiomers visualization called method 'chiral ordering agents'. The team also develops new tools for NMR in isotropic and anisotropic environment to optimize the detection of insensitive, exotic nuclei and low concentrated compounds.

The ERMN team published 47 articles in peer-reviewed journals, corresponding to 1,61 articles / full-time equivalent researcher; the average impact factor was 4.35. Team members also reported their results through 14 lectures, 34 oral communications, 27 poster presentations and 14 invited seminars.

Since 2013, four main research areas have been conducted i) Methodological and analytical and development of anisotropic deuterium NMR ii) Development of frequency spatially encoded pulse sequence experiments ii) Quick and sensitive multidimensional NMR pulse experiments iv) Conformational analysis of (bio)-compounds using NMR in chiral oriented solvent

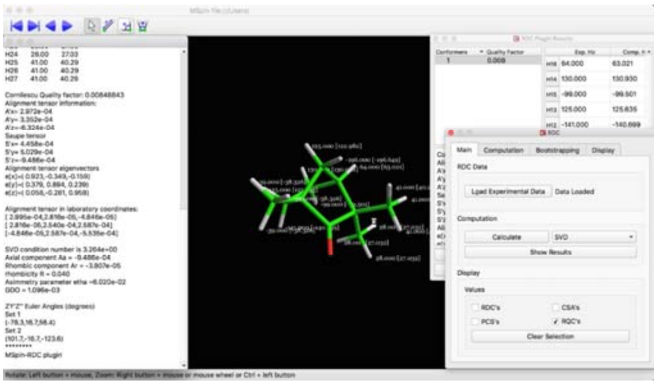
1) Analytical and methodological development of deuterium NMR

Among all quadrupolar nuclei, deuterons play a distinctive role in NMR for two reasons: i) it possesses intrinsic NMR properties (unusually small nuclear quadrupole moment) that can be efficiently exploited; ii) it is naturally present (0.0155 % on average) in all (bio)organic compounds and hence can be used as a remarkable tracer in analytical chemistry without any isotopic enrichment. From a practical view, recent instrumental advances (high magnetic fields, cryogenic probes, hardware) have significantly boosted the sensitivity and the potentialities of natural abundance deuterium NMR (NAD NMR). Besides when isotropic solvents are replaced by anisotropic media (lyotropic (chiral) liquid crystals), we have access to ^{2}H-residual quadrupolar couplings (RQC) of deuterated analytes or at NAD level. Interestingly, this order-dependent NMR interaction can be exploited for numerous analytical purposes (visualisation of enantiodiscrimination, determination of enantiopurity, (^{2}H/^{1}H) isotopic analysis, structural determination, study of orientational mechanisms, ….). In this context, ICMMO possesses a unique (worldwide) instrument (since 2007), namely a 14 T NMR spectrometer equipped with a ^{2}H selective cryoprobe, that is mainly dedicated for research activities (in particular at ERMN group), but also for routine ^{2}H analyses.

Over the last five years, the activities on this theme were focussed on two concomitant research axes whose key idea/concept is to provide new specific and original analytical solutions for bio-, geo- and organochemists by combining ^{2}H or NAD (1D/2D) NMR and weakly aligning (chiral) media: i) innovative methodological developments (NMR reaction monitoring, acquisition methods such as NUS or Ultrafast), ii) dedicated/specific applications (characterization and enantiopurity measurement of the chiral acyl chains in tetra-acylated sulfolipid analogues or axially chiral biaryls, analysis of (^{2}H/^{1}H) isotopic distribution of geobiomarkers or food aroma molecules, study of mesogenic ionic electrolytes). Both aspects leaded to fruitful national and international collaborations with various researchers from French universities (Orleans, Nantes, Lille, Strasbourg) and Institutions (ENS, Curie, CEA), as well as foreign universities (Giessen, Southampton, Warsaw) or prestigious Institutes (IISC in India, Max Planck of Heidelberg, Weizmann and Technion in Israel), thus showing the broad interest of this research activity. Quantitatively, 12 research articles in peer-review international journals (*ACIE, Analyst, AC, CC, CPC, FFJ, MRC NJC, JOC, JPCA,* …) and 5 book chapters (*eMagRes, ESS, MMR (2), EAS*) and a full review (45 pages) have been published to CSR. In terms of international/national visibility, five articles were highlighted by different ways: i) three were considered by Journal's Editors as "VIP" papers (*Analyst* **2014**, *ACIE* **2015** and *ChemPhysChem* **2017**, with two "cover pages"); ii) two of them, *AC* **2013** and *Geochimica Acta* **2015**, were highlighted by WEB media («*Chemical & Engineering News*» of ACS and «*Spectroscopy Now*» website in 2013) and INC/INSU CNRS / Paris-Sud website in 2015, respectively.

From the methodological viewpoint, two important achievements have to be mentioned. The first one is the « *in situ* and real-time » monitoring of the interconversion of isotopically enriched enantiomers (*L*- and *D*-alanine-d_3) by alanine racemase directly observed by the variation of intensity of their ^{2}H-RQC on ^{2}H-{^{1}H} NMR spectra recorded in a chiral, liquid-crystalline environment made of short-length DNA fragments. The robustess/interest of this new method was demonstrated by the extraction of the turnover numbers of the enzyme by using the Michaelis-Menten model, whose values are coherent with values obtained by classical methods, thus leading to a change of paradygm in the domain (*Anal. Chem.*, **2013**, *85*, 4694). An inherent drawback of this approach is the experimental time required to record spectral data for monitoring the time-dependent variations of all compounds in the mixture, in particular for extremely fast and/or multiple (cascade) chemical transformations for which an extremely fast identification and/or quantification of ^{2}H signals of products (reactants, (un)stable intermediates, products, …) (chiral or not) require highly short-time 2D NMR experiments. Non-uniform acquisitions combined with covariance/compressed sensing processing have been explored to reduce the acquisition time of anisotropic NAD (QUOSY-type) 2D-NMR experiments. (*Analyst*, **2014**, *139*, 2702). However, the time saving is not enough to monitoring too fast multiple (cascade) chemical transformations, that demand 2D experiments with sub-minute time resolutions or below. In this context, we have demonstrated that subsecond homonuclear anisotropic deuterium ultrafast 2D experiments (ADUF) are possible and compatible with the basic gradient units implemented on routine NMR spectrometers, and allow recording ^{2}H signals of weakly aligned deuterated solutes in sub-second experimental times. (*Chem. Commun.*, **2016**, *52*, 2122). The second major achievement is the design a ^{2}H-RQC/DFT-based integrated computational protocol for the evaluation of the order parameters of aligned solutes via singular value decomposition using ^{2}H-RQC extracted from anisotropic NAD (ANAD) 2D-NMR spectra (**Figure 1-1 and 1-2**). The idea here is to benefit of the advantage of ^{2}H-RQCs (which are formally equivalent to one-bond $^1D_{CH}$ (^{13}C-^{1}H)-RDCs) for calculation of the Saupe order matrix, furnishing acute information to study molecular structure and orientational behaviour, and so detected tiny differences in the molecular alignment of enantiomers in CLC, for instance. The power of this hyphenated approach and in particular to understand the alignment processes and the role of molecular shape in the ordering mechanism through the determination of inter-tensor angles between alignment tensors and inertia tensors was revealed (*ChemPhysChem*, **2017**, *18*, 1252).

(a)



```
H24    28.00    27.03
H25    41.00    40.29
H26    41.00    40.29
H27    41.00    40.29

Cornilescu Quality factor: 0.00848843
Alignment tensor information:
A'x= 2.972e-04
A'y= 3.352e-04
A'z=-6.324e-04
Saupe tensor
S'x= 4.458e-04
S'y= 5.029e-04
S'z=-9.486e-04
Alignment tensor eigenvectors
e(x)=( 0.923,-0.349,-0.159)
e(y)=( 0.379, 0.884, 0.239)
e(z)=( 0.058,-0.281, 0.958)

Alignment tensor in laboratory coordinates:
[ 2.995e-04,2.816e-05,-4.846e-05]
[ 2.816e-05,2.540e-04,2.587e-04]
[-4.846e-05,2.587e-04,-5.535e-04]

SVD condition number is 3.264e+00
Axial component Aa = -9.486e-04
Rhombic component Ar = -3.807e-05
rhombicity R = 0.040
Asimmetry parameter etha =6.020e-02
GDO = 1.096e-03

ZY'Z'' Euler Angles (degrees)
Set 1
(-78.3,16.7,56.4)
Set 2
(101.7,-16.7,-123.6)
********
MSpin-RDC plugin
```

Conformers	Quality Factor
1	0.008

	Exp. Hz	Comp. Hz
H16	84.000	83.021
H14	130.000	130.930
H15	-99.000	-99.501
H13	125.000	125.835
H12	-141.000	-140.099

Figure 1-1 : (a) Screenshot showing different graphical components of the integrated MSpin-RQC program.

(b)

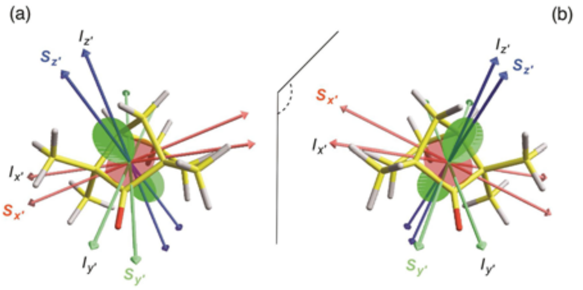


Figure 1-2 : Example of vizualization of principal axis system of Saupe (Sx', Sy', Sz') and inertia tensors (Ix', Iy', Iz'), and the Saupe tensor surface associated with two enantiomers (Fenchone).

From a more applicative aspect, and among results published, the wealth of ANAD 2D-NMR in polypeptide-based liquid crystals has been nicely revealed through two analytical achievements associated with the investigation of the natural site-specific (^{2}H/^{1}H) isotopic profile of (achiral or enantiopur) biocompounds of interest. The key idea here is to combine the advantage of simplified analysis of 2D maps with a more favourable distribution of ^{2}H signals on the anisotropic spectra (quadrupolar doublets instead of singlets when recording isotropic ^{2}H NMR (SNIF-NMR), thus limiting peak overlapping. The first concerns the isotopic analysis of molecular biomarkers (Miliacin, a pentacyclic triterpene of the amyrin family) preserved in sedimentary archives, in order to provide clues about the evolution of past climatic conditions (paleoenvironmental information). Contrarily to irm-MS approach, that provides a global molecular (^{2}H/^{1}H) value, the resulting isotope profile for miliacin shows, for the first time, that large variations in (^{2}H/^{1}H) ratios of methyl groups of the molecule was compatible with its biosynthetic processes, thus experimentally validating the reaction pathway proposed. This work revealed that ANAD 2D-NMR has also the potential to permit predicting possible fractionations during the diagenesis process of pentacyclic terpenes (degradation) in soils (*Geochim. Cosmochim. Acta*, **2016**, *173*, 337). The second one deals with the evaluation of intramolecular ^{2}H isotopic composition of vanillin (the most used food aroma) as an illustrative example of the analytical challenges associated with molecular authenticity/traceability investigations in food products, as well as the determination/understanding of metabolic/synthetic pathways. So far isotopic fractionation of vanillin remains incomplete due to the overlap of two aromatic ^{2}H resonances, and the impossibility of separating these fortuitous isochronous sites by isotropic

NMR. Exploiting the analytical potential of ANAD 2D-NMR, we have shown that all aromatic monodeuterated isotopomers can be spectrally discriminated on the basis of ^{2}H-RQC, thus enabling the determination of their relative proportions for the first time. These new isotopic data on vanillin, never exploited so far, provides an original tool for investigating/discriminating between the precursor origins of vanillin (natural versus synthesis origin), and subsequently fighting against the counterfeir, in combination with other existing NMR approaches such as analysis by ^{13}C irm (*Flavour and Fragrance Journal*, **2018**, *33*, 217).

Finally, the analytical potential of ANAD NMR was also used to evaluate the relative solute-fiber affinities (through distribution coefficients) toward two homopolypeptides (of same chirality) in lyotropic bipolymeric oriented systems, thus enriching our understanding of interactional/orientational behaviour of weakly polar, (prochiral) bicyclic molecules. In particular, we have pointed out that because the solute distribution is a property of the whole molecule, it affects in the same way all molecular local properties, from ^{2}H quadrupolar splittings to the diagonalized Saupe's order matrix. (*J. Phys. Chem. A*, **2016**, *120*, 6076).

2) Development of frequency spatially encoded pulse sequence experiments

In this second research theme, the aim is to simplify the ^{1}H spectrum to easily and accurately extract the couplings (scalar and dipolar couplings). After the development and optimisation of the Selective Refocusing pulse sequence (SERF) the team has developed new pulse experiments combining selective experiments and spatial encoding (G-SERF) to extract the coupling between one selected proton with the other protons of the compound (Figure 2-1a). The 1D encoding has been extended to 2D encoding permitting to combine *J*-edited and correlation spectroscopies permitting to extract easily the overall couplings of the ^{1}H spectrum multiplets (*Chem Eur J*, **2013**, *19*, 12221). This experiment is based on an original use of selective refocusing techniques, in the frame of a multi-dimensional sample frequency encoding, that results in a -fully resolved- spatial edition of the whole coupling network through the NMR sample (PCR COSY, Figure 2-1b).

To going further to simplify the ^{1}H spectrum and to increase the sensitivity of these encoded experiments, theoretical simulations using Spin Dynamica program (developed by Levitt's group at Southampton) have been made to know the evolution of the coherences during the selective pulse and the gradient pulses. This permit to demonstrate that there is a magnetic field dependence of the magnetic field and the quality of the spatial frequency encoding (*PCCP*, **2016**, *18*, 22827; *Magn. Res. Chem*, **2015**, *53*, 836). In chiral liquid crystals, enantiomers have not the same NMR spectrum. Then it is possible to visualize them in G-SERF experiment, for instance. It is possible to perform a quantitative chiral analysis by simulating accurately dipolar edited spectra of enantiomers dissolved in a chiral liquid crystalline phase then these simulations are used to calibrate integrations that can be measured on experimental data. The quality of the simplification has been tested on Oligomeric Saccharides and it is demonstrated that the combinaison of pure shift and *J*-edited spectroscopies greatly simplify the work on highly crowded proton spectra (Push-G-SERF).

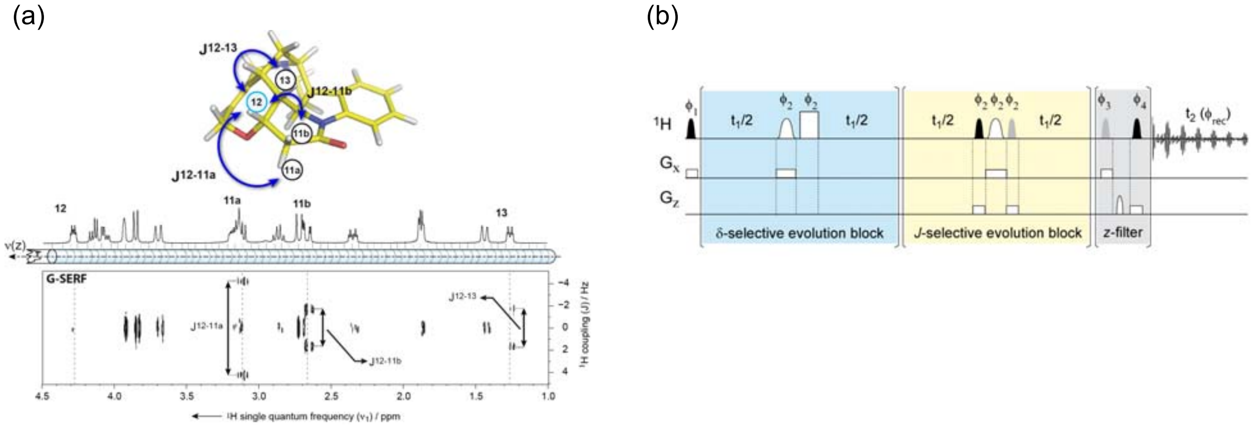


Figure 2-1 : (a) 2D G-SERF map (b) PCR-COSY pulse sequence diagram

3) Quick and sensitive multidimensional pulse experiment

The team in this theme has worked on the use and the development of robust NMR experiments to obtain in the minimum experimental times the structural information or to give more sensitive experiments. To reach this goal the team has used fast-repetition NMR experiments (Figure 3-1). One option is to reduce the relaxation delay between each pulse sequence block of a 2D NMR experiment. This is particularly well adapted for heteronuclear HMQC type experiments (SOFAST and IMPACT experiments). For instance, a sensitive NMR tool has been successfully developed here to probe the H-bond network in *beta*-sheet or helix secondary structures of peptides (H^{N}-CO SOFAST HMBC experiment). Based on selective pulses allowing reducing T_1 relaxation times for amide ^1H, it reduces the recycling time and provides a significant gain of accumulation time, which in turn enhances the sensitivity by a factor of two (*Org. & Biomol. Chem.*, **2013**, *11*, 7611). New NMR sensitive experiments able to suppress the huge signal of the polymer in PEG-linked compound spectra have been developed. These techniques called SENSASS NMR allowed reducing signals with the help of semi-selective pulses or WATERGATE sequences, and enhancing the sensitivity with methods such as fast-pulsing techniques. SENSASS NMR allowed the reduction of the polymer signal until 99 % and enhancements up to 480 % in sensitivity (*J. Magn. Reson.* **2013**, 237, 63). This kind of methodology has successfully revealed the presence of a hydrazino turn conformation in dipeptides derived from N-aminoazetidinecarboxylic acid. The different applications have demonstrated that this newmethodology is particularly well adapted to push back the limit of NMR spectroscopy and permitted to provide information to which the chemist had no access until now.

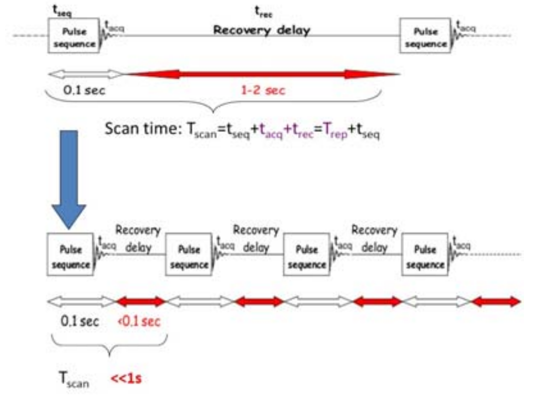


Figure 3-1 : Fast-repetition NMR experiment

4) Conformational analysis of (bio)-compounds using NMR in (chiral) oriented solvent

The conformational study of bioactive molecules is becoming increasingly important in order to maximise and control the effects of drugs at a biological level. Indeed, analogues of a given bioactive solute could have different biochemical activities *e.g*. phenylsalicilic acid and diflunisal (Figure 4-1a, *J. Phys. Chem. B*, **2014**, *118*, 9007). Even more interesting is the enantiomeric discrimination of flexible molecules with chiral centres. As a matter of fact, due to the specificity of the biological receptors it is well known that within a couple of enantiomers one could be an eutomer whereas the other is a distomer like naproxen (Figure 4-1b) whose *S*-enantiomer is 28-fold more active as an anti-inflammatory drug than the *R*-isomer, reported to be a liver toxin and to incidentally causes gastrointestinal disorders. It is, therefore clear that the conformation that a solute adopts in solution could give insight into the biological solute-receptor interactions. It is known that their biological role originate from their specific binding to target proteins and is evidently driven by the spatial arrangement they adopt at the active sites. In this perspective, from 2012 within a well-established collaboration with the LXNMRSCAn group (Universita della Calabria) we have focused on this topic, and designed a robust and efficient methodology derived from the NMR data obtained in (chiral) liquid crystalline solvent *via* the Additive Potential-Direct Probability Distribution (AP-DPD) approach able to model the solute-solvent interactions (Figure 4-2, *New J. Chem.*, **2015**, *39*, 9086; *Eur. J. Pharm. Sci.*, **2017**, *106*, 113). We firstly have investigated the therapeutic class of Non Stereoidal Anti-Inflammatory drugs (NSAID) with various simple but widely used commercial drugs – salycilates and profens, increasing : i) the number and complexity of torsional degrees of freedom from diflunisal (one torsional degree of freedom) to naproxen (two non-cooperative torsional degree of freedom) or ketoprofen (two cooperative torsions), and ii) the NMR difficulties due to fluorine nuclei that led us to develop when necessary new NMR pulse sequences as the GET-SERF (*J. Magn. Reson.*, **2013**, *234*, 101).

Following these successful preliminary results, proof of concepts, we are aiming to continue to exploit and develop the analytical potential of NMR in (chiral) weakly ordered solvents in order to deliver an efficient tool for elucidating conformational equilibria and distributions of small (chiral) molecules and solve stereochemical challenges. Ideally it would be a tool for drugs screening and design. Three peculiar activities are aimed :i) investigating more complex or different systems (coupled & independent rotors) in various domains; ii) getting insight into structure-activity relationships comparing the in-solution conformational distribution of analogues or couple of enantiomers of different bioactivities as the chiral anisotropic solvent allows to statistically orient them in a different way and leads to spectral enantiomeric differentiation; iii) exploiting enantiotopic spectral differentiation in chiral anisotropic solvent to over-express NMR data for prochiral solutes. Test molecules would be taken within commercial and widely used antihistaminic drugs as they possess all the features we would like to investigate (Figure 4-3). Phenylbutazone is currently under investigation to evaluate the feasibility of this project.

(a) (b)

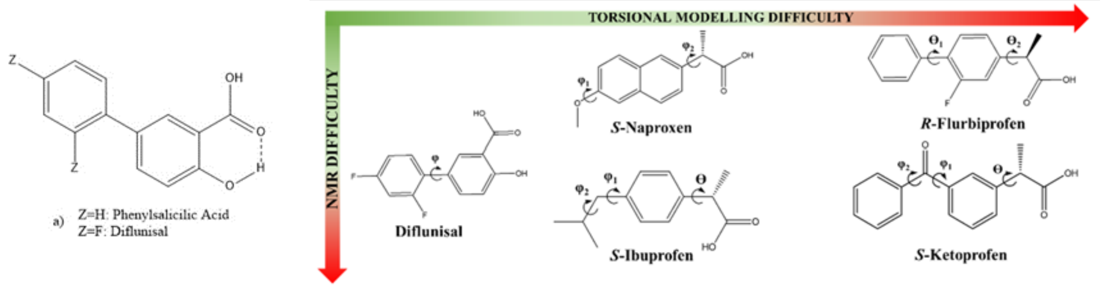


Figure 4-1 : Chemical structure of (a) Diflunisal and its non-fluorinated analogue and (b) various commercial NSAID successfully studied by NMR in liquid crystals combined to AP-DPD approach

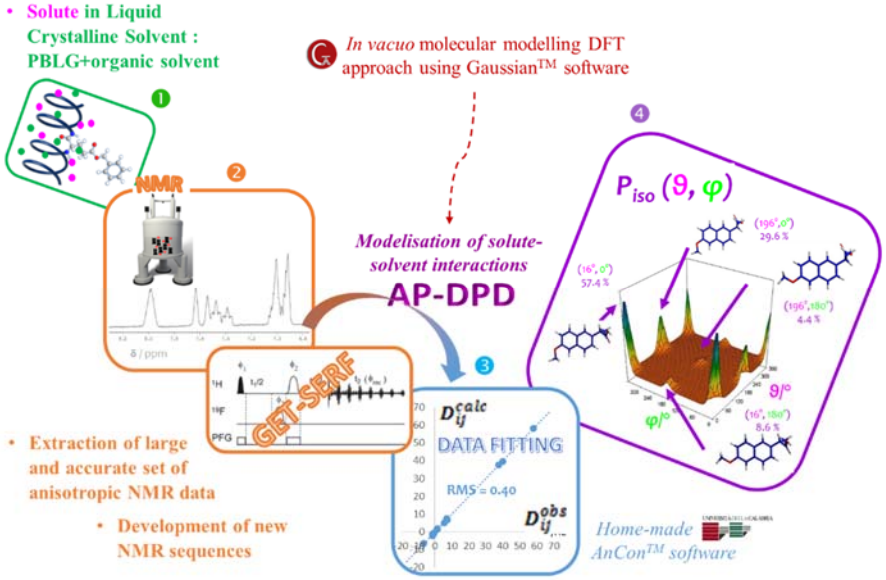


Figure 4-2 : Analytical methodology combining NMR in oriented media to AP-DPD approach to determine in-solution conformational distribution of (chiral) solutes

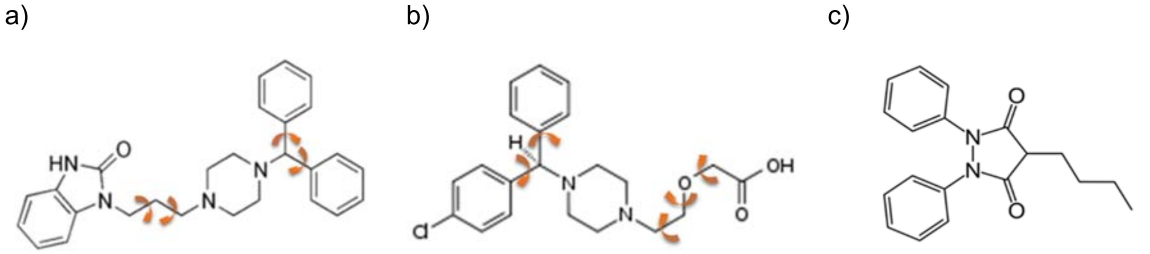


Figure 4-3 : Test molecules to be studied : a) oxatomide; 1st generation of antihistaminic, b) (levo)cetirizine, (2nd) 3rd generation of antihistaminic, c) phenylbutazone (NSAID)

It is important to note that even if all the research themes have been developed initially by the team members, all these developments have been used in collaboration with other ICMMO's research teams and other nationally or internationally collaborations.

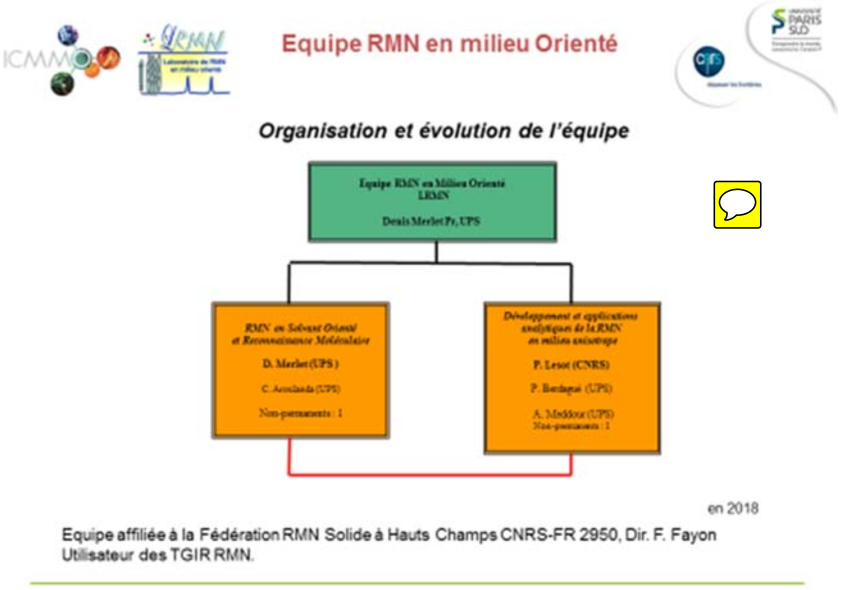
Highlights

1) It is important to note that over the last five-year the team "RMN en milieu orienté" has changed a lot of the permanent staff: Dr. Ouvrard (CR) is in sickness leave, Dr. Farjon (CR) has moved in Nantes University, Dr. Giraud (MCF IUT) has been recruited as Full Professor in P5 University, and Dr Bayle (MCF UFR) is in retirement. A recruitment should be done this year (IUT). Another MCF position is requested for next year (UFR).
2) A number of publication has been recognised as VIP or Hot articles including cover pages (*Analyst* **2014**, *Angew. Chem. Int. Ed.* **2015**, *NJC* **2015**, *ChemPhysChem.* **2017**) or has been highlighted press releases in ACS news *Anal. Chem.* **2013**) or in CNRS and Université Paris-Sud websites (*Geochim. Cosmochim. Acta* **2016**).
3) The high involvement in different scientific committees (INC-CoNRS S-12, CNU S-32, FR RMN-GBP, Alpine conference, GERM).
4) It is important to note that even it is not accounted into the quantitative production of the ERMN, two students of Analytical Professional Licence have been recruited by Sanofi (in collaboration with the team) to implement on their own spectrometers our new frequency spatially encoding pulse sequence experiments. Moreover, a Master degree student and concomitantly permanent staff of Servier has used the enantiomeric analysis by NMR in oriented media. This demonstrates the interest of the industrial community toward our research themes.

2 Organisation and life of the research team

Management, organisation and scientific animation

The team is organized around two areas of research as depicted below in the organization chart. It is important to note that all of the team permanent members contributes to the animation of these axes that are not therefore classified easily within a group but to all the staff of the team. Due to the number of leaving and depending of the arrivals, the organization chart will change. The choice of the team as a whole (budget, PhD thesis, master and scholarship application) is done in a collegial manner.



Equipe RMN en milieu Orienté

Organisation et évolution de l'équipe

en 2018

Equipe affiliée à la Fédération RMN Solide à Hauts Champs CNRS-FR 2950, Dir. F. Fayon
Utilisateur des TGIR RMN.

3 SWOT analysis

Strengths	**Weaknesses**
• Developments of new NMR methodologies • Numerous application analytical domains • Active local, national and international collaborations • International visibility • Quality of ICMMO’s NMR instrumental plateform • Competitive research axes	• Variation of the number of permanents over the last period • Interaction with the local eco-system • No participation to European funding program
Opportunities	**Threats**
• Permanent staff arrival • PhD arrival in dialogue with the PhD school • The creation of the Université Paris-Saclay (2020)	• Positioning of ERMN towards the Université Paris-Saclay targets • Continuous recruitment of students of quality (Highly competitive ED context) • Difficulties in pursuing a long-term fundamental research in a limited context of calls for “oriented” proposals • International competitive domain

4 Scientific strategy and projects

The organization of the team will remain identical for the next period depending of the number of arrival, as well as the research themes for which the objectives are described below.

1) Analytical and methodological development of deuterium NMR at natural abundance level

During the next period, two main axes will be investigated by the team: i) development of new specific analytical tools for studying natural compounds in the frame of the fight against counterfeit. For instance, the implementation of NUS experiments and/or selective decoupling of the organic co-solvent NAD signal present in lyotropic aligned systems will be performed to reduce the experimental times and/or improve the sensitivity of NAD 2D-NMR experiments in chiral liquid crystals; ii) application of integrated NMR protocol (“MSpin-RQC programme”) in the structural elucidation of complex natural bio-compounds (such as artemisinine, strychnine, …).

2) Development of frequency spatially encoded pulse sequence experiments

During the next five years, the methodology will be extended in chiral liquid crystals to test the robustness of the experiments and to help to extract the dipolar coupling for enantiomers which will be used in the next theme. From a methodological point of view, an improvement of the PUSH-GSERF pulse sequence will be generalized to obtain a fully resolved correlation experiment, in the spirit of the PCR-COSY. These spatially encoded experiments can have a lack of sensitivity due to the fact that the NMR signal comes from only a part of the sample and not from the whole sample. A gain in NMR sensitivity can be obtained by exploiting the *para*-hydrogen technique, for instance. A dedicated experimental apparatus is available within the team.

3) Conformational analysis of (bio)-compounds using NMR in chiral oriented solvent

The project is to apply this methodology on compounds structurally more and more complex in terms of number of flexibility. Couples of non-rigid enantiomers will also be tested. If in PBLG mesophase, the chirality of the phase induces a difference in the conformational potential it will allow us to observe two different conformational behaviours for both enantiomers. If no difference is observed, the measurements obtained on both enantiomers spectrally differentiated will increase the number of experimental data to determine more accurately the conformational potential.

Self-assessment document

Team 7 - ECI

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Chimie Inorganique**
Acronym:	**ECI**
Director's name (current contract):	**Talal MALLAH**
Director's name (future contract):	**Ally AUKAULOO**

SELF-ASSESSMENT DOCUMENT

Scientific policy

1 Research products and activities (to be filled first for the unit and then for each team or theme)

The Inorganic Chemistry team (https://www.icmmo.u-psud.fr/Labos/LCI/) focuses on the development of materials that possess original and smart chemical and physical properties in order to address societal challenges in the area of sustainable energy, information storage, new electronic materials and medicine. We design materials at the molecular and the nanometric scale using organic chemistry, coordination chemistry and soft chemistry. We use different characterization tools including large instruments (Synchrotrons SOLEIL and ESRF, Laboratoire National des Champs Magnétiques Intenses at Grenoble and the National High Magnetic Field Lab at Tallahassee-USA) in order to investigate the physical properties of our systems. We rely on theoretical calculations (*ab initio*, DFT) to rationalize our experimental results and as guide for the design of new systems with targeted chemical and physical properties.
The members of the team (see organizing chart in section 2) published 150 articles in international peer-reviewed journals with an average impact factor of 5.365. This corresponds to a number of 2.93 publications/ETPC/year. The members of team were invited to 46 conferences among them 26 out of France. They gave 46 invited seminars in French and Foreign laboratories.

Scientific output

In the following, we present a focus on our results; the name of the PI of each project is highlighted.

1-Artificial photosyhnthesis (**A. Aukauloo**, Z. Halime, M. Sircoglou)

The focus of the thematic of Artificial Photosynthesis is to use solar energy to extract electrons and protons from water coupled to the production of H_2 or the reduction of CO_2. In order to reach these targets, we develop molecular complexes and molecular assemblies to capture and convert solar energy to realize charge accumulation and therefrom perform multi-electronic catalysis. The main discoveries from our group in the domains are as follows:

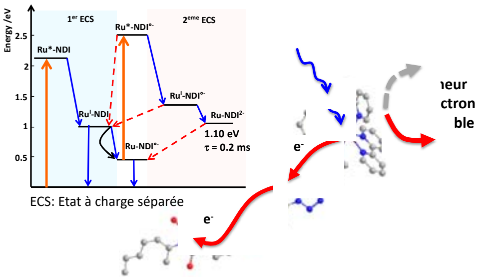


Figure 1. Energy levels for the Ru-NDI sequential charge transfer

To date, only a few studies have addressed the question on deciphering the stepwise process of charge accumulation in artificial systems. We have chosen a molecular dyad containing a naphthalenediimide (NDI) moiety that can act as a reversible reservoir for two electrons linked to a $[Ru(bpy)_3]^{2+}$ chromophore (Fig. 1), abbreviated as Ru-NDI. We have, in collaboration with a team from Institut des Sciences Moléculaires d'Orsay (ISMO; Univ. Paris Sud/ Paris-Saclay), developed for the first time in France a pump-pump probe set up in order to address this challenging issue on tracking a two-electron charge accumulation. We have successfully been able to decipher the kinetics for the constructive and deleterious pathways upon the sequential accumulation of two electrons (Fig. 1). (Work highlighted in *En direct des labos de l'INC* http://www.cnrs.fr/inc/communication/direct_labos/aukauloo6.htm.

In Photosystem II, a special pair of amino acids the TyrosineZ and Histidine 180 acts as electron relay between the photoactive units (P680) and the Oxygen Evolving Complex (OEC), the Mn_4Ca cluster. Since the last X-ray structure of Shen (Nature 2011), it was proposed that these two amino acids could also act as a proton exit from the OEC and not only a sheer electron relay functioning following a former proposal termed as the 'rocking proton mechanism'. In this reported model, we found that water is playing the role of a gatekeeper for a one-electron two-proton transfer from the imidazole-phenol (Fig. 2). A proton is expelled from the phenol ending its journey in the porphyrin chromophore. This study constitutes the starting point for further analysis of the fate of protons in both models of PSII and the natural enzyme. (Angew. Chem. Int. Ed. **2018**, 10.1002/anie.201804498).

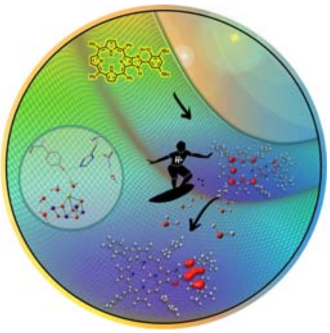


Figure 2. Water gating an E2PT process

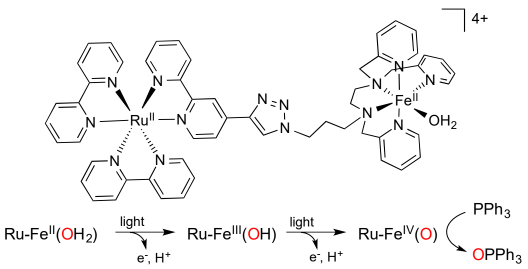


Figure 3. Ru-Fe dyad for the photoactivation of water

In Artificial Photosynthesis, water stands as the source of electrons and protons. We have been investigating on the possibility to use water to photogenerate an Fe^{IV}-Oxo, a highly oxidizing species, starting from an Fe^{II}-OH$_2$ complex. The system developed in collaboration with F. Banse is shown in Fig. 3. It consists of a chromophore-Fe(II) catalyst. We have been able to evidence the formation of the chromophore- Fe^{IV}-Oxo intermediate (Fig. 3). The latter was able to transfer its oxygen atom to an organic substrate. This result is a proof of concept that water can be used to supply the O atom in oxidation of organic substrates. (Chem. Sci. **2015**, *6*, 2323; highlighted at the *Journal du CEA-Saclay* 2015).

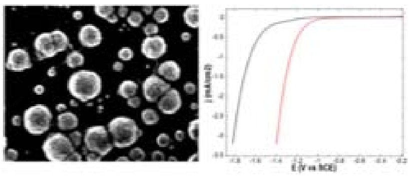


Figure 4. Nanoparticles of Ni from a molecular nickel complex

There is an urgent need in developing cost-effective catalysts for the production of H$_2$ in order to troubleshoot the issues with the use of noble metal such as platinum as catalyst for the production of H$_2$. In a previous study from our group on cobalt complexes, we evidenced that the molecular complexes suffered electrochemical alteration to end in the formation of highly catalytic nanoparticulates. We have studied the nickel glyoximato complexes with this mindset. We have shown that the glyoximes ligands are the preferential centers for the addition of both electrons and protons leading to the departure of the molecular system to nickel based nanoparticles, that were acting as efficient catalyst for the H$_2$ production (Fig. 4). This study is a cautionary tale on the intimate nature of the catalytic species in the field of molecular catalysis for H$_2$ production.

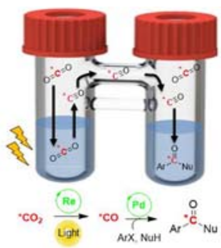


Figure 5. Two chambers device for CO$_2$, reduce, reuse, recycle

In the field of CO$_2$ reduction, we have investigated as the proof of concept of CO$_2$ valorization strategy based on its photocatalytic reduction to CO and the direct use of the produced CO in a palladium-catalyzed aminocarbonylation reaction (Fig. 5). This approach provides a means for more efficient application of ^{13}C-isotope and ^{14}C-radioisotope-labeled CO$_2$ in pharmaceutically relevant drug labeling. This work was carried out in collaboration with the Laboratoire de Marquage au Carbone 14 Institut des Sciences du Vivant Frédéric-Joliot, CEA-Saclay. (ChemPhotoChem **2018** 10.1002/cptc.201800012).

2-Bioinspired nonheme molecular and supramolecular Fe complexes (**F. Banse**, J.-N. Rebilly, K. Sénéchal-David)

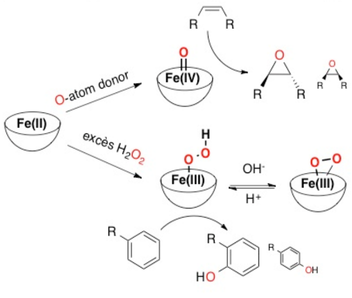


Figure 6. Generation and reactivity of reaction intermediates

As an alternative to the conventional methods implementing harmful reactants and/or harsh conditions, our general approach aims at developing iron complexes as catalysts for the oxidation of small organic molecules by mild oxidants (H$_2$O$_2$, O$_2$). Starting from these complexes, reaction intermediates such as high-valent iron-oxo and iron-(hydro)peroxo can be obtained either using (i) chemical oxidants or (ii) O$_2$ in the presence of a stoichiometric amount of chemical reductant. These intermediates are active for the oxidation of several organic substrates (Fig. 6). Nonetheless, two limitations remain: 1) these species may display a lack of selectivity and efficacy, and 2) transposing the stoichiometric activation of O$_2$ into a catalytic process requires controlling the delivery of the electrons, in order to avoid the unproductive reaction of the oxidizing intermediates with the reductant. To overcome these drawbacks, we get inspiration from metalloenzymes that perform the fast and selective oxidation of their substrates by O$_2$, where (i) the active site contains some aminoacids that anchor the substrate and some other in the second coordination sphere of the metal center that promote the formation of the reaction intermediates; (ii) the oxidation of the substrate by O$_2$ is coupled to a controlled input of electrons.

Supramolecular systems and second coordination sphere. We have developed an original system in which the catalytic unit (iron complex) is covalently linked to a substrate binding pocket (calixarene capped by a trisimidazole Zn complex, Fig. 6). We have shown that the reactivity of the Fe complex and the host-guest properties of the Zn-calixarene moiety are interlocked: encapsulation of a linear alkylamine alters the Fe coordination sphere and thus promotes the formation of the Fe^{IV}O, mirroring an allosteric effect that is ubiquitous in metalloenzymes but for the first time in a model system (coll. O. Reinaud, Univ. Paris Descartes; Inorg. Chem. **2013**, *52*, 69; Chem. Eur. J. **2017**, *23*, 2894; N. Ségaud PhD thesis).

Along the same line, we have developed artificial metalloenzymes by inserting, covalently or not, metal complexes in a protein. We have reported the use of these systems as catalysts for the oxidation of sulfides by H_2O_2 or their photoinduced oxidation by water (Dalton Trans. **2016**, *45*, 706; Catalysts **2016**, *6*, 202; coll. J.-P. Mahy, ICMMO; C. Buron PhD thesis).

The 2nd coordination sphere also plays a synergetic role with Fe in O_2/H_2O_2 activation. We have appended a non-coordinating amine to a conventional Fe^{II} complex, thus drastically modifying its reactivity with H_2O_2 (Fig. 7). Whereas conversion of Fe^{II} to $Fe^{III}(OOH)$ is usually observed, appending the 2nd sphere amine results in a direct conversion of Fe^{II} into $Fe^{IV}O$. The amine acts as a proton shuttle between the proximal and distal oxygen atoms of Fe^{II}-bound H_2O_2, allowing O-O bond cleavage, thus mimicking the role of histidine in peroxidases (coll. F. Avenier, ICMMO; J. Am. Chem. Soc., under revision).

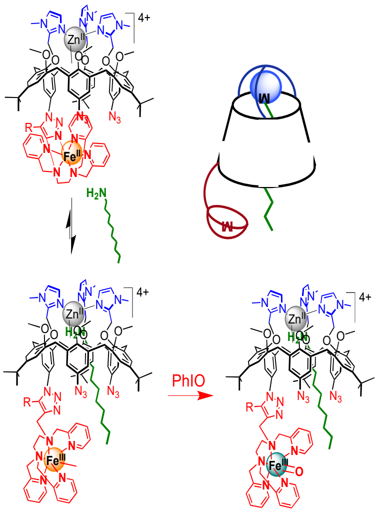


Figure 7. Structure and reactivity of the supramolecular Zn^{II}-Fe^{II} complex

Reductive activation of dioxygen by Fe^{II}. To decipher the mechanism of the reductive O_2 activation by Fe^{II} centers, we used cyclic voltametry as an analytical tool and as a way to deliver electrons to the system. After determination of electrochemical signatures of the possible $Fe^{IV}O$, $Fe^{III}(OOH)$ and $Fe^{III}(OO)$ intermediates isolated at low temperature (for the two latter, these are the first and unique data reported in the literature for non-heme complexes), we have performed a thorough cyclic voltametry study of the reaction between an Fe^{II} complex and O_2. The voltamograms of O_2 / Fe^{II} samples of various composition have been simulated according to a mechanism involving the above-mentioned intermediates (Fig. 8). The mechanism shows some similarities with that frequently reported for porphyrinic complexes, but most importantly, it provides guidelines to improve our systems to develop electro-assisted catalytic reactions. (coll. E. Anxolabéhère, Univ. Paris Diderot; Chem. Sci. **2015**, *6*, 639; N. Ségaud PhD thesis). We have reported a related study using a porphyrinic Fe complex during the same period (Inorg. Chem. **2016**, *55*, 12204).

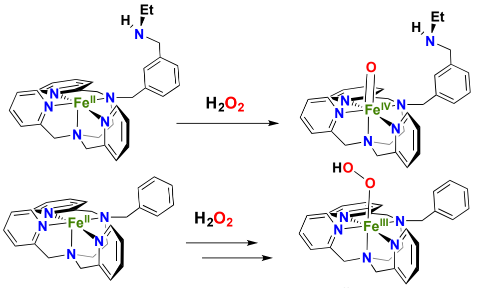


Figure 8. The reaction between Fe^{II} and H_2O_2 is triggered by second sphere interactions

3-Magnetic and photomagnetic hybrid (nano)materials (**A. Bleuzen**, A. Bordage, G. Fornasieri)

Molecular (photo)magnetic materials offer appealing perspectives towards high-density data storage. Nevertheless, the bistability properties are usually observed at low temperature and the compounds are obtained in powder or single-crystal forms. Therefore, their integration into devices for genuine application necessitates i) a better understanding of the photo-induced phenomena in order to push up the operating temperature from below 150 K to room temperature, ii) the development of manufacturing processes that would allow exploiting the bistability properties at the nanoscale in a real device and iii) the knowledge and mastering of the effect of the processing step at the nanoscale on the switching properties. In this context, we are engaged i) in the fundamental study of photomagnetic Prussian blue analogs (PBA) and the CoFe PBA constitute for us a series of model compounds and ii) in the use of porous sol—gel oxides as hard templates to elaborate nanocomposites which would allow studying and then exploiting the properties of the functional coordination polymers in real applications.

Regarding the fundamental study of the photomagnetic effect in Prussian blue analogs (PBA), our understanding of the role played by the redox potential of the transition metal (TM) ions involved in the electron transfer led us to evidence a magnetic switching triggered by a proton coupled electron transfer (PCET) assisted by long-range alkali cation transport in the alkali cation free CoFe PBA (J. Am. Chem. Soc. **2014**, *136*, 6231)**.** PCET reactions constitute a key point in contemporary challenges such as energy conversion and have been intensively studied in solutions, proteins, and electrochemistry. To our knowledge, this is the first example of PCET reactions in a porous coordination polymer with such spectacular changes in the magnetism. The adjustment of the bistability temperature range goes through the fine-tuning of the redox potentials of the TM ions, which can be achieved by gently distorting the Co-NC-Fe linkages, for instance by applying an external pressure. The quantification of such slight structural distortions hardly detectable by standard techniques is therefore crucial. By studying the effect of an external pressure on a series of NiFe PBA, we have shown that X-ray Magnetic Circular Dichroism (XMCD) at the TM K-edges is a relevant technique to quantify such distortions (J. Phys. Chem. C **2013**, *117*, 19645)**.** A CNRS researcher, A. Bordage, has been recruited to carry out the ambitious project aiming at establishing a quantitative link between XMCD signals and photomagnetic effect.

Regarding our strategy based on the use of sol-gel oxides to integrate the functional coordination polymers into real devices, we have shown that i) ordered mesoporous silica monoliths constitute a relevant versatile platform for the study of the processed (photo)magnetic PBA nanoparticles (Eur. J. Inorg. Chem. **2017**, 1303) and ii) a macroscopic magnetic anisotropy can be induced by the combined control of size, shape and organization of NiFe PBA nanoparticles in an ordered mesoporous silica monolith opening up new opportunities for the development of original nanostructured materials exhibiting anisotropy in their properties at the macroscopic scale (Fig. 9) (ChemNanoMat **2017**, *3*, 833)**.**

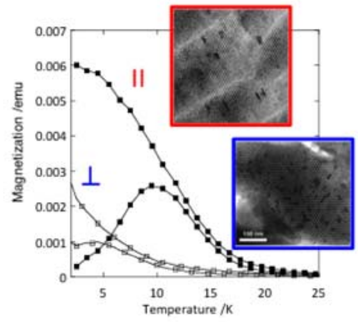


Figure 9. Magnetic anisotropy of the NiFe nanoparticles within the ordered mesoporous silica monoliths

4-Spin-crossover molecular and (nano)materials (**M.-L. Boillot**)

Matrix effect. Recent works focusing on the relationship between the cooperativity of spin transition and the particle size have provided general trends and a few puzzling observations. The difficulty arises from the combination of other factors including the particle surface and its interaction with the surrounding environment. First, we observed that the embedding in polymeric or vitreous matrices of microcrystals characterized by abrupt transition was non-innocent. The transition curves are either shifted and smoothened or are non-reversible leading to atypical thermal hysteresis. From the magnetic study performed with physicists (coll. E. Enachescu, Univ. Iasi, Romania), it was shown that the hysteresis loop didn't result from cooperativity but from (i) particle-matrix elastic interactions (b) that were modeled by negative variable pressure effects, (ii) their cutting off (c) – restoration (a) according to the change of volume driven by the spin transition and the glass transition (Fig. 10; Appl. Phys. Lett. **2014**, *104*, 031909). At low temperature, the particle environment influences the spin switching induced by light as shown by the kinetics of the LIESST relaxation, observation also modeled with a variable pressure effect (Appl. Phys. Lett. **2016**, *109*, 031908). The matrix being active, the non-trivial question to be studied now concerns the combined effects of interface, matrix and confinement taking place in the case of spin-transition nano-objects.

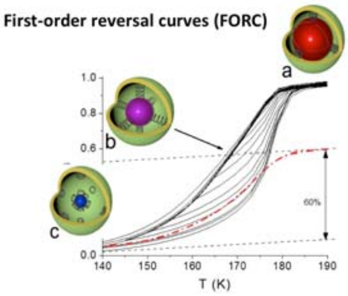


Figure 10. First-Order Reversal Curves (FORC) analysis of the hysteresis loop revealing a matrix effect rationalized with a combination of a variable negative pressure effect and the switching on/cutting off of elastic interaction.

Cooperativity. One challenge in Materials Science is to control the cooperative phase transformation occurring in solids on ultra-short time scales. Bistable spin-transition materials that may be switched with light according to the LIESST effect are good candidates for this mechanistic and dynamical study done with physicists (coll. E. Collet, IPR, ANR-13-BS04-0002 project) and theoreticians (coll. C. Enachescu, Iasi Univ., Romania, Brancusi Program). This phenomenon takes place via the coupling between the electronic change (spin multiplicity) and the molecular volume at the origin of cooperativity (Fig. 11). Therefore, the simultaneous excitation of a large number of molecules within a spin-transition material, which requires nanocrystals and a femtosecond optical technique, generates an elastic wave capable of self-amplifying the ultra-fast photo-switching of the material (Nat. Mater. **2016**, *15*, 606; http://www.cnrs.fr/inp/spip.php?article4521). This elastically-driven cooperativity triggered by a light pulse leads to an efficient route towards the generation and stabilization of photoinduced phases in volume-changing

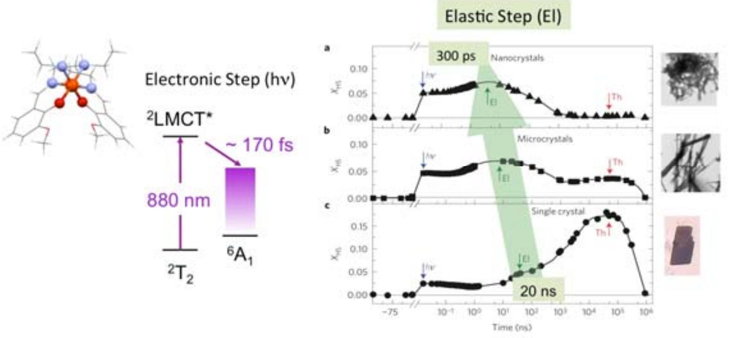
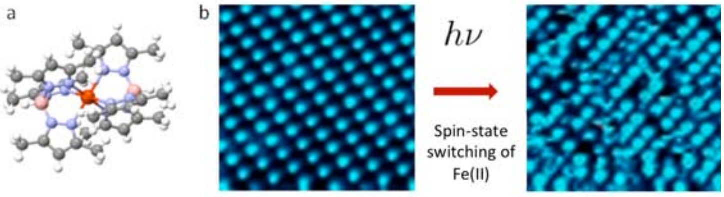


Figure 11. Dynamic characterizing the low-spin to high-spin transition triggered by a femtosecond laser pulse in an Fe^{III} spin transition material in the form of single-crystal, micro- and nanocrystals



materials.

Figure 12. STM images (4 K) showing a self-assembled monolayer of spin-crossover molecules on a gold surface and the blue light effect of the spin-state switching of Fe^{II}

Bistability at the single molecule level. Spin-crossover molecules, whose spin states switch in response to an electric field and a light irradiation, are promising for spin electronics (or integration into electronic devices). For these objectives, it is mandatory to preserve the switchability on metallic surfaces at the scale of a few molecules (or single molecule), that is scarcely observed. This question was studied with T. Mallah in the project (ANR-BLANC-12 BS10006) gathering Scanning Tunneling Microscopy (STM) specialists (V. Repain, MPQ, Paris-Diderot Univ.) and theoreticians (C. Barreteau, CEA Paris-Saclay), aiming to modulate the spin-polarized current by switching the magnetic moment of a spin-crossover molecule or vice versa. The formation of self-assembled monolayer of molecules on a gold surface was exploited to determine by STM, a local technique, the electronic structure of molecules and its change upon light irradiation. Besides the spin-state photoswitching within the monolayer and its dynamics (Fig. 12; *Nat. Commun*., **2016**, *7*, 12212; http://www.cnrs.fr/inp/spip.php?article4747), we have confirmed the S = 2 iron(II) signal and the thermal spin-crossover by X-ray Magnetic Circular Dichroism and X-ray absorption spectroscopy measurements (J. Phys. Chem. C **2018**, *122*, 727). These observations raise the question of the importance of interactions between metal surface and molecules with respect to molecule-molecule interactions.

5-Magnetic Nanosystems

5.1-Single Molecule Magnets (V. Campbell, J.-J. Girerd, F. Lambert, **T. Mallah**, E. Rivière)

Single Molecule magnets as qubits. A qubit is an object that can be described as a two-levels system, this is the case of the electronic spin in the presence of a magnetic field. For a qubit to be useful, its coherence time must be long enough in order to be able to perform a quantum calculation. We are involved in the design of molecules that possess these two characteristics. Coordination complexes are good candidates for qubits. For example, the electronic spin of a Ni(II) complex (spin S = 1) may behave as a two-levels system if one is able to design a complex where the three-fold degeneracy of the S = 1 electronic spin is lifted in such a way that the $m_S = \pm1$ levels lie lower in energy than the $m_S = 0$ level. This can be achieved for given geometry and symmetry of the coordination complex. During the last few years, we have addressed the question concerning the control of the nature and the magnitude of the zero-field splitting (ZFS) in mononuclear and then polynuclear complexes. The challenge of controlling the coherence time will be addressed later.

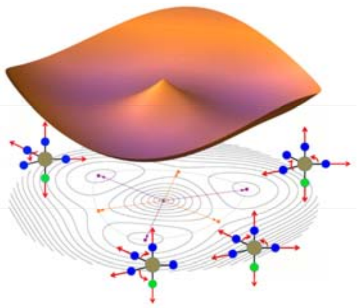
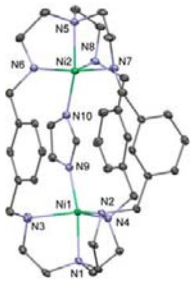


Figure 13. Representation of a moat around a Jahn-Teller C_3 crossing showing the three symmetry-equivalent minima and transition states of the trigonal Ni(II) complex

ZFS is a consequence of the simultaneous effects of spin-orbit coupling and low symmetry (axial for instance in comparison to cubic) of the coordination sphere of coordination complexes. Based on these ideas, we demonstrated that a Ni(II) complex with a trigonal bipyramid symmetry (three-fold axial symmetry) undergoes a first order spin-orbit coupling that lead to a giant ZFS and thus to very large magnetic anisotropy (Fig. 13; J. Am. Chem. Soc. **2013**, 135, 3017). The analogous complex where Ni(II) is replaced by Co(II) (S = 3/2) has the $m_S = \pm3/2$ lower in energy than the $m_S = \pm1/2$ ones leading to a blocking of its magnetization. The axial magnetic anisotropy is revealed by a magnetic hysteresis cycle at zero applied field (Chem. Sci. **2014**, 5, 3418). A deep understanding of the nature of the magnetic anisotropy was gained thanks to *ab initio* calculations carried out with the collaboration of N. Guihéry from Toulouse University.

To perform quantum calculation, it is necessary to build a quantum gate. One possibility to do so is to couple two qubits in order to achieve entanglement. This can be done by designing a binuclear Ni(II) complex where two the two Ni(II) ions are antiferromagnetically coupled and where each Ni(II) ion possess a large ZFS (Fig.14). Such binuclear Ni(II) complex was prepared using a bis-macrocyclic ligand that imposes a pentacoordinate sphere around the Ni(II) ions with a geometry close to the trigonal bipyramid necessary to keep the large uniaxial anisotropy and thus the qubit behavior. The molecule showed all the basic properties to behave as two entangled qubits (Inorg. Chem. **2017**, *56*, 10655). We are now measuring its coherence time.



Single-molecule magnets on magnetic surfaces. In the perspective of addressing a small collection of molecules and ultimately a single molecule, we developed a strategy for grafting magnetic coordination complexes on the ferromagnetic Fe_3O_4 substrate. Its consisted of designing Ni(II) and Co(II) complexes with organic ligands bearing phosphonate groups able to simultaneously coordinate to the metal ions and to the oxide substrate as depicted below. The structure of the complexes ensures the orientation (to some extent) of the molecules on the substrate necessary to preclude a random distribution of their magnetic axes relatively to the substrate surface. X-ray Magnetic Circular Dichroism at the metal $L_{2,3}$-edges studies performed at SOLEIL on a sub-monolayer of the molecules reveals the presence of a hysteresis cycle of the Co(II) complex (Fig. 15); Nat. Comm. **2016**, 7, 13646).

Figure 14. View of the structure of the binuclear Ni(II) complex

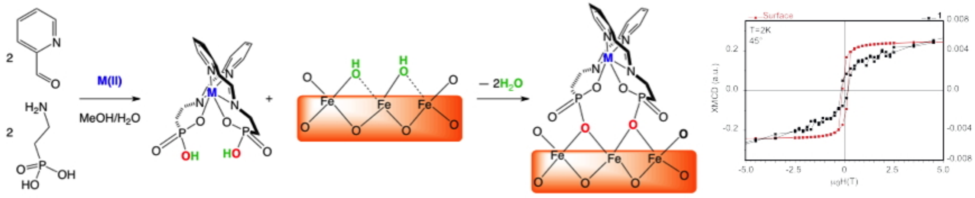


Figure 15. Schematic view of the complex formation and its grafting on the iron oxide substrate (left) and XMCD hysteresis loop on the Co and the Fe edges showing an opening of the loop for the Co complexes

5.2-Coordination Nanoparticles (**L. Catala**, **T. Mallah**, S. Mazerat)

Size and magnetic properties control of coordination nanoparticles. The separation between the nucleation and the growth processes in Prussian blue analogue nanoparticles allows controlling the size of the objects at the molecular level. We demonstrated the controlled growth of particles based on CsNiCr from 6 to 30 nm keeping the same shape and aspect ratio (Fig. 16). It was then possible by thoroughly studying and analyzing their magnetic properties to experimentally determine the magnetic single domain size found equal to 20 nm. Beyond this size the objects possess a magnetic multi-domain behavior (Adv. Funct. Mater. **2014**, 24, 5402).

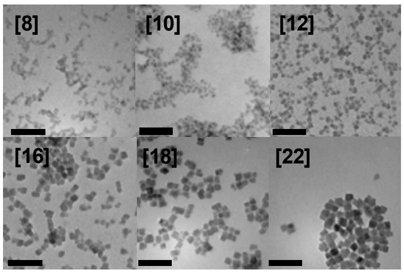


Figure 16. TEM images of the CsNiCr nanoparticles; scale bar = 100 nm.

Coordination nanoparticles for imaging. A new theme has been developed within the laboratory, focusing on the design of nanoparticles within 5 nm size by a green process leading to a preferential localization of active ions (Gd(III), Mn(II)) at the nanoparticles' periphery. This strategy allows exalting the longitudinal relaxivity of the nanoobjets by optimizing the proportion of these ions. Rapid cell internalization was demonstrated by confocal fluorescence microscopy when the nanoparticles were coated with a fluorescent polymer (Dextran-TRITC). The strong stability of the Prussian blue analogues severely limits the ions release.

Excellent contrasts in T1 are obtained at low concentration in active ion and this even at high magnetic field, well beyond the performance of clinical agents (Fig. 17; Chem. Commun. **2014**, *50*, 6740). Preliminary *in vivo* tests were carried out.

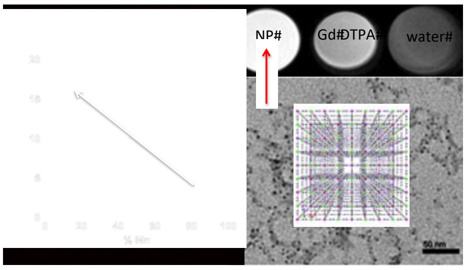


Figure 17. Confocal Fluorescence Microscopy showing cell internalization of MnInFe NPs and evolution of longitudinal relatixivity depending on the Mn content and high T1-weighted contrast for the NPS, GdDTPA (0.2 mM of GdIII for both) and water and TEM micrographs

6-Photochromism and photo-switchable systems (A. Léaustic, **P. Yu**)

Our research mainly focuses on the design of novel photo-responsive systems by using photochromic molecular switches, especially those derived from the very popular family of organic photochromes called diarylethene. A wide range of functions and properties can be potentially photo-controlled by the reversible structural changes of such switches. Coordination chemistry offers a particularly appealing playground as use of appropriate photochromic ligands would provide a convenient way to design novel metal complexes displaying various photo-switchable functions or properties. We have synthesized a ter-thiazole-based photochromic ligand capable of reacting with different metal ions due to the presence of a salen-like cavity (Fig.18a). Such a photochromic ligand is particularly appealing as it combines two competing photochemical processes: the expected 6π electrocyclization and cycloreversion that switches the ligand between its two thermally stable open form (OF) and closed form (CF) and an ultrafast ESIPT (Excited State Intramolecular Proton Transfer) process endowing the open form (OF) with a large Stokes-shifted fluorescence. Although its copper and nickel complexes are found to show neither photochromism nor fluorescence, a combined theoretical and experimental study allowed us to identify the MLCT as the main inhibiting factor (Chem. Eur. J. **2014**, *20*, 12279). In a stark contrast, the zinc containing complex is found to be both photochromic and fluorescent. Moreover, an interesting light-induced release and uptake of zinc(**II**) ions in solution is clearly demonstrated and this process is also accompanied by a reversible fluorescence modulation (Fig. 18b). Theoretical calculations support the very large difference observed in the coordinating ability toward the zinc(**II**) ion between the open and closed forms, and suggest the potential of such ligands in the photo-regulation of concentration of different metal ions in solution (Chem. Asian J. **2017**, *12*, 853).

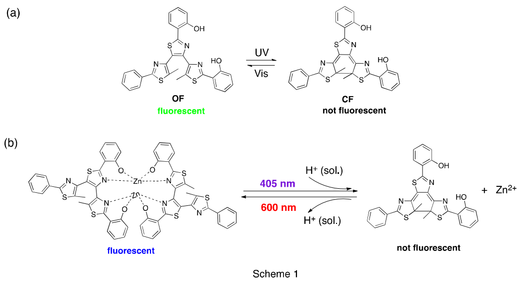


Figure 18. (a) Schematic view of a photochrom whose fluorescence is different in the open and closed form and (b) example of Zn^{II} release

7-Carbon nanotubes with targeted electronic properties (**V. Huc**)

Carbon nanotubes from calixarene. We developed, for the first time, the synthesis of short segments of carbon nanotubes of "zig-zag" geometry, with controlled diameters (Fig. 19, in red). We use Calixarenes as templates (Chem. Eur. J. **2016**, *22*, 3105). This opens up real prospects for the total synthesis of carbon nanotubes of perfectly defined electronic properties "a priori".

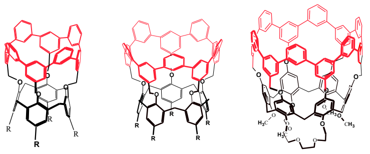


Figure 19. Examples of carbon nanotubes segments with “zig-zag topology

Coordination nanoparticles for CVD carbon nanotube growth. We have developed, with L. Catala, a new approach for the preparation of nanoalloys for CVD growth of carbon nanotubes. Pyrolysis of PBA nanoparticles self-assembled films leads to nanoparticles of metal alloys and then by a CVD process to very high-quality carbon nanotubes (Fig. 20; Carbon, **2017**, *123*, 583). This is the first clear demonstration of the growth of carbon nanotubes from well-defined metal alloys. This new approach could eventually allow the control of the structural and electronic properties of carbon nanotubes during the growth process.

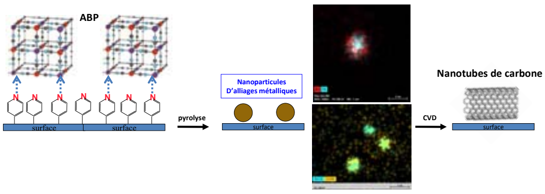


Figure 20. Coordination nanoparticles catalysts self-assembled on a substrate for the growth of carbon nanotubes

Highlights

ANR JCJC. The ANR *MagDiDi* « Photomagnétisme et distorsions structurales – Le mystère levé grâce au XMCD dans la gamme des X durs » (ANR-17-CE29-0011, 01/01/2018 – 31/12/2021 (212 247€)) was awarded to A. Bordage. A. Bordage joined the team during the past five-year plan. This project will provide her the support to develop her ambitious project that aims at quantifying small structural distortions from transition metal K-edges X-ray Magnetic Circular Dichroism (XMCD) and bring a fundamental understanding of this spectroscopy. This is a necessary step towards the design of room temperature photomagnetic materials and thus a prerequisite for devices and applications.

Blaise Pascal International Research Chair. The chair was awarded to Pr. E. Coronado in 2014 upon the proposal by T. Mallah, P. Seneor (Unité Mixte de Physique, Univ. Paris-Saclay) and A. Proust (Institut Parisien de Chimie, Sorbonne-Univ.). Pr. Coronado spent 12 months (2014-2016) in the Region Ile de France and gave several seminars on different subjects in the area of molecular magnetism, molecular spintronics and 2D materials. He also gave a series of lectures in Master 2 classes. His presence allowed the organization of the "VIII European School on Molecular Nanoscience" in Paris (http://www.icmol.es/esmolna2015/), aimed at promoting interactions between young master 2 and PhD students with experienced researchers. The presence of Pr. E. Coronado was an excellent opportunity to strengthen the links between his research group and several Ile de France groups by the exchange of mainly PhD students.

Strategic Research Initiatives of Paris-Saclay University. MOlecules and Materials for the ENergy of TOMorrow (MOMENTOM) is one of the selected projects of the Paris-Saclay SRI (http://cearc.fr/content/projet-momentom-irs-paris-saclay-2017-2020). It gathers 26 research laboratories and 10 institutions that will focus their research efforts to address two aspects within the "New energies and society" challenge: (i) using cell fuels to convert chemical energy into electric power and vice-versa and (ii) developing new materials to convert solar power into electric power/solar. A. Aukauloo is involved in the organization and the promotion of the project.

4-Technology transfer (Fig. 21). During the past period two start-ups (AJELIS (http://www.ajelis.com/), September the 23rd 2014 and NOVECAL (http://www.novecal.com/) March the12th 2018) were created by V. Huc and his colleagues. AJELIS is specialized in the preparation of fiber-based filtering materials for the recovery of pollutants and strategic metals from industrial water, while NOVECAL aims at producing catalysts with excellent efficiency and high and reproducible metal content that are easy to eliminate. The active molecules in these materials are based on calixarene whose size can be easily tuned and that can be produced in high yield. The research involving these molecules that were designed and prepared in our laboratory by V. Huc had a completely different aim, but were found to have a high added-value that justified the transfer of knowledge from fundamental research to real applications.

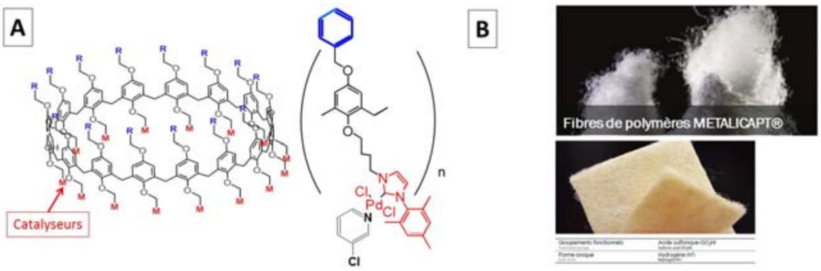
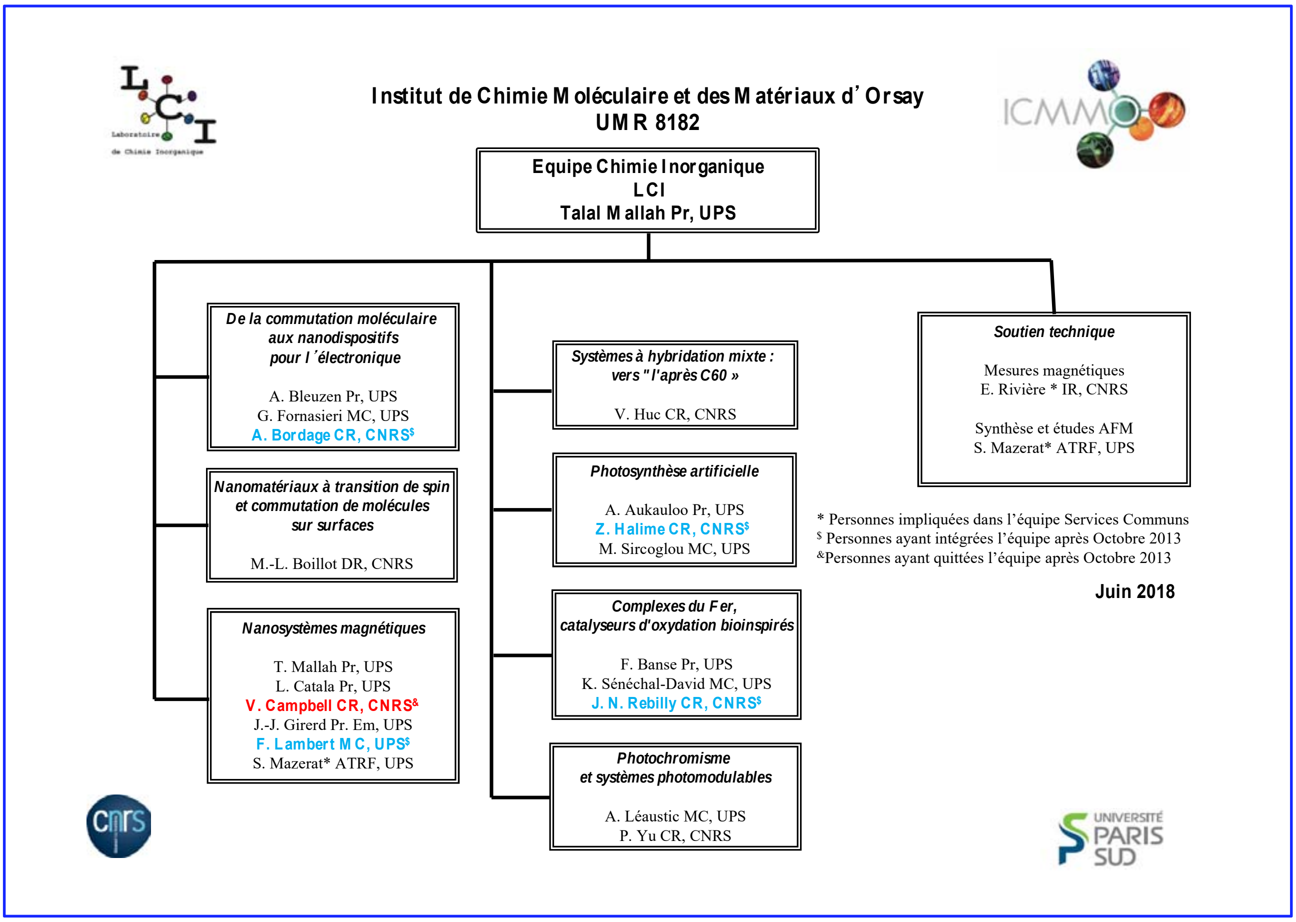


Figure 21. (A) Catalysts supported by calixarene macrocycles marketed by NOVECAL and (B) fibers for cations extractions based on calixarenes marketed by AJELIS

5 Organisation and life of the research unit (or the team/theme if relevant)

The team (https://www.icmmo.u-psud.fr/Labos/LCI/) is organized in 7 groups as schematized below.



Four permanent persons (3 CR and 1MCF; in blue) joined the team and one CR (in red) left the team during the 2013-2018 period.

Departures		Arrivals	
V. Campbell	October 2014	A. Bordage	January 2014
		Z. Halime	October 2016
		J.-N. Rebilly	January 2016
		F. Lambert	Januray 2018

Despite this organization in groups, there are intergroup research projects as can be seen from publications and from the projects proposed for the next period.

There are continuous scientific meetings within and between the groups on ongoing projects. At the level of team, there is a meeting every two weeks including post-docs, PhD students and internships students with two parts: (i) discussing any problem that may have arisen during the last two weeks followed by (ii) a quasi-formal scientific presentation by in most cases a post-doc or a PhD student.

Every month, we invite an external scientific personality to give a seminar.

Several meetings gathering permanent researchers are planned within the year to discuss several issues related to equipment acquisition and particularly to define policy for PhD recruitment and proposals to recruit CNRS researchers or faculties when a position is available.

T. Mallah, the actual responsible of the team, will be replaced by A. Aukauloo, Professor at the University, for the next period.

6 SWOT analysis

Strengths	Weaknesses
↑Success in ANR projects (14 for the past 5 years) ↑Technology transfer and creation of two start-ups ↑Strong collaborations with physicists and biologists within Paris-Saclay and at the international level ↑State-of-the-art research in renewable energies and single-objects information storage	↓Weak participation to European projects (only 1) ↓Very few ANR projects as coordinator (only 2/14) ↓A slight decrease of the number of publications ↓Difficulty to keep foreign young CNRS researchers (one departure) ↓Absence of a specialist in theoretical calculations
Opportunities	**Risks**
✳Develop new ambitious risky research projects ✳Use in-lab expertise to address highly challenging and contemporary research areas ✳Benefit from the Paris-Saclay dynamics to enhance international visibility ✳Recruit a young CNRS researcher	★Random success in projects at the national level ★Overwhelming administrative tasks ★Losing focus on long term research targets ★Lack of University politics for PhD recruitment

7 Scientific strategy and projects

For the next 5 years the team will mainly focus on the following challenges:

1. developing efficient molecular catalysts for the selective reduction of CO_2 in a first place to CO,
2. achieving the reductive activation of dioxygen via the modulation of molecular and supramolecular properties of non-heme Fe complexes for the development of electro-assisted oxidation catalysis,
3. developing of a new transition metal K-edge X-ray Magnetic Circular Dichroïsm tool that enables reaching a photomagnetic effect at room temperature for high-density information storage,
4. designing single layers of switchable molecules in contact with metallic surface that can be addressed by an electric field,
5. designing coordination complexes that behave as qubits for quantum computing devices
6. developing new conducting/ferromagnetic two-dimensional (2D) coordination networks
7. designing coordination nanoparticles for theranostics and gas sensors
8. designing suitable photochromic systems for the photo-regulation of the concentration of different metal ions, in particular those involved in various biological processes,
9. designing photochromic molecules as spacers in light controlled spintronic devices
10. designing and synthesising of ring-like conjugated molecules as precursors for the total synthesis of carbon nanotubes with targeted electronic properties.

<u>1-Artificial photosyhnthesis (**A. Aukauloo**, Z. Halime, M. Sircoglou)</u>

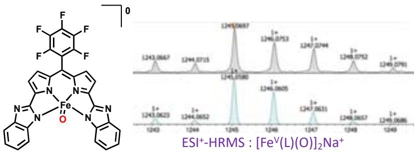


Figure 22. Fe(V)=O species intercepted in mass spectrometry

For the coming five years we will focus on three main topics based on the advancement realized during the last period, in line with an ongoing **ANR project Multiplet** (PI: A. Aukauloo), aiming to develop an autonomous photocatalytic system coupling a dyad for the light activation of water and a laccase, an enzyme that reduces O_2 to H_2O. Our task here is to develop robust molecular complexes for activating metal-aquo complexes to their corresponding metal-oxo derivatives through a two-electron and two-proton abstraction using a photosensitizer. We have designed new tetradentate ligands holding a dipyrrin motif, a feature from the porphyrin chemistry, to stabilize highly oxidized metal oxo species (Fig. 22). Preliminary results have already comforted the chemical generation of an iron(V)-oxo species as depicted below. We will perform a full-fledged investigation on the spectroscopic and reactivity pattern of such species. Our target will be to photogenerate such reactive species using light and water as sole sources of energy and oxygen atom donor respectively. Z. Halime has joined the laboratory in October 2016 as a CR1 CNRS researcher on the theme of CO_2 reduction, with the target to develop efficient molecular catalyst for the selective reduction of

CO_2 in a first place to CO. In order to reach this target, we are developing porphyrin based catalysts holding different functions that would help in the activation of the substrate. Preliminary results are supportive for this strategy and a noticeable shift of the over-potential for the CO_2/CO transformation by 500 mV has been evidenced (Fig. 23)!

Following our investment in the set-up of a pump-pump probe experiment in collaboration with Dr. T. Pino (ISMO Univ. Paris Sud/Paris-Saclay) to investigate the charge accumulation processes, we will pursue our effort to use this unique technique to interrogate photocatalytic two-electron transfer processes such as O_2, H_2O and CO_2. These fundamental studies will provide indispensable knowledge for the design of efficient photocatalytic systems. Indeed, we want to gain a complete map of the various constructive and deleterious pathways upon photo-activation of the catalysts.

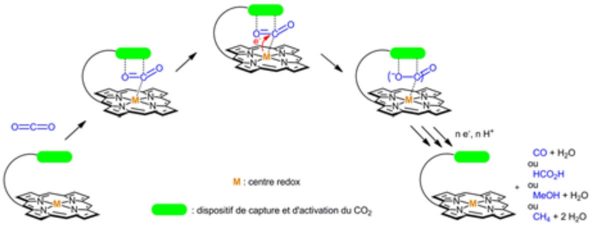


Figure 23. Metalloporphyrins decorated with secondary activating functions for CO_2 reduction

We are also devoted to develop intra-lab and inter-lab projects in ICMMO. We are currently collaborating with the group of A. Bleuzen to develop Prussian Blue Analogues (PBA) confined in mesoporous silica for the generation of new photocatalytic materials for water splitting.

Our approach consists in the formation of controlled PBA nanoparticles and therefrom upon oxidation leads to the formation of catalytic metal oxides particles. We demonstrated that under visible light in presence of a photosensitizer and an electron acceptor we can perform the photo-oxidation of water (Fig. 24). We will pursue our effort with the defining target to reach heterobimetallic metal oxides with very efficient catalytic properties.

In collaboration with E. Schulz (ICMMO), we are currently developing supramolecular assemblies of a photosensitizer and a catalyst to perform photocatalytic asymmetric epoxidation of alkenes with water as the oxygen atom donor.

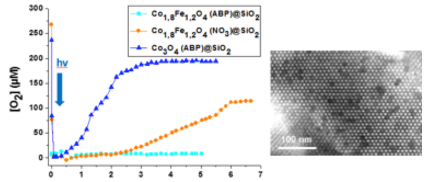


Figure 24. Nanoparticles of Co_3O_4@SiO_2 for photooxidation of water

2-Reductive O_2 activation. Modulation of molecular and supramolecular properties of non-heme Fe complexes: towards electro-assisted oxidation catalysis (**F. Banse**, J.-N. Rebilly, K. Sénéchal-David)

Our recent results on the determination of the reductive O_2 activation mechanism provided guidelines to design much more efficient systems to activate O_2 and use them in oxidation catalysis.

The reduction potential of the Fe/O_2 adduct must be increased, for energetic reasons, and in order to avoid its over-reduction.

-*1st coordination sphere modulation*: the adduct in our reference system is best described as Fe^{II}-O_2. Addition of electron withdrawing groups (EWG) should thus enhance Fe^{II} Lewis acidity, coordination of O_2 and favor the reduction of the Fe^{II}/O_2 adduct. On the other hand, electron donating groups (EDG) should favor the Fe^{II}-to-O_2 electron transfer to yield an adduct described this time as Fe^{III}-superoxo. Additionally, after electron input into the adduct, the electronic properties of the ligands are expected to modulate the evolution of the resulting $Fe^{III}OO^-$ intermediate, leading to different active species (with different reactivities): high valent Fe^VO ensuing from heterolytic O-O cleavage (EDG) or stabilization of $Fe^{III}OO(H)$ species (EWG).

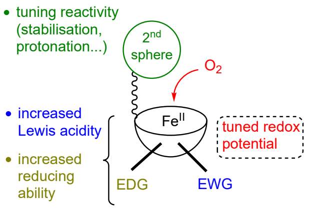


Figure 25. Schematized structure with modulation of the first and second coordination spheres

-*2nd sphere modulation*: independently from 1st sphere modulation, addition of 2nd sphere groups can favor Fe^{II}/O_2 reduction and direct the evolution of the resulting species towards O-O cleavage (pull effect). This can be achieved by adding H-bond donors, cationic groups, or Lewis acids in the vicinity of the distal oxygen atom of Fe^{II}-O_2, in order to stabilize its Fe^{III}-OO^- reduced form. We also plan to append non-innocent groups (quinones, phenols…) or redox complexes (Cu^I) as 2nd sphere groups, which could act as electron relays and redox cofactors for iron.

Simple synthetic modifications will be provided to our ligands to explore these aspects. Rationalization of the reactivity of these new complexes will be obtained by thorough electrochemical studies and simulations performed in collaboration with E. Anxolabéhère and F. Kanoufi (Univ. Paris Diderot). The new systems will be evaluated in electro-assisted oxidation catalysis of classical organic substrates (cyclohexane, cyclooctene, aromatics). Finally, these systems could be applied to supramolecular catalysis by using their 2nd sphere groups as recognition sites for more specific substrates (by H-bonding, charge-charge interaction or coordination). In that case, region-selectivity in oxidation (with O_2, H_2O_2 or O-atom donors) could be expected, as a result of substrate preorganization (Fig. 25).

3-Magnetic and photomagnetic hybrid (nano)materials (**A. Bleuzen**, A. Bordage, G. Fornasieri)

New TM K-edge XMCD tool that will enable reaching a photomagnetic effect at room temperature for high-density information storage. We showed previously that the switching temperature range of CoFe Prussian blue analogs can be tuned by slightly distorting their structure, for instance under an external physical pressure or an internal chemical pressure. We recently showed that TM K-edges XMCD is highly sensitive to such distortions and could allow for their quantification in relation with different chemical or physical parameters, which is a prerequisite for the design of room temperature photo-switching compounds. Nevertheless, the information contained in the XMCD signals at the TM K-edges is not yet satisfactorily known. Therefore, we first aim at quantifying the XMCD signals at the TM K edges by using PBA as model compounds to disentangle the information contained in the signals (**ANR JCJC;** Coordinator: A. Bordage). This ambitious project will be conducted in strong interaction with the ODE beamline scientists at Soleil and experts in X-ray absorption spectroscopy of the 'Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie' (IMPMC, Paris). Such a tool would bring new insight into magnetic systems and should interest diverse scientific communities.

Fundamental study of new materials exhibiting properties induced by the collective behavior of magnetic nanoparticles. Ordered mesoporous silica monoliths exhibiting 2D hexagonal porosity are great tools to induce anisotropy in functional nanoparticles as the particles' shape can be determined by their rather narrow (typical diameter of 5–8 nm) and long (length up to a few hundred microns) cylindrical pores. In addition, when using a mesoporous silica monolith instead of the more frequently used ordered mesoporous silica powders, a parallel organization of the pores can be achieved over whole macroscopic fragments of the monolith, in which the spreading of the magnetic anisotropy of the nanoparticles to the macroscopic scale should induce completely new properties (preliminary results in ChemNanoMat **2017**, *3*, 833).

Ordered nanostructured thin films, models of high-density recording media. We are engaged in the development of an unconventional method for the elaboration of versatile ordered nanostructured thin film made of ordered functional nano-perforated oxide films, the perforation of which are filled with functional islands made of coordination polymer, oxide or metallic alloy. The elaboration method involves surfactant-assisted sol-gel processing and self-directed heterogeneous nucleation-growth of a coordination polymer followed by a possible further transformation of the coordination polymer into the corresponding mixed metal oxide or metal alloy. The proof-of-concept has recently been established (Nanoscale **2017**, *9*, 5234) and we are now aiming i) at converting this first successful synthesis into a versatile approach in terms of chemical composition of the both components and nanostructuration, ii) at demonstrating the relevance of such an approach to prepare tailor-made functional and multifunctional materials and iii) at exploring the possibilities regarding high scale fabrication.

4-Spin crossover molecular and (nano)materials (**M.-L. Boillot**)

Spin-crossover nanoparticles. We will study of how the surface-related and the volume-dependent properties determine the spin-crossover behavior at the nanoscale. This work will be pursued with nanocrystals of molecular nature whose specificities with respect to the spin-transition nanoparticles of coordination polymers will be searched for.

Mechanism and dynamic of the spin transition. It consists in the investigation of the multi-scale processes triggered by light in spin-transition nano- and microcrystals by using femtosecond Infra-Red spectrometry (coll. M. Lorenc Univ. Rennes, J. Kubicki, Univ. Poznan). This experimental technique is expected to provide new information on the activation of the molecular vibrational modes upon the photo-, elasto- and thermo-induced processes occurring in the crystalline lattice.

Molecular spin-state switching on metallic surfaces. The topic will be developed with V. Repain (Univ. Paris-Diderot), P. Sainctavit (IMPMC, Paris and SOLEIL), C. Barreteau (CEA Paris-Saclay). We will explore the molecule-metal and molecule-molecule interactions that determine the electronic properties, the organization and the possible collective effects. For that, it is necessary to develop the chemistry of sublimable spin transition molecules assembled on different metallic substrates. Moreover, we plan to study molecule/metal interfaces whose spin state may be switched by light at high temperature by designing functionalized molecules that can be chemically anchored on metals. We will take advantage from the chemisorption to implement the light-induced transition according to the Ligand-driven light-induced spin change (LD-LISC) approach. The latter uses the structural isomerization of the ligand for modulating the ligand field and the Fe(II) spin state (coll. P. Yu).

5-Magnetic Nanosystems

*Polynuclear complexes as entangled qubits (J.-J. Girerd, F. Lambert, **T. Mallah**, E. Rivière).* Mononuclear complexes behaving as two-levels systems will be thoroughly studied by pulsed EPR and will be coupled to microwave resonators in order the assess their potential as qubits; this will be carried out in collaboration with physicists group in Spain and Italy. We will also investigate the ability of a Co^{II} mononuclear complex as a nuclear spin qubit. We have shown that the nuclear spin of Co (I = 7/2) is coupled to its electronic spin (Chem. Sci. **2014**, *5*, 3418) leading to the possibility to obtain of a qudit (d = 8). This study will be carried out on a single molecule in collaboration with the group of W. Wernsdorfer (Karlsuhe Institue of Technology, Germany). We will also design polynuclear complex as potential three-qubit systems. Preliminary results are encouraging as shown by the trinuclear Ni(II) and Co(II) complexes where each metal ion of the trinuclear unit plays the role of a two-level system and the antiferromagnetic coupling ensures entanglement necessary to build a quantum gate (Fig. 26). Inelastic Neutron Scattering and Terahertz spectroscopy are under investigation in order to determine the energy level spectra of these molecules.

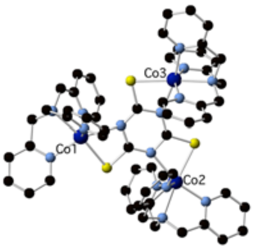


Figure 26. View of the structure of a trinuclear Co^{II} complex

*Magnetic/conductive 2D coordination networks (Z. Halime, **T. Mallah**, S. Mazerat).* The design of coordination networks confined in two-dimensions using organic ligands with delocalized π-electron systems may allow the occurrence of conductivity if an efficient electronic coupling can be achieved between the metal ions and the ligands. Along this line, we aim at developing original 2D coordination networks that combine conductivity and magnetic properties that may be used as magnetic electrodes in spintronic devices. Ultimately, we aim at isolating single layers that can be transferred to different substrates for the design of devices. Preliminary results along this direction are encouraging as shown in the Atomic Force Microscopy (AFM) image where an ultrathin film of 1.4 nm thickness and large surface area was obtained (Fig. 27). Transport studies are under investigation in collaboration with the Centre of Nanoscience and Nanotechnology (C2N) at Univ. Paris-Saclay.

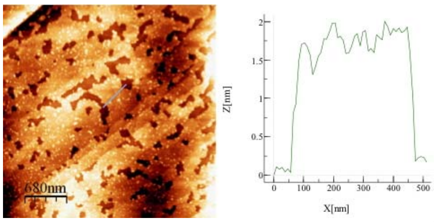


Figure 27. Atomic Force Microscopy image of a 2D coordination network with 1.5 nm thickness corresponding to 3 or 4 monolayers

*New switchable nanoparticles (**L. Catala**, **T. Mallah**, S. Mazerat).* New nanostructures associating active dies (electro, photo, thermo...) and spincrossover nanoparticles are envisaged to achieve the control of the spin transition at ambient temperature by various stimuli. In particular, insertion detection within microporous networks (NO_x, SO_x and other gases) will be targeted. Preliminary results were obtained concerning the design of core-multishell nanoparticles where two ferromagnetic networks are separated by a paramagnetic spacer leads to a magnetic coupling between the core and the outer shell that can be switched by a magnetic field (Fig. 28).

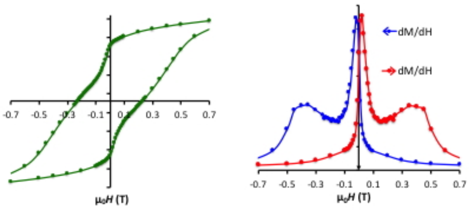


Figure 28. Magnetic hysteresis cycle of a core-two shell nanoparticles (left) and its derivative (right)

*Development of new theranostic agents (**L. Catala**).* We will design core-shell coordination nanoparticles with a core active in therapy associated with an active ion-enriched surface for MRI. The target sizes remain well below 10 nm to facilitate renal elimination. In particular, systems associating a core of Prussian blue for photo-assisted hyperthermia are being developed and optimized. Stability in physiological environments requires in particular an optimization of the coating. Another direction is the evaluation of the potential of bimetallic nanoparticles including heavy ions (Pt, Au, Pd) for use in hadrontherapy and radiotherapy. Finally, systems including the combination of these therapies with chemotherapy are envisaged, in particular for the release of drugs assisted by hyperthermia. This work will be done in interaction with specialized and recognized teams at the local level (IRS Nanotherad, Univ. Paris Diderot) and at the international level (Univ. Mons, Belgium).

6-Photochromism and photo-switchable systems (A. Léaustic, **P. Yu**)

We aim at designing suitable photochromic systems for the photo-regulation of the concentration of different metal ions, in particular those involved in various biological processes. Novel organic and coordination systems displaying photo-switchable chiro-optical responses will also be designed and prepared.

Within the **ANR project SpinFun** (2018-2021; PI T. Mallah), we will develop both light and redox sensitive diarylethene-based molecular switches targeted to be anchored on ferromagnetic substrates in order to build light and electro- sensisitive spintronic devices (coll. Unité Mixte de Physique, Univ. Paris-Saclay). The design of the molecules will be guided by theoretical calculations (Univ. de Mons, Belgium).

We will develop in the framework **ANR project Swist** (Switchable fluorescence hysteresis by light; 2018-2021; PI: Y. Pei) the design of diarylethene-based switches with desired photochromic properties and functions (coll. ENS Paris-Saclay).

7-Carbon nanotubes with targeted electronic properties (**V. Huc**)

Synthesis of conjugated molecular rings. We will continue our work on the synthesis of conjugated molecular rings, derived from cyclacènes. These compounds could indeed present remarkable electronic properties such as superconductivity in the solid state. The approach (based on the use of Calixarenes) already enabled us to reach a number of important milestones towards this goal (development of new families of Calixarenes, new Calixarenes functionalized, etc...).

Towards the total synthesis of carbon nanotubes. The synthetic strategy of the "zig-zag" carbon nanotubes segments will be generalized to "elongated" segments by adding additional aromatic units. This will pave the way for the total synthesis of carbon nanotubes of perfectly controlled structural and electronic features.

Transfer of technology. The 2013-2018 period saw the creation of two start-ups directly resulting from the fundamental work in the laboratory (in close collaboration with the CEA-Saclay in the case of the AJELIS start-up). This has resulted in the hiring of 5 post-doctoral students in indefinite contracts.

The development of these start-ups will continue to be based on the fundamental work carried out within the team (synthesis of new extractors, new catalysts, etc...).

Département d'évaluation de la recherche

Self-assessment document

Team 8 – SP2M

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Synthèse, Propriétés & Modélisation des Matériaux**
Acronym:	**SP2M**
Director's name (current contract):	**Nita DRAGOE / Jerome CREUZE**
Director's name (future contract):	**Nita DRAGOE / Jerome CREUZE**

SELF-ASSESSMENT DOCUMENT

1- Research products and activities

Scientific output

The Synthesis, Properties and Modeling of Materials team (SP2M) was created on January 1, 2014 from the two former teams of the Institute's "Materials Science" research topic: *Non-equilibrium materials* team and *Physical chemistry of the solid state*. This re-organization was motivated by our close research themes and was intended to give more coherence to the material science activities within the Institute.

A major effort has been made to disseminate our work nationally and internationally, with the publication of more than 300 articles, with a significant number in high-level international journals (Science, Nature Physics, Physics reports, Energy & Environmental Science, Journal of the American Chemical Society, Physical Review Letters...). A selection is given in Appendix 4. We note that about two thirds of our papers are published in scientific journals in the top 25% of their category and almost all (92%) in journals belonging to the top 50% of their category. Some of our articles are frequently cited: two of our articles published since 2013 are now ranked "*Highly cited papers*" by ISI Web of Science. The average impact factor of all our papers is 3.32 and the number of papers per ECTP per year is 3.61. The average citations for all our papers for the period of reference is 8.1.

Since its creation, the team consists of about 30 permanent staff and is organized into five research groups:

-**Numerical simulations** (NS) with main activities as methodological developments for the study of thermodynamics and kinetics of metal alloys, determination of the electronic and vibrational properties of complex oxides by *ab initio* calculations and the development of a realistic semi-empirical interaction model for the simulation of oxides. Some of these activities are related to experimental activities in SP2M team.

-**Functional Thin Films** (FTF) with objectives related to the synthesis and characterization of oxides thin films with controlled stoichiometry and microstructure, to the study of the relationships between synthesis parameters, structures and properties and to the determination of the stability of the obtained films.

-Functional Materials (FM) with primary activity the synthesis of functional materials at any scale, from nanoparticles and nano-structured materials to single crystals of centimeter size, and study of their properties, including electrical, thermal and magnetic as well as coupled properties, for applications such as thermoelectricity, ferroelectricity, superconductivity, etc.

-**Advanced Materials for Photonics** (AMP) with an interest in the interaction between powerful but very brief laser pulses (femtoseconds) and optical glasses, focusing on understanding the fundamental mechanisms operating in the material on the one hand and to the use of the induced optical properties, on the other hand. The innovative nature of this method comes from the fact that the beam is focused and that all the rays, coherent, can be arranged to "sculpt" the material by acting collectively: It is a kind of material science by laser in confined media.

-**Microstructure and Properties (MP) of metallic alloys** with research directions related to the understanding of the mechanisms of formation and evolution of microstructures of metals and alloys, addressed by means of experimental analyses and numerical simulations.

There are strong scientific interactions between these groups. A brief selection of important results obtained during this five-year period and illustrating the activity of the team is subsequently presented in the same order of the research groups used above.

In the **Numerical Simulations** group, we have continued to develop collaborations with the team's experimentalists both in the activity of the calculations of band diagrams and Infra-Red spectra by ab initio methods, but also by making first attempts to describe the structure of high entropy oxides.

For example, we performed a spectroscopic study of $SrTiO_3$ on Si(001) templates coupling experimental and ab initio investigations. The infrared spectra of strained samples and relaxed samples of different thickness show that both the mechanical stress and the thickness play major roles: higher energy modes evolve as soft modes in thinner strained films. Dynamical *ab initio* calculations allowed showing that the ferroelectricity is mainly due to the soft O-Ti-O bending mode which develops at the TiO_2-terminated surface of the film. Two critical parameters may be controlled to obtain this result: the thickness of the film and the in-plane strain. The thicker the film, the larger the (compressive) strain needed to develop ferroelectricity.

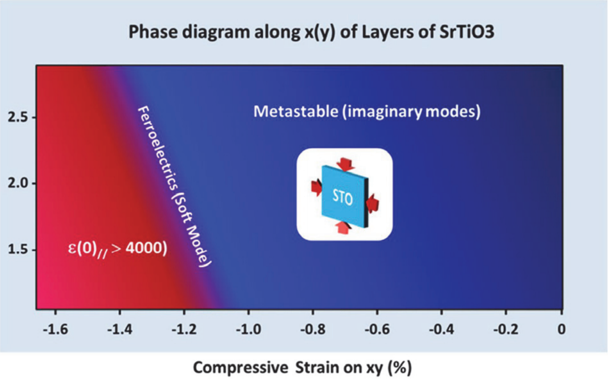


Figure 1. Phase diagram of SrTiO3.

We also conduct studies in collaboration with experimentalists from other laboratories (structure and chemistry of surface alloys, influence of small molecules on superficial segregation...). As an example, we studied bimetallic copper-gold nanoparticles at high temperature. By linking a macroscopic model to experimental HRTEM data, we show that the surface energy varies linearly with the composition in the liquid state of Cu-Au nanoalloy, i.e., it follows a Vegard's rule-like dependence. Atomistic Monte Carlo simulations using N-body interatomic potentials confirm the Vegard's rule-like behavior of the surface energy obtained from experiments combined with macroscopic modeling.

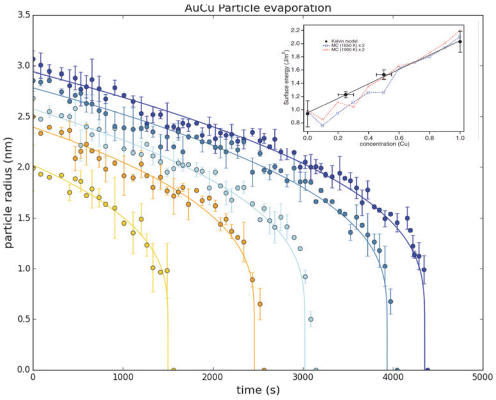


Figure 2. Evaporation curves of liquid $Cu_{50}Au_{50}$ NPs at 700 °C. Experimental data (circles), macroscopic model (full line). Inset: Surface energy as a function of Cu concentration. Experimental (black), MC simulations (red and blue).

In parallel, the group continued its core activities:

-The development of an integrated method based on ab initio calculations and up to Monte Carlo simulations to optimize the system, both in relation to structural variables (optimization of the crystalline defects structure, and more generally atomic positions) and chemical ones (optimization of the spatial distribution of the constituents of the alloy). The coupling with rigid lattice-based approaches allows determining the energetic driving forces of the studied phenomena. An original analysis on an effective lattice (effective model of site energies) leads to the characterization of the driving forces over the whole range of concentration. This lattice model allows the development of Monte Carlo simulations on a rigid lattice, giving access to unforeseeable time-space scales so far for models based on the electronic structure and taking into account atomic relaxations. As an illustration, this approach shows that phase separation is mainly driven by the elastic contribution for Au-Ni and by the chemical contribution for Ag-Cu. Furthermore, rigid-lattice Monte Carlo simulations lead to phase diagrams that are in good agreement with both those obtained by off-lattice SMA-MC simulations and the experimental ones.

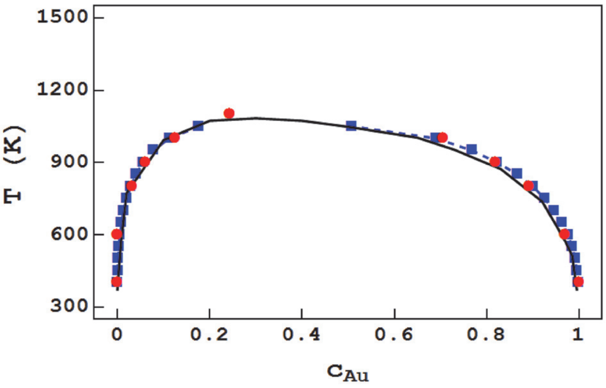


Figure 3. AuNi Phase diagram. Black : experimental, red : off-lattice, blue : rigid-lattice.

-The development of numerical tools (Mean-Field Approximation Site Kinetics, MFASK) adapted to the studies of nanoalloys kinetics. Generally nanoalloys are obtained under non-equilibrium conditions leading to metastable structures which should evolve in time towards a thermodynamically stable configuration. Detailed studies of their stability over long time scales, including their environment, are necessary to well characterize their properties. The MFASK is a powerful tool for the analysis of the kinetics and to identify the main paths of the kinetic process (Figure 4).

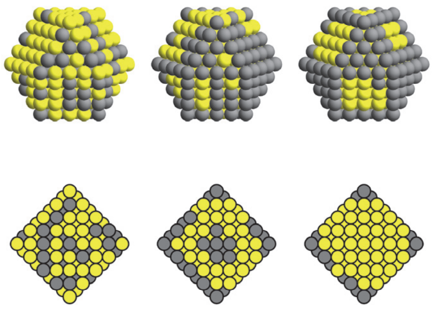


Figure 5. Time evolution of AgCu configurations. Left : random, center : onion, right : core/shell.

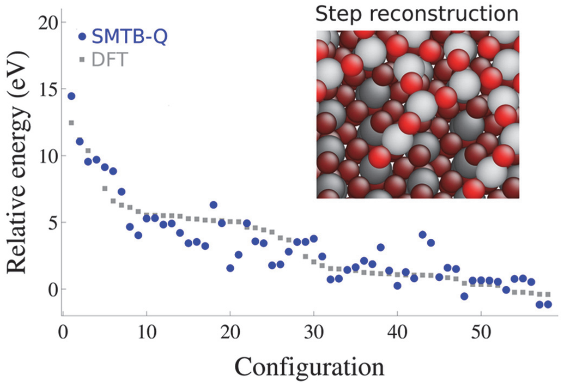


Figure 5. SMTB-Q vs DFT global minimum search as a function of the number of tested configurations.

-Development of interatomic potentials for oxides. So far, the realistic modeling of atomic interactions with empirical potentials in solids such as TiO_2 which have mixed ionic and covalent bonding is still a challenge. A second moment tight-binding charge equilibration model (SMTB-Q) for TiO_2 has been refined by comparison with results of density functional theory (DFT) calculations. This model successfully reproduces the experimental properties of TiO_2 crystal as well as the surface energy of low index surfaces. In particular, we demonstrate that the refined model is useful in global optimization studies by using it to search for reconstructions of the ⟨11-1⟩ step on the rutile (110) surface (see Figure 5).

The **Functional Thin Films** group is interested in the synthesis and study of metal oxide thin films and layers of controlled stoichiometry and microstructure. The goal is to understand the relationships between synthesis parameters, chemical composition, microstructure and functional properties, as well as the role of constraints on thermodynamic, chemical and mechanical stability. Our studies are based on a multi-physical and multi-scale experimental approach and coupled with numerical modeling. They focus on materials with high technological potential for applications such as microelectronics and optics (thin layers of zirconium oxides, vanadium oxide and perovskite), corrosion protection at high temperatures (complex metal alloys), nuclear applications (natural oxidation of zirconium alloy Zy4) or electrochemical sensors (tin oxide as a layer for electrochemical grafting).

The main results obtained in this period are:

-The mastering of ternary oxide layers elaboration by Metal-Organic Chemical Vapor Deposition (MOCVD).

Thin layers of zinc tin oxide were synthesized from two organic metal precursors one containing Sn and the other Zn. We tested different experimental conditions which allowed us to obtain thin layers of amorphous oxides of different stoichiometry. We also undertook to make these same layers from one heteronuclear precursor containing the two metals. Several stoichiometries as well as different structures (crystallites size, phases) were obtained. Since 2017, an extension of our activities has been initiated

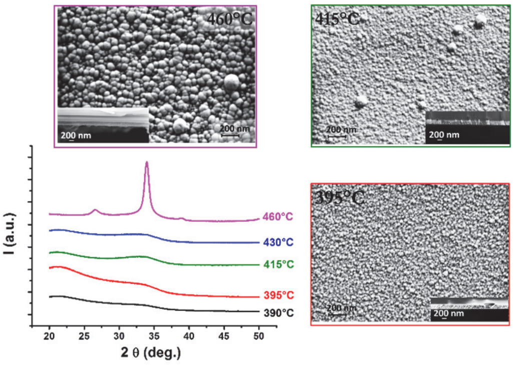


Figure 6. Surface morphology and XRD spectrum of $ZnSnO_3$ obtained by MOCVD with different synthesis temperatures.

towards the study of heterojunctions TiO_2/Co_3O_4 for applications in the field of energy.

-The mastering of the elaboration by MOCVD of SnO_2 layers for electrochemical grafting for thermoelectric applications and sensors.

This work was part of collaboration between our group, which developed the nanostructured films of SnO_2 by MOCVD and the Lambe Laboratory in University of Evry, which functionalized these surfaces via an electrochemical reduction of diazonium salts. The surfaces thus functionalized are then used as electrodes to quantify contaminants (copper, uranium...) in water by analyzing an electrochemical signal. The operating conditions were optimized to control the thickness of the layer, its stoichiometry in oxygen (EDX, SIMS and XPS), its nano-structuring (GIXRD) and finally its chemistry (FTIR).

Two typical texturations were selected, associated with two different microstructures. IR spectroscopy confirmed that low and high temperature deposits contain SnO_2 and/or SnO_x as well as hydroxyl and carboxylate groups. The electrical resistivity measurements of the films chrono-amperometry (current density as a function of time) showed that grafting of diazonium salts occur on the oxide surface sometimes with a mixed grafting mode (2D-3D).

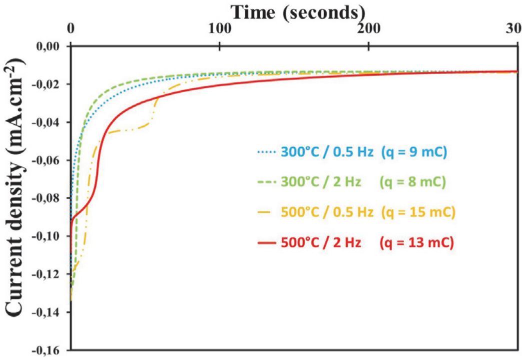


Figure 7. Current density evolution vs. immersion time of SnO_2 thin layers obtained by MOCVD with different elaboration conditions.

-Mastering of synthesis by CVD assisted by microwaves

A collaboration agreement was signed during the reference period between the SP2M team and TE-OX company to develop new materials in the form of thin films, heterostructures and nanowires and/or nanotapes of metal-insulating phase transition oxides, such as VO_2, and then to study and adapt their physical properties to integrate them into new electronic and optical components. In this context, one of the MOCVD reactors has been specially modified to develop vanadium oxide-based nanostructured layers, relying on plasma activation of the more reactive radical gas species at lower temperatures. The parametric study clarified the experimental conditions favorable to the production of nanostructures of vanadium oxides (wires, stars, platelets, rods) as shown in Figure 8.

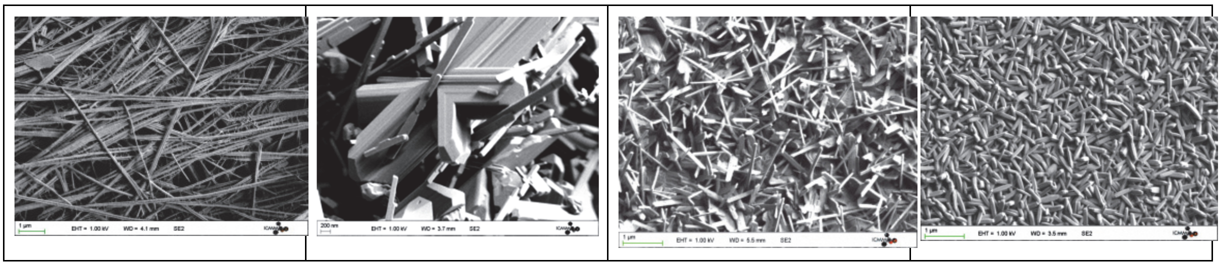


Figure 8. Nanostructured morphologies of VO2 obtained by MOCVD assisted by microwaves.

-Study of the mechanisms of oxidation of metal alloys in humid atmosphere

This work aims to understand both the influence of water vapor during the high temperature oxidation (600 °C - 900 °C) of metal alloys (Inconel 600 and Fe-17Cr) and the role of internal stresses, such as residual stresses, growth constraints as well as thermal and chemical stresses. A special feature of these stress studies is the coupling of X-ray diffraction with $\sin^2\psi$ law analysis, in-situ and operando deflection measurements and theoretical approaches.

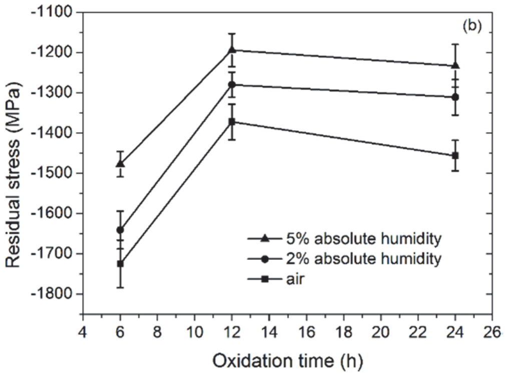


Figure 9. Residual stress evolution in oxide layer of Fe-17Cr alloy oxidized at 800°C with different absolute humidity.

Our results showed that the oxidation rate decreases in the presence of water vapour for the same temperature and the same oxidation time. On the other hand, the kinetics follows a parabolic evolution below 800 °C and become more complex above this temperature as in dry environment. These results allow us to assume that the presence of chromium would promote interaction with water. The distribution of chromium is much more homogeneous between the grains and the interface of the substrate in the wet-air configuration, thus justifying slower oxidation kinetics.

-Synthesis and mechanical behavior of ZrO_2 thin films

Over the reference period we continued our activities on ZrO_2 thin films. It is an interesting oxide for its functional applications but also for the nuclear industry: these layers are formed naturally on the fuel claddings of nuclear power plants and the resistance of the claddings is essential for the Security. The main advances obtained are described below.

-Polycrystalline models of ZrO_2 made it possible to estimate the internal micro-stresses. We showed that the thin films textures observed following the oxidation of the Zy-4 alloy are those that correspond to the lowest deformation energy associated with the metal-oxide transformation. Until now, this result was obtained only by mechanical computations of polycrystalline aggregates (Figure 10).

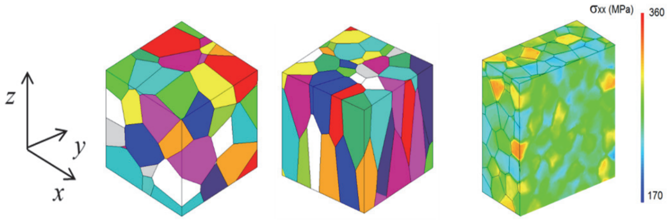


Figure 11. Polycrystalline models for ZrO_2 films to estimate internal stress.

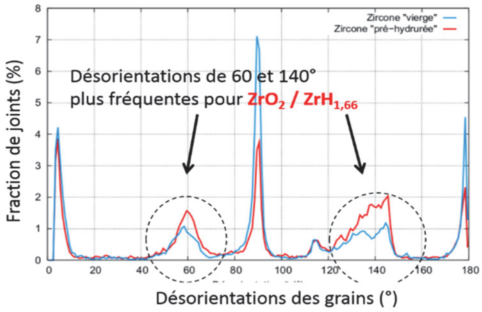


Figure 11. Volume proportion of grain boundary vs. grains orientation (disorientation).

-The study of corrosion-diffusion in Zr-based alloys, taking into account the mechanical-diffusion coupling, has shown in particular that the oxide developing on a Zr hydride has finer and more disoriented grains than that the one on a Zr alloy. This result was obtained through the analysis by electron microscopy of thin blades cut by FIB. This type of result is very rare in the literature (only 1 paper published in 2015), Figure 11.

-Thin layers of ZrO_2, developed in the laboratory by different growth modes and on different substrates, were tested for multi-fragmentation by bending in a scanning electron microscope. These studies, coupled with finite element simulations, showed that the thickness of the layer is the major parameter concerning the appearance of cracks and their multiplication. These two characteristics are independent of the residual stresses and the proportion of quadratic or monoclinic phase of ZrO_2.

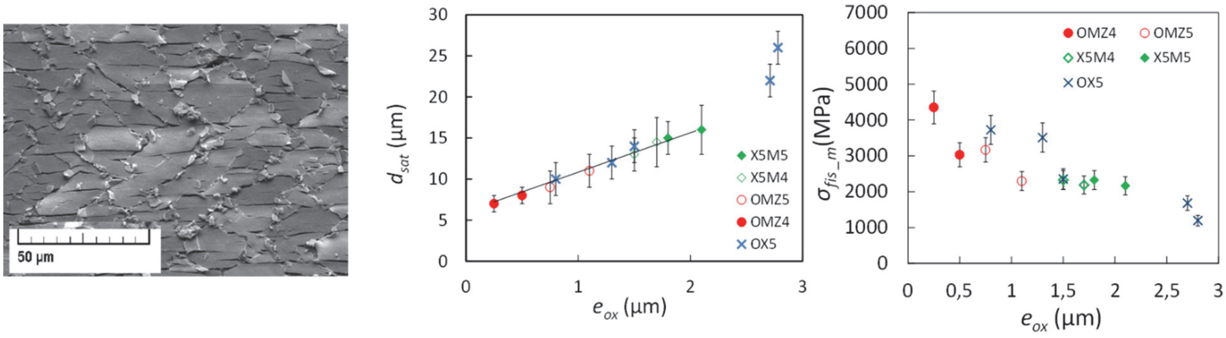


Figure 12. Surface morphology (left), lattice parameter (middle) and residual stress evolution (right) of ZrO_2 layers with different thickness.

The **Advanced Materials for Photonics** group continued the study of the laser-glass interaction both by trying to understand the involved mechanisms and in order to "build" new optical properties.

Ultrafast silica oxide destabilization and nano-gratings formation: The changes created by the femtosecond laser in silica are such that a strong birefringence is observed. As shown in Fig 13a, we demonstrated that it is mainly related to nanoporous layers (200-300 nm spacing and 20-30 nm thick). We have largely studied this microstructure and its dependence with the laser parameters, but especially with the chemical composition. Applications can be numerous in the field of fast material processing by producing nanoporous mater at the micron scale, decisive for space variant birefringent devices (inset of Fig 13a).

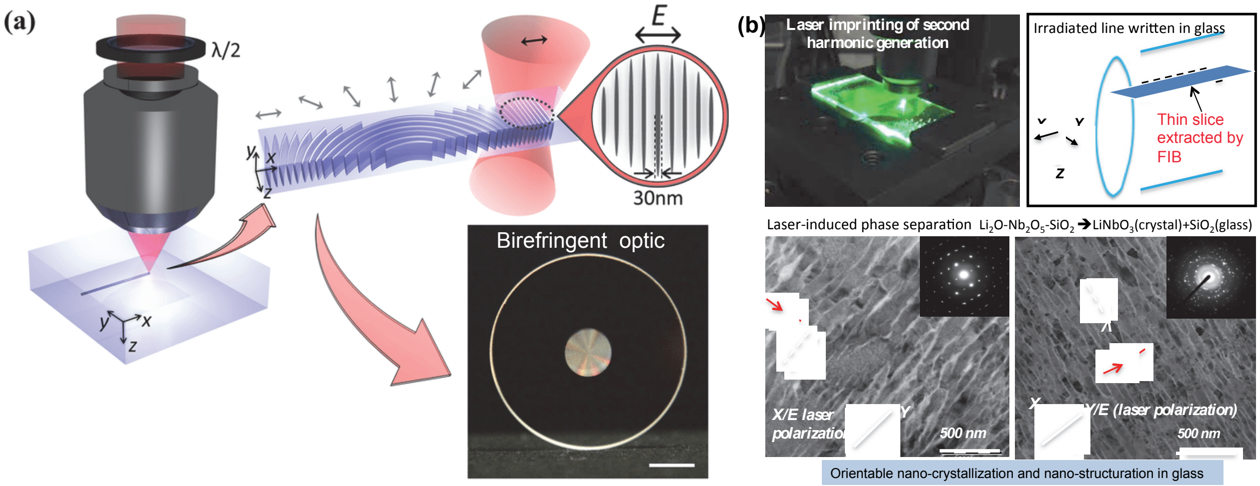


Figure 13. (a) Ultrafast silica oxide destabilization and nano-gratings formation; (b) Oriented nano-crystallization in glasses and second-harmonic generation.

Oriented nano-crystallization in glasses: The precipitation of micro and nanocrystals in the vitreous domain of the Li_2O-Nb_2O_5-SiO_2 system was also studied using femtosecond laser. This part was carried out thanks to the collaboration with the MP group of the team that brought his expertise in EBSD. Thus, we have followed the evolution of textures and achieved an advance by showing the possibility of orienting the crystallites and thus second harmonic generation (see Fig. 13b) using the polarization of the laser. This is the first time that the action of the light polarization is evidenced to orient crystallization in materials. The orientation of non-linear optical properties for integrated optics is thus mastered. This is one of the results of the thesis of J. Cao who received the thesis award of the Department of Physics of University Paris-Saclay.

The MAP group also leads industrial development activities:

- Application of our skills on photosensitivity mechanisms of the germanosilicates glasses to UV light in order to realize refractive index gratings, called Bragg gratings for optical telecommunications. We have published several papers on glass transformation kinetics, which leads to lifetime prediction for Alcatel, ITF and 3S photonics companies.

- Fictive temperature T_f is a parameter that characterizes the structural disorder of a glass. We recently lead a study, which includes fluctuations of this parameter as a contribution to the Rayleigh scattering and to propose specific chemical compositions to the Draka-Comteq company that allow to get rid of it: a novelty in the field.

Finally, because silica is a glass, it is centro-symmetric and therefore it is achiral. However, we found special conditions in which chirality can be induced by femtosecond laser irradiation. This important result (invited paper in Light: Science & Applications in 2017), which apparently breaks the Curie principle, will be detailed at the end of this chapter in the highlights section.

During the reference period, the **Functional Materials** group obtained several major results, including the evidence of the influence of the electric field on the growth of single crystals in an image furnace. These studies have necessitated original, innovative and novel instrumental developments, such as the establishment of a high-voltage crystal growth device in an image furnace, which enables various fields of several kV/cm to be applied during the crystallization at high temperature. Thanks to this prototype, we have shown that an external electric field can modify the solid-liquid equilibrium (displacement of the boundaries in the phase diagrams), and also plays a role in the section and the orientation of the domains (application to the ferroelectricity in particular). In addition to the above-mentioned electric-field crystalline growth device, we have also developed a high-temperature Hall effect measurement device using an alternate field created by a Halbach-type magnet attached to a rotating platform. This device, unique at this moment, enables very fast measurements of the type and carrier concentrations at high temperature.

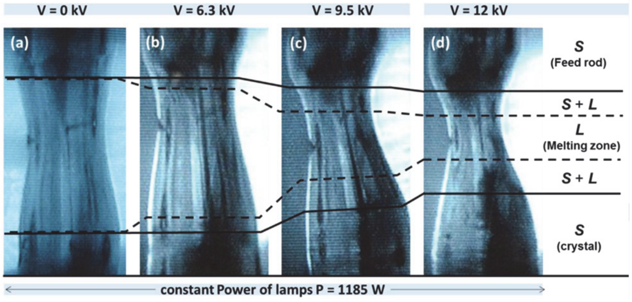


Figure 14. Evolution of the solid-liquid equilibrium with the application of an external field, with a reduction of the width of the melted zone.

A key activity of this group is the growth of single crystals of centimeter size and of high crystalline quality, which generates strong collaborations with teams of physicists in the nearby environment. This expertise has led to important results regarding two activities: heat transport in one dimensional (1D) cuprates and magnetic properties of oxides of pyrochlore structure.

One interesting specificity of the 1D cuprates is their extremely high "ballistic" thermal conductivity, with heat being mainly carried by magnetic excitations propagating in the direction of the spin chains (1D thermal transport). This peculiarity results in extremely large and anisotropic values of the thermal conductivity, Both of these characteristics are extremely promising for "thermal management" or "thermal device" applications.

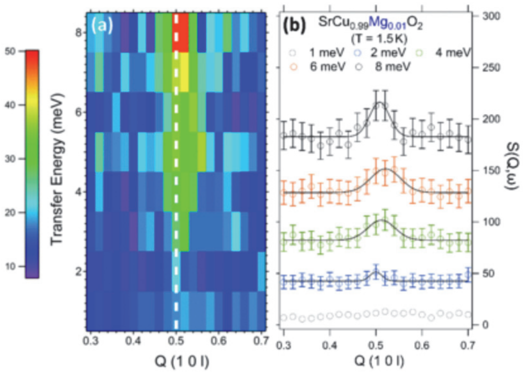


Figure 15. Neutrons scattering evidencing the opening of a spin pseudo-gap.

Study of the 1D heat transport mechanism in cuprates has been performed by thermal conductivity measurements, coupled to inelastic neutrons scattering (magnetic excitations and phonon spectra) at low and high temperatures respectively. This enabled us to probe the effect of the introduction of a controlled concentration of impurities on the propagation of spinons and phonons and to predict their impacts on the heat transport properties in these materials. In particular, we showed the "chain breaking" effect of impurities and their dramatic influence on thermal conduction by introducing impurities into the spin chains. We also evidenced the opening of a spin pseudo-gap at low-energy in these cuprates, in response to the segmentation of the spin chains. A part of this work was obtained during the PhD thesis of D. Bounoua who received the French Neutrons Society Prize in 2018.

Regarding the oxides of pyrochlore structure, two new research routes were opened:

-An original approach in the study of quantum spin ice by taking into account the stress due to the structural disorder and its influence on the behavior at very low temperature, which was enabled by the extension for the first time of the crystal growth of $Ln_2Zr_2O_7$ pyrochlores to various *Ln* rare-earths beyond Pr, as seen in Figure 16.

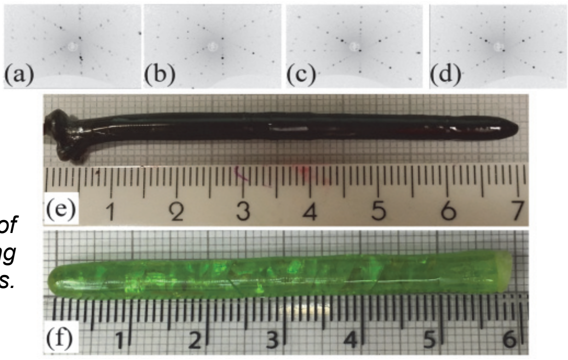


Figure 16. Single crystals of titanate (e) and zirconate (f) of pyrochlore structures, and Laue XRD patterns (a-d) showing the good crystalline quality of the crystals.

-The original use of THz spectroscopy (synchrotron radiation) in the study of oxides of pyrochlore structure with frustrated magnetism for the $Tb_2Ti_2O_7$ system. The obtained results suggest that the lattice vibrations are the driving force responsible for the transition from quantum spin ice to quantum spin liquid in this system.

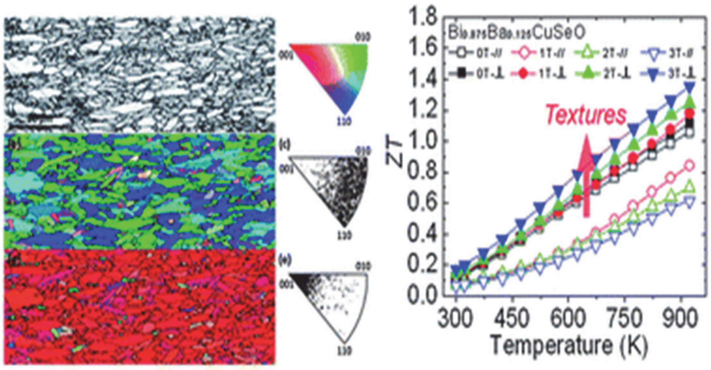


Figure 17. Texturation of a BiCuSeO-based sample (left) and influence of the texturation on the thermoelectric figure of merit.

We also extended our previous works, which had evidenced the excellent thermoelectric properties of BiCuSeO-type materials. These materials, whose potential for thermoelectric applications has been evidenced for the first time in our group, are today among the most efficient polycrystalline p-type materials in their temperature range. Thermoelectric figure of merit (ZT) greater than unity were obtained in this system.

Their development has led many research teams around the world to devote their activities to their optimization or to the development of new materials of the same family, as shown by the high number of citations of our articles (3 papers cited more than 100 times in the last five years). In particular, we have shown that their performance can be significantly improved by preferential orientation of the crystallites using texturing processes (figure 17). We have also extended our studies to other selenides families and shown that very promising thermoelectric performance can be obtained in materials such as $AgBiSe_2$ or $BaCu_2Se_2$.

Last, a new activity started in the team with the study of a new class of materials, high entropy oxides. A remarkable result in this activity (invited talk at ICTMC-2016, Halle, Germany) will be detailed at the end of the chapter, in the highlights section.

The research activities of the **Microstructure and Properties of metallic alloys** group are linked to the understanding of the mechanisms of formation and evolution of microstructures and textures during the thermo-mechanical treatments of metals and alloys. These studies are approached through experimental analyses and numerical simulations. The research activities incorporate fundamental and applied aspects. The final objective is the optimization of the mechanical or functional properties in relation to the processes of elaboration, shaping or assembly.

One of the research axes is the understanding of the formation of microstructures during solidification and post-treatment. This theme is related to the rapid development of additive manufacturing in recent years. This process makes it possible to generate parts with complex geometries that are inaccessible with conventional processes. Guaranteeing the use properties goes through the control of the manufacturing process (power, displacement of the source...) to control the microstructure (texture, absence of defects...). Even if this process is innovative, we rely on the experience already acquired with the studies underwent on welding or cladding which mechanisms are very close. These studies are carried out in the framework of the project SOFIA (Solutions for industrial Additive Metallic Manufacturing).

Our research also continues on understanding the mechanisms of texture formation during deformation and recrystallization by studying the mechanisms related to primary recrystallization and grain growth. These studies are carried out both from a fundamental point of view and in the framework of collaborations with several industrial partners.

In particular, we are interested in the mechanisms that promote the development of the "Cube texture". The strong growth of the superconductor cable market opens up prospects for research on Ni-W hypertextured metal substrates. The production of second-generation superconducting cables requires the epitaxy deposition of YBaCuO on a hypertextured substrate. Previous studies have shown a clear improvement in the critical current density circulating in the superconducting layer for a textured substrate with the Cube orientation ({100}<001>). The crystallographic texture, intimately linked to the values of use of functional layers (conversion efficiency, critical current...) is therefore an indispensable lever to make the product efficient and attractive. The study concerned in particular the effect of the chemical elements on the twinning and the trigger temperature of the abnormal growth of the grains detrimental to the epitaxy of the deposit. The influence of sulphur content on the development of Cube texture following recrystallization is shown in the following figures.

The sulfur content increase tends to decrease the twin boundary fraction (about 0% for 40 ppm of sulfur) and to increase the Cube fraction (about 100% for 40 ppm of sulfur).

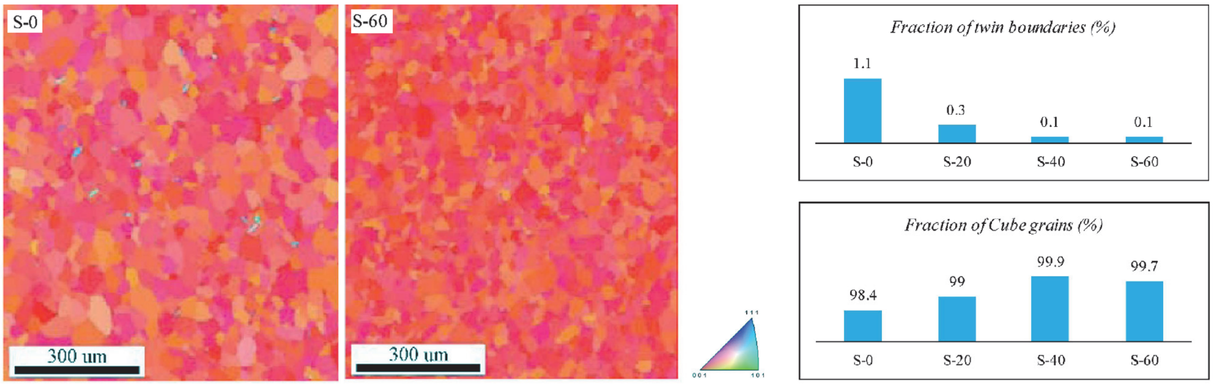


Figure 18. Orientation maps ({100} // rolling plane) of samples with 0 and 60 ppm of sulfur after full recrystallization. Fraction of twin boundaries and of Cube grains with deviation lower than 10°.

The control of the nature of the grain boundaries makes it possible to optimize some properties such as corrosion resistance. In this aim, a study on twinning has identified the influence of strain and grain size on the number of twins obtained per grain after recrystallization. An influence of strain and grain size on the number of grain boundaries is shown in the following figure. Both strain and grain size tend to increase the twin number per grain.

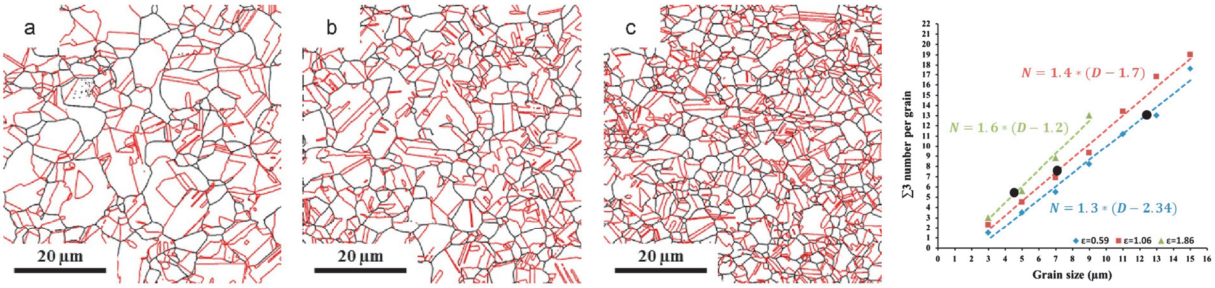


Figure 19. EBSD maps for the samples after three deformation states: (a) ε=0.59, (b) ε=1.06 and (c) ε=1.86, followed by an annealing at 900 °C during 4 min. (grain boundaries in black and ∑3 type boundaries in red). ∑3 Number per grain versus the grain size for each strain amount.

Titanium alloys forged in the α + β phase domain may exhibit abnormal grain growth during annealing in the β-domain. The difficulty is to be able to characterize the microstructure existing at high temperature. For this study, the ARPGE method was used to reconstruct the β microstructure from the EBSD characterizations performed on the α phase present at ambient temperature. These analyses allowed us to develop a scenario for the development of a single texture component during forging. This scenario was confirmed by numerical simulations from a Monte Carlo model, which allowed to test the influence of dispersion around this single orientation and the presence of grains with other orientations on the appearance of abnormal growth.

The last research axis concerns colamination. The colamination of sheet metal is an assembly technique for associating different materials in order to take advantage of the combination of their respective properties (thermal expansion, hardness, magnetic properties). The physical phenomena responsible for the adhesion between the plates during plating/consolidation by colamination are studied. This also makes it possible to develop new assemblies. In particular, this work allowed developing tubes by colamination (Project of the SATT Paris-Saclay).

An extension of this process is the multi-colaminating or ARB (Accumulative Roll Bonding), one of the numerous Severe Plastic Deformation methods to elaborate highly distorted materials. The goal is to obtain interesting mechanical properties: a high elasticity limit, as well as a strong tenacity thanks to the development of ultrafine grain structures. ARB consists of superposing two sheets in order to laminate them by 50%, which results in their welding by diffusion during this warm deformation. The sheet thus obtained, is cut into two pieces of equal size which are superimposed and re-inserted into the rolling mill, and so on... Then, an ultra-fine grain sandwich plate is obtained. As shown in the following figure, the fine-grained microstructure of two different aluminum alloys is achieved from two cycles of colamination.

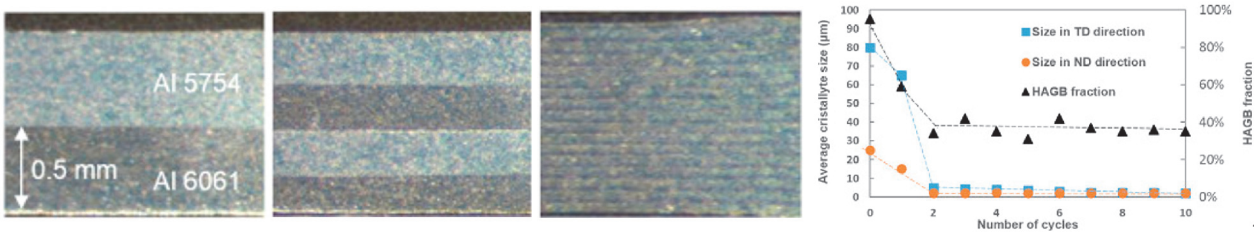
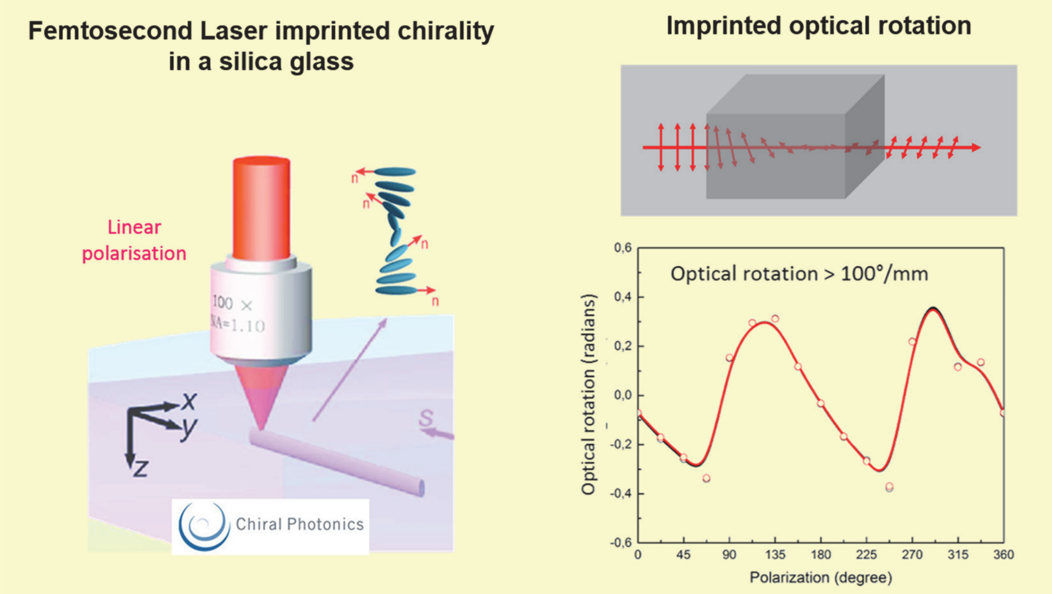


Figure 20. Samples of aluminum 6061 and 5754 obtained after 1, 2 and 5 cycles and evolutions of grain sizes and fraction of boundaries of high disorientation (HAGB, high Angle Grain Boundary) according to the number of cycles.

Highlights

During the reference period several important results were obtained. We list here two major results among our scientific achievements. We select two important results, of international recognition, that are obtained in collaboration with two other teams of the Institute.

As shown on the scheme below, we have demonstrated the production of an optical chirality in silica glass using femtosecond laser irradiation in linear polarization. This results from the action of force fields produced by the light, which restructures the material at the ten's nanometer scale. Circular optical properties, such as optical rotation and dichroism, are thus created. This new phenomenon is of magnitude comparable to that of quartz and can lead to important applications, knowing that the effect can be modulated with the polarization of the laser. This important result led to the start of a project to perform chiral restructuring in organic glass or crystals. This subject thus achieves a transverse cooperation in the institute between the activities of the material research group and a group of organic chemistry (MS&MT).


Femtosecond Laser imprinted chirality in a silica glass

Imprinted optical rotation

Figure 21. Femtosecond Laser imprinted chirality.

Also, we were the first to highlight the remarkable properties of a new class of materials discovered in 2015, high entropy oxides, which according to their composition can present notably colossal dielectric constants or large ionic conductivities. These properties make them very promising for applications, for example in the field of energy storage and it is a work in cooperation with the ERIEE team of ICMMO. It is important to note that this is not just a new material class but a new paradigm in the development of new functional oxides that uses high configuration entropy of a complex mixture in order to stabilize new phases.

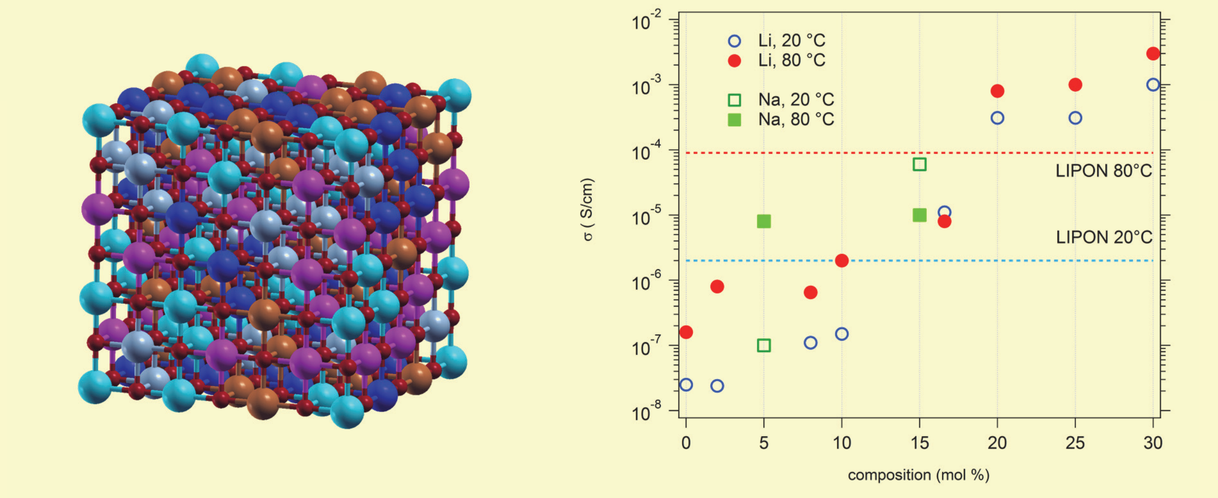


Figure 22. Left: "Simple" crystalline structure obtained by mixing 5 binary oxides at high temperature, under the effect of high configuration entropy. Right: ion conductivity of Li^+ and Na^+ in high entropy oxides, compared to that of "classical" solid electrolytes.

2- Organisation and life of the research team

Management, organisation and scientific animation

The SP2M team was created on January 1, 2014 from the two former teams of the institute's "Material science" topics: Non-Equilibrium Materials and Physico-Chemistry of the Solid State. It has, today, 30 permanent members (20 academics, 4 CNRS researchers, 6 engineers) and 16 post-docs, PhD or CDD; 15 team members are habilitated to direct research (HDR). Because of its large size it is represented by two team leaders to all Institute meetings. The team leaders are elected by the permanent personnel at the beginning of the contract.

During this five-year period, two persons arrived in the SP2M team: Tassadit Nait (T, Univ Paris Sud), Christophe Racic (T, Univ Paris Sud) but several departures took place: MG Barthes (DR, CNRS, retired), Alexandre Revcolevschi (Emeritus Professor Univ Paris Sud, retired), Severinne Le Moal (MdC Univ Paris Sud, transfer), Isabelle Braems (CR CNRS, transfer), Gaël Sattonnay (MdC Univ Paris Sud, transfer), Mickaël Herinx (AI, CNRS, retired).

The team is organized into five thematic groups, with strong scientific interactions. Each group is animated by a permanent member co-opted by the members of the group and who is the privileged interlocutor with the team leaders. The team operates without an elected council but on the basis of an operating charter agreed upon and adopted at the beginning of the contractual period by all of its members. This charter stipulates the creation of three committees within the team on subjects relating to "finances", "laboratory space" and "laboratory life" and stipulates partial pooling of all contractual resources.

Decisions are taken following monthly team meetings, interspersed with scientific meetings in which permanent and non-permanent seminars are held. In addition, a "Non-permanent Day" organized each year, is an opportunity for all non-permanent members to present their scientific activities. The "recurring" financial resources of the team are pooled and managed by "Finance committee". In particular, we have a proactive policy of participation in the major scientific congresses of our field. To this end, about one third of the recurrent financial ressources are intended to support participation in these congresses, especially for doctoral students who must submit their work to an international conference before their defence.

3- SWOT analysis

Strengths	**Weaknesses**
Multidisciplinary. *Close proximity of resources, external collaboration and strong integration.* *Important scientific production in high-impact journals (Science, Nature Physics, Energy & Environmental Science, Physical Review Letters).* *International recognition (Invited lectures, seminars).* *Strong research activity related to social and economic actors facilitating the professional insertion of our young doctors.*	*Success rate for national and European calls for projects not high enough, with 1 ANR JCJC contract and 1 European Marie-Curie Individual fellowship contract over the reference period.* *Low attractiveness of universities to attract students (mainly PhD and post-doctoral candidates).* *Thematic dispersion.*
Opportunities	**Threats**
Emergence of Paris-Saclay foreseen in the next five-year contract (Centrale Supélec, CEA Saclay, Soleil,...). *Improvement of the image of metallurgy among students linked to the various national actions (National Metallurgy Network) or regional (FERMI).* *Association, partnership, collaboration with other laboratories of Paris-Saclay.*	*Marginalization of materials science in a biology/pharmacy/chemistry cluster.* *Lack of visibility of our activities within the University of Paris-Saclay.*

4- Scientific strategy and projects

As recalled in Chapter 3, the creation of the team Synthesis, Properties and Modeling of Materials at the beginning of this contract, from the two former "materials" teams of the ICMMO, was motivated by the desire to give more coherence to the materials science’s activities the Institute. This project seems to be a success and the existence of this team is now re-conducted as is. We therefore wish to continue to maintain the same organisation and to intensify the collaborations resulting from this grouping. The team will therefore again include five thematic groups with the following staff:

-Numerical Simulations (1 Emeritus DR CNRS, 1 DR CNRS, 1 PR, 1 MC)

-Functional Thin Films (2 PR, 3 MC, 1 T)

-Advanced Materials for Photonics (1 DR CNRS, 1MC)

-Functional Materials (3 PR, 4 MC, 1 IE, 1 AI CNRS)

-Microstructure and Properties of metal alloys (1DR CNRS, 4 MC, 1 AT)

In addition to this workforce, a T and an AI have support activities for all of the team's thematic groups.

Finally, before the end of this contract we note a retirement of one of the researchers of the numerical simulations group together with the fact that a professor from the functional materials group will become Emeritus. His position has been requested to the university and we hope to be able to recruit a new professor in one of the experimental groups. Considering the already low and decreasing number of CNRS personnel in our team we will pursue our attempts to recruit CNRS researchers.

The group **Numerical Simulations** will continue to acquire fundamental knowledge about the crystallographic structure, the physical properties and the distribution of elements in an alloy, all in the vicinity of faults and interfaces. In particular, we propose the following three main orientations:

● Further development of the SMTB-Q model coupled with *ab initio* calculations for the study of oxides and their interfaces for applications in fields such as nuclear materials, ionic superconductivity in high entropy oxides that are studied experimentally in the team, storage information with the study of complex perovskites deposited in thin film on silicon and whose properties are studied experimentally by IR spectroscopy. The mastery gained in the development of semi-empirical potentials allows us to consider valuing this activity with the creation of a database.

● Exploiting Monte Carlo simulations with relaxation to extract the relevant energetic quantities that control the chemical equilibrium configuration in the case of alloys. The coupling with a site-energy formalism recently developed in the group identifies the driving forces and contributions due to local order and lattice vibrations. This formalism proves to be very promising for a systematic analysis of the thermodynamics of the alloys and their defects. In addition, it will allow developing much faster simulations on effective lattice (equilibrium or kinetics), while retaining most of the role of relaxations. We are also considering developing this methodology to study ternary oxides and non-stoichiometric oxides from simulations using the SMTB-Q potentials developed in the group.

● The study of the thermodynamic behaviour of metal nanoalloys in the framework of the IRN “Nanoalloys” and the GDR “Nanoperando”, with two main objectives related to the desire to approach to the actual conditions of use of these nanoalloys. The first concerns the development of approaches that allow for an increasingly realistic approach to account for the environment, primarily the interaction with the molecules of a gas. The second concerns the study of the stability of nanoalloys during hardening or annealing. This activity will allow us to keep in touch with experimental work carried out in the context of various ongoing collaborations.

The objective of the **Functional Thin Films** group is still to study nucleation, growth and stability of thin (deposited and natural) layers in relation to their structures, microstructures and mechanical characteristics. Correlations between synthesis parameters and processes, structural state, residual stress state and phase transitions will be sought. The structural and functional evolution of these layers during ageing and damage phenomena will also be studied, in order to control their behaviour and their stability. This work will be based on a multi-technical and multi-scale experimental approach, from the growth of films to the nano-scale to the use in service of these materials, often demanded by a strong thermal stress field, mechanical or thermo-mechanical. They will carry both on model materials and on materials with high technological potential (perovskites, complex metal alloys and amorphous alloys). Mechanical modeling will also be developed to predict the cracking behaviour and damage to the layer/substrate systems. We propose three main thematic axes:

● The development of new nanostructured materials by chemical methods by pursuing the study of ceramic materials oxides either binary AO_2 or ternary perovskite type ABO3, developing them by different chemical methods: hydrothermal synthesis, CVD thermal from organometallic precursors and plasma-assisted CVD. In the latter case, this allows to reduce the thermal budget and to consider deposits on substrates that do not tolerate heating (such as polymers). The main objective will be the synthesis of nanostructured dielectric materials with high permittivity or phase transition. The key synthesis parameters will be optimized so as to master/understand the chemistry, structure and microstructure of the material to achieve the physical and/or optical properties referred to.

● The study of residual surface stresses of oxidized or treated alloys. In the case of oxidation, that of metal alloys under wet air remains poorly studied, although humidity is present in almost all industrial applications. The kinetics of growth of oxide layers under wet air and the associated atomic diffusion mechanism will then be studied using multi-scale and multi-technical approaches (TGA, thermodynamics, SIMS, XRD, SEM/EDX). Residual, growth and thermal stresses will be analyzed by experiments (XRD and/or in-situ deflection) and numerical modeling. The effect of thermal cycling will be studied in terms of microstructure, kinetics, diffusion mechanism and mechanical stresses. In the case of surface treatments of alloys (shot blasting, laser shock, etc.), these are generally applied in order to improve the fatigue resistance of metal components, due to residual stresses and induced hardening. We will seek to better identify the associated mechanisms, mainly by XRD. The analysis of the shape of the diffraction peaks will quantify the microstructural evolution of the hardened layer and their position tells us about the residual mechanical state of the alloy. The thermal stability of the treated areas will also be studied.

● The study of the mechanical damage of the layer/substrate systems, the main characteristic of which being the cracking of the layers and which can occur during their elaboration or during their use. Our recent results show that one cannot be satisfied with an "average" measure of these stresses in the layer and that the texture and gradient (structural and mechanical) of the layer are to be taken into account. We therefore wish to use polycrystalline aggregate calculations to assist in the interpretation of XR diffraction patterns in the presence of crystallographic texture. These simulations will also separate the effect of crystallite size of the effect of micro-strains. By comparing the results obtained by XRD, we can then identify the state of macroscopic and microscopic stresses, even in the case of textured materials and complex stresses. Moreover, the characterization of the rupture is often carried out by tests of multicracking. The relationship between this phenomenon and the properties of the layer/substrate system is often addressed by analytical models, whose main limitations lie in not leading to quantitative analyses. More complete modeling by finite elements will thus allow to refine the effect of the substrate on the process of multicracking and to take into account a gradient of stresses in the layer. These simulations can then be associated with experiments on various systems, such as oxide/metal or metal/polymer.

In terms of scientific objectives, the **Functional Materials** group wishes to continue the development of the themes for which it has acquired international recognition and those which it has made emerge during the period 2013-2018, which can be described as below:

● The study of high entropy oxides, an activity initiated during the period 2013-2018 and for which we are among the pioneers. As part of this activity, we wish to extend the study to neighbouring or more complex systems (oxides of different crystalline structures or polycationic structures) as well as to different chemical systems, including chalcogenides, while contributing to the understanding of the properties of the already discovered systems.

● Methodological and instrumental developments for the growth of single crystals of oxides, in particular by the application of an electric field during growth. Our objective is both to understand the mechanisms by which the electric field plays on the crystalline growth, but also to benefit from an additional parameter for the growth of single crystals of improved properties. We also plan to couple the method of growth in image furnace to online analysis devices.

● The continuation of the activities for which we are recognized, in particular the development of new thermoelectric materials of the chalcogenides types, for which we have obtained excellent results over the period 2013-2018, the study of frustrated magnetism, both by pursuing our studies of pyrochlore-type model materials but also by extending them to new systems with complex magnetic structures, and finally studying the mechanisms of thermal conduction in connection with magnetism in spin-chain or spin-ladder compounds.

In order to improve the integration of the group, we also want to develop crystalline growth techniques complementary to the technique of melting of the zone in image furnace, to extend these activities of growth to new systems, including chalcogenides, antimonides, or arsenides. The techniques envisaged are of the type Bridgman or flux, which allow performing syntheses in controlled atmosphere in sealed tubes. We also want to extend the crystal growth activities of oxides to high entropy oxides, and conversely use our skills in the study of transport properties, in particular thermal ones, to study those of single crystals of spin-chain or spin-ladder materials prepared by zone melting in an image furnace.

The perspectives of the group **Advanced Materials for Photonics** are based on the group's achievements in the field of materials for optics since now 1996. Thus, the study of the fundamental aspects of photosensitivity to femtosecond IR laser made it possible to highlight during the period 2013-2018 the possibility of orienting nanocrystals at will simply by controlling the direction of polarization of the irradiation laser light, in the case of a particular glass. We want to extend this possibility to other inorganic glass, but also to organic glass for which the experimental parameters will be very different. A much more important challenge will be to "play" with the light to "play" with the chirality of matter. For this, we will use organic single crystals made by our colleagues in organic chemistry of the Institute. Moreover, having shown the possibility of producing chiral structures in the solid without using a circular light, we imagine being able to realize in the following years chiral selected photo-reactions from racemic mixtures, by controlling the electromagnetic fields of ultra-short pulse light via nonlinear interaction. This program is part of the ERC AdG project submitted in 2017. Finally, the potentialities of the method of modifying glass with the femtosecond laser begin to reveal themselves (start-up project IdEx Paris-Saclay). The developments will be carried out in connection with the industrial engineering sector of the Institute of Optics or Polytech Paris Sud.

The projects of the group **Microstructure and Properties of metallic alloys** are linked to the research guideline corresponding to the identified scientific locks, in particular by the GDR "recrystallization". They concern certain aspects associated with dynamic recrystallization, primary recrystallization, grain growth of conventional or nanostructured materials. Thus, our projects will continue to revolve around a main axis which concerns the control of microstructures and textures in relation to chemistry and manufacturing processes in order to optimize the mechanical and physical properties.

We will be interested in plating of sheets of different materials and in particular the mechanisms of adhesion to the interfaces between sheets. This process is of particular interest for the elaboration of "leadframes", magnetic materials, magneto-harmonic labels, bi-or tri-blades with special deflection, electromagnetic temperature sensors... There is currently an analytical model to describe the adhesion of sheets of identical materials. This model will need to be enriched by an experimental approach and finite element simulations in order to reflect plating of different materials. This process will also be extended using jagged rolling mill cylinders in order to develop, not only flat products, but bundles of half tubes or tubes for heat exchanger applications, particularly in the field of electronics. These studies will be carried out in collaboration with other laboratories in Paris-Saclay, proficient in magnetism and electronics.

Moreover, in recent years there has been a strong enthusiasm for the themes related to additive manufacturing. This activity involves other actors not directly related to metallurgy (robotics, production of laser or electron sources,...) and helps to develop interactions with academic and industrial partners. Studies are needed to understand the interactions between energy sources and matter in order to master the fusion of metal powders. In addition, our expertise in the field of understanding grain growth mechanisms and phase transformations makes it possible to propose manufacturing strategies to generate materials with controlled textures. This work will be done in the context of ongoing project (project SOFIA) or in the start-up phase (projects FAPS manufacturing additive Paris-Saclay and AFH Additive Factory Hub).

Département d'évaluation de la recherche

Self-assessment document

Team 9 - ERIEE

EVALUATION CAMPAIGN 2018-2019

GROUP E

INFORMATION

Team name:	**Recherche et Innovation en Electrochimie pour l'Energie**
Acronym:	**ERIEE**
Director's name (current contract):	**Pierre MILLET**
Director's name (future contract):	**Pierre MILLET**

SELF-ASSESSMENT DOCUMENT

1- Research products and activities

Scientific output

The Eriée team (Team of Research and Innovation in Electrochemistry for Energy applications) was created at the beginning of the five-year 2013-2018 evaluation period, to address issues in material science and physical chemistry for energy applications. The team is the continuation of the former "Energy" group which was part of the LPCES team in the previous contract, and was already working on similar research topics. There are only 5 Profs and Associate Profs (no technical support and no CNRS researcher). Over the 2013-2018 period, an Emeritus Professor (M. Guymont) has left the team in 2016. An associate professor of the team (S. Franger) has been nominated Professor in 09-2014 and a new associate professor (L. Assaud) has joined the team in 09-2015. The research effort focuses on three reactions of great societal interest: (i) water dissociation (electrochemistry and photo-electrochemistry); (ii) carbon dioxide reduction; (iii) lithium intercalation for batteries. The ambition of the team was (and still is) to address basic science issues in material science and physical chemistry (elaboration and characterization of innovative materials and nano-structured interfaces of electrochemical interest) but also to develop innovative devices and to value technological outcomes in the industry sector. The different activities are classified into 4 major themes.

Theme 1-a. Water electro-dissociation for hydrogen production

Water dissociation by electrolysis is a significant and historical research topic of the team. The focus is on near-ambient temperature applications (acidic-polymer electrolyte and liquid-alkaline electrolyte). Our activities cover both basic research (in material science to develop innovative electrocatalysts) and applied research (device and prototype developments, electrochemical engineering). Over the 2013-2018 period, main team contributions were made in material science (elaboration, synthesis, and characterization of innovative materials and nano-structured electrochemical interfaces), in physical-chemistry (multiphysics characterization of these interfaces) and in electrochemical engineering (prototype conception, design, development and technology transfer). The need for innovative electrocatalysts is justified by cost (especially in acidic environments where expensive noble metals predominate) and efficiency improvements. Examples of team contributions to the state-of-art are (i) the development of polymetallic alloy nanoparticles on carbon substrates (**Fig. 1**); (ii) the reduction of noble metal loadings (**Fig. 2**); (iii) the functionalization and implementation of transition metal inorganic complexes (e.g. clathrochelates (**Fig. 1**), polyoxometalates, polyoxothiometalates, etc.) for the hydrogen (HER) and oxygen (OER) evolution reactions and their application in polymer electrolyte cells; (iv) the development and optimization of coating processes (**Fig. 3**). A large set of experimental techniques have been used to characterize these systems: electrochemical techniques (e.g. impedance spectroscopy and rotating ring-disk electrodes; some of them like pulsed impedance spectroscopy have been developed within the team), and physical (e.g. exafs/xanes at Soleil, **Fig.4**; more recently an AFM-SECM setup has been installed in the team).

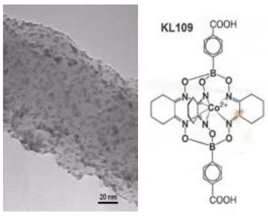


***Fig.1**: PtPd nanoparticles on carbon nanofibers and chemical structure of a Co clathrochelate.*

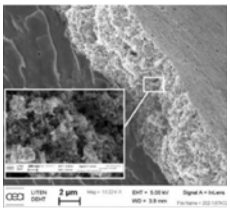


***Fig.2.** SEM image of IrO_2 catalytic layer in PEM water electrolysis cell.*

***Fig.3.** Laboratory catalytic ink printer.*

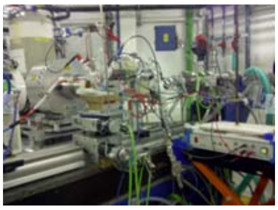


***Fig.4.** in-situ exafs setup used at SOLEIL for in-situ experiments.*

Key facts

National collaborations: universities of Versailles, Rennes, Grenoble, Nice, Montpellier, Reims, CEA Saclay.
International collaborations: universities of Tokyo, Moscow, Santa Cruz, Hannover.
Key research projects: ANR (HydroPEM, 2011-2014; Aitoiles, 2011-2015; Chalcocat, 2016-2019; Moïse, 2017-2020), IRS IDEX Paris-Saclay (MOMENTOM), Charm3at Labex (AMicE).
List of PhD thesis (N. Mbemba, C. Rozain, B. Verdin, B. Bensman) and post-docs (A. Villagra, G. Mouchaham, A. Pradon).
Main outcomes: research papers, international conferences and invitations, national and international research contracts in basic science.

Innovation and applications

The team is also involved in electrochemical engineering (cell conception, prototype development and testing, technology transfer, modeling, diagnostic tools). These activities take place in the frame of various collaborations with the industry sector. An ATEX test platform (GenHyTech) has been designed and developed to test prototype PEM water electrolysis cells and stacks (**Fig. 5**). A spin-off company (CETH) has been created in 2005. Massive investments have been made in 2010 (SPTI) and 2014 (Aréva + ADEME) to develop and put on the market MW-scale electrolyzers (**Fig. 6)** and technical collaborations are on-going. In addition, P. Millet has been working 2 years in the PS2E energy transition institute to qualify multi-MW PEM water electrolysis plant for grid services (management of the FlexiPEM 1 and 2 projects, **Fig. 7**).

Fig. 5. *Atex platform developed and installed at ICMMO.*

Fig. 6. *300 kW PEM water electrolyser (collaboration ArévaH$_2$Gen).*

Fig. 7. *7-MW PEM water electrolysis platform at EnergiePark, Mainz, Germany (collaboration Siemens).*

Key facts
National collaborations: Air Liquide, EDF, ArévaH2Gen, Conseil Général de l'Essonne, ADEME.
International collaborations: ITM-power (UK), Siemens (Germany), Hydrogenics (Canada), ProtonOnsite/NEL (USA).
Key research projects: ANR (HydroPEM, 2011-2014), ADEME (Mhyel, 2017-2019; Méthycentre, 2018-2021), PIA (FlexiPEM1, FlexiPEM2, 2015-2019), industry (AH2Gen).
List of PhD thesis (C. Rozain, B. Verdin) and post-docs (A. Villagra, A. Pradon).
Main outcomes : development of strong links with the industry sector attracting significant financial support, several technical book chapters, international expertise for the industry and the European Commission.

Theme 1-b. Water photo-dissociation for hydrogen production

This research sub-theme started in 2014 and specific experimental setups have been developed since then in the team **(**e.g. **Fig. 8)**. Collaborations have been developed with eminent international research laboratories in the field of semiconducting materials (Japan; e.g. chalcogenide thin films, **Fig. 9**) and molecular chemistry (Russia). Eriée is concentrating its effort on the manufacturing (e.g. **Figs 10, 11**) and multiphysics characterization of nanostructured photo-electrochemical interfaces. Various approaches are used for surface binding of charge transfer co-catalysts: physisorption, chemisorption (grafting), gas phase deposition. Regarding the characterization, several specific test benches have been developed and various impedance spectroscopies are used to analyze the reaction mechanisms and identify rate determining steps.

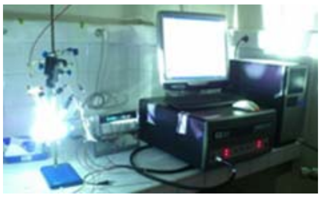


Fig. 8. *Photograph of the photo-electro-chemical setup.*

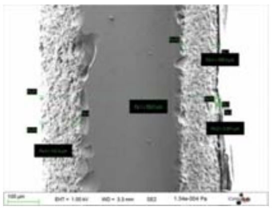


Fig. 9. *Cross-section of a CuGa$_3$Se$_5$ thin film photoelectrode.*

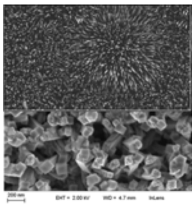


Fig. 10. *TiO$_2$ nanorods covered by (top) Co/Ni hydroxide nano-flowers; (down) cobalt ZIF67, for water photo- oxidation.*

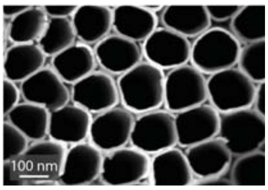


Fig. 11. *TiO$_2$ nanotubes obtained by anodization for water photo-oxidation.*

Key facts
National collaborations: UVSQ and Rennes Universities (Pr. E. Cadot, Dr. D. Favre), SOLEIL (Dr. A. Zitolo).
International collaborations: University of Tokyo (Japan, Prof. K. Domen), Tokyo University of Science (Japan, Prof. A. Kudo), Beni-Suef University (Egypt, Prof. M.H. Khedr), University of Erlangen-Nuremberg (Germany, Prof. J. Bachmann).

Recent research projects: ANR (ChalcoCat, 2011-2014), French-Egyptian scientific cooperation program STDF-IFE, French-German joint collaboration program (CCUFB, 2016).
List of PhD thesis (A. Villagra, M. Antuch) and post-docs (W. El Rouby from Egypt, P. Büttner from Germany).
Main outcomes: research papers, international conferences and invitations, national and international research contracts in basic science.

Theme 2-a. CO_2 electro-reduction

This theme started in 2009. The idea was to extend the know-how gained in water electrolysis (material science and devices) to CO_2 electro-reduction, a topic of significant interest in the industry. The challenge is to develop electrocatalysts operating in aqueous media, to increase reaction selectivity and avoid the parasite hydrogen evolution reaction. Most of the effort is made on molecular electrocatalysts such as transition metal complexes (**Fig. 12**), metal-porphyrines, MOFs, and POMs. The efficiency is measured using conventional electrochemical techniques (**Fig. 13**) and the reaction selectivity is analyzed by gas chromatography (**Fig. 14**).

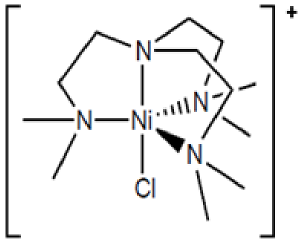


Fig.12. *Structure of nickel tris 2-diméthylaminoéthyl amine.*

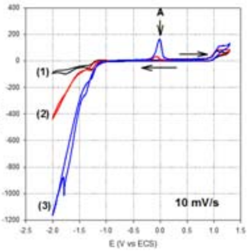


Fig.13. *CVs in ACN/0.1 M TBAP + 0.5 mM Ni(Me_6tren)Cl^+ : (1) Ar ; (2) CO_2; (3) CO_2 + 0.5 mM H^+.*

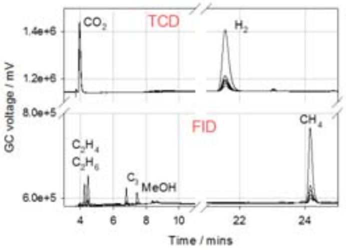


Fig.14. *Typical reaction products detected by gas chromatography during a chrono-amperometry.*

<u>Key facts</u>
National collaborations : PS2E Institute, Italcementi Co., UVSQ, Rennes.
International collaborations : Russian Academy of Science (Moscow, Prof. Y. Voloshin).
Recent research projects: European (CEOPS, 2013-2015); ANR (ChalcoCat, 2011-2014).
List of PhD thesis (F. de Guglielmo, A. Ragupathy, A. Villagra) and post-docs (K. Ramirez, C. Thibault, P. Vorburger, R. Zakari).

Theme 2-b. CO_2 photo-reduction

As for water electrolysis, the topic of CO_2 electro-reduction has been extended to CO_2 photo-reduction. Some specific setups have been developed within the team, mainly with the support of PhD students (**Fig. 15**). Our efforts focus on the elaboration of nano-structured semi-conducting materials (**Fig. 16**), surface coated with co-catalytic compounds of appropriate properties, and their multi-physics characterization. Molecular co-catalysts (e.g. metalo-porphyrines, molecular complexes, graphene quantum dots or graphene-derived nanosheets, **Fig. 17**) are mostly used for that purpose. CO_2 photo-reduction is investigated using either photo-reactors or photo-electrochemical reactors (**Fig. 18**).

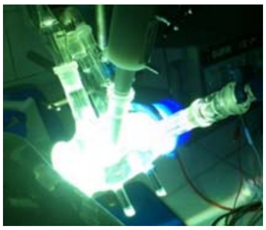


Fig.15. *CO_2 photo-reduction setup developed in the team.*

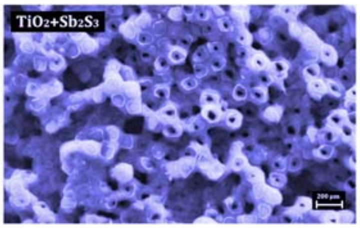


Fig.16. TiO_2/Sb_2S_3 photoelectrode for CO_2 photo-reduction

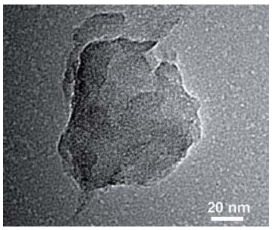


Fig.17. TEM image of C_3N_4–Ru–F nanosheets.

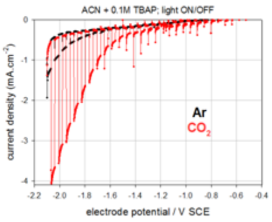


Fig.18. *photo-assisted CO_2 reduction into CO using $CuGa_3Se_5$ thin film..*

The focus is on nano-structuration and the coupled measure of topological/property photo-electrochemical properties at the nanometer scale. In 2015, a PhD student of the team (A. Villagra) has obtained a grant from the French Ambassy in Japan to spend one month in the laboratory of Prof. A. Kudo at Tokyo University of Science: he has been trained on photochemical procedures to analyze reaction mechanisms in order to improve the efficiency as well as the reaction selectivity (**Figs. 18**). Another PhD student (Yi Peng) from Santa Cruz

University, CA, has been laureate of a Chateaubriand mobility grant and has spent 6 months in the lab (first semester of 2018). More recently, a collaboration has been launched with Greenfish Co. (Belgium) to elaborate semiconducting photo-electrodes by deposition of Sb_2S_3 nano-cristals atop TiO_2 nanotubes for CO_2 photo-reduction (**Fig. 17**).

Key facts
National collaborations: Italcementi Co; Universities of Versailles and Rennes.
International collaborations: Tokyo University of Science (Japan, Prof. A. Kudo), Santa Cruz university (USA, Prof. S. Chen), National Tsing Hua University (Taiwan, Prof. R.A. Radoong), GreenFish Co. (Belgium).
Recent research projects: ANR (ChalcoCat, 2011-2014); joint PhD thesis with Univ. Santa Cruz and Taiwan.
List of PhD thesis (A. Villagra, Y. Peng, S-M. You, P. Allazov) and post-docs (W. El Rouby).
Main outcomes: research papers, international conferences and invitations, national and international research contracts in basic science.

Theme 3. Electrochemical energy storage: batteries, microbatteries, solid state batteries

The team has developed an expertise in the field of energy storage, in terms of active materials synthesis (oxides, phosphates…), characterization (XRD, SEM/TEM, BET) and electrochemical characterization (voltammetry, impedance spectroscopy). Research activities focus on conventional batteries (commercial) modelling (behavior, state of health, ageing) thanks to some specific lab facilities (100 A cycling tests, climatic chambers, large band impedance analyzers) (**Fig.19**). Since 2015, an intensive collaboration (projects, student exchanges) with Indian partners is ongoing. Projects in electric mobility (partnership with PSA, Renault) and large scale energy storage systems (partnership with EDF) led to innovative battery ageing modelling with a fatigue approach (weighted Ah-throughput model) (**Fig.20**). Another research activity concerns the development of microbatteries (lithium µbattery, lithium-free µbattery) in partnership with ST Microelectronics (1 patent for fast conformal 3D thin film deposition) (**Fig.21**). In this domain, projects are dealing with materials studies, innovative architectures (3D) and systems (Li-free), full µbattery characterization by impedance (reliability process). More recently, a new research topic has emerged, regarding solid state batteries after demonstration of superionic conductivity of new high entropy oxide materials (lithium and sodium conduction) (**Fig.22**). The Greenfish Company (Belgium) is involved in this field, dealing with full solid state battery assembly and solid/solid interfaces characterization by electrochemical impedance spectroscopy.

Fig.19. *Batteries cycling room facilities.*

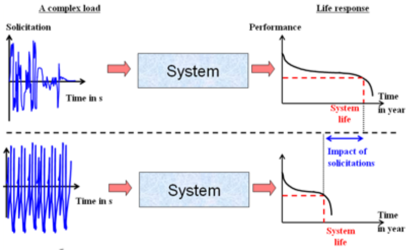


Fig.20. *Batteries ageing modelling.*

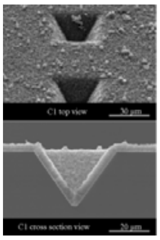


Fig.21. *3D micro-batteries.*

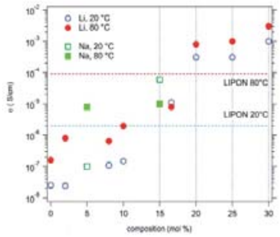


Fig.22. *Li/Na superionic conductors for solid electrolyte.*

Key facts
National collaborations: IMN (Nantes), LRCS (Amiens), ICMPE (Thiais), IPREM (Pau), Chimie-ParisTech (Paris), CEA/Saclay, CEA/Grenoble, PSA (La Garenne-Colombes), Renault (Guyancourt), Saft (Bordeaux), EDF (Moret), ST Microelectronics (Tours).
International collaborations: CECRI/Karaikudi (India), IISc/Bangalore (India), IIT/Jodhpur (India), IIT/Patna (India), Greenfish/Brussels (Belgium).
Recent research projects: ANR Pepite (2015-2019), ANR Helios (2016-2019), CNRS Energie (2017, 2018)
List of PhD thesis (N. Besnard, S. Larfaillou, P. Bernard, G. Piana), international student exchanges (A-K. Meena, A. Bhatia, V. Sundaram, S. Karrupiah, R. Pongilat, L. Sharma) and post-doc (C. Bongu).
Main outcomes: research papers, national and international research contracts in basic science and applications in collaboration with the industry sector.

Theme 4. Development of new experimental tools and modeling

Various experimental techniques have been developed in the team to investigate and elucidate multi-step chemical, electrochemical and photo-electrochemical reaction sequences. For example, the concept of electrochemical impedance spectroscopy has been extended to gas-phase reactions (**Fig. 23**) in order to analyze metal hydrogen interactions in the presence of strong hysteresis (**Figs. 24, 25**). Practical applications are found in hydrogen storage in hydride-forming materials and hydrogen purification by permeation. Another example is the development of non-harmonic electrochemical impedance spectroscopy (**Fig. 26**). The technique has been used to characterize multi-layer cylinders for selective hydrogen purification/compression.

Fig.23. *Gas-phase impedance setup developed in the team.*

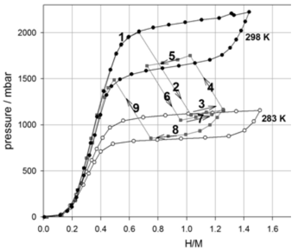


Fig.24. *Hysteresis of the $LaNi_5$-H_2 system.*

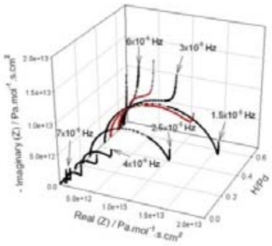


Fig.25. *Gas-phase impedance diagrams ($LaNi_5$-H_2).*

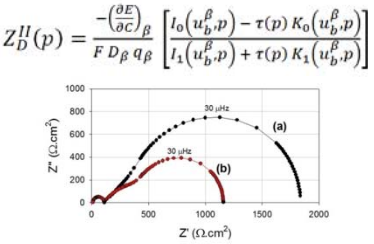


Fig.26. *Analytic expression and graph of the impedance of a bi-layer hollow cylinder.*

<u>Key facts</u>

National collaborations: CentraleSupélec, university of Grenoble, LITEN CEA Grenoble.

International collaborations: SINTEF (Norway, Dr. T. Peters), Mahnken & Partner GmbH (Germany, Dr. S. Reck).

Recent research projects: ADEME (Vitrhydrogène, 2017-2020).

List of PhD thesis (C. Decaux, R. Ngameni) and post-docs (R. Ngameni).

Main outcomes: research papers, international conferences and invitations, national and international research contracts in basic science.

Characterization platforms

Over the years, the Eriée team has developed a rich contracting activity (≈ 3.0 M€). A significant part of it has been used to hire post-doc fellows. All the scientific and technical resources available in the team have been purchased in the frame of research contracts. In addition to the acquisition of conventional research equipment, two specific scientific platforms have been developed:

1. The **AMicE** platform: a new multi-purpose AFM characterization platform has been purchased and installed in the team in March 2018. The equipment (ICON Bruker, ≈ 260 k€, **Figs. 27-29**) was purchased using fundings from the industry (≈ 70%), UPSud (≈ 20%) and the Charm3at Labex (≈ 10%). This equipment can be used (**Figs. 30-32**) for Atomic Force Microscopy (AFM), Quantitative Nanomechanical mapping (QNM) analysis, Scanning Electrochemical Microscopy (SECM), Kelvin Probe Force Microscopy (KPFM), in tapping and peakforce tapping modes. This equipment will play a central role in the scientific activities of the Eriée team during the next contract.

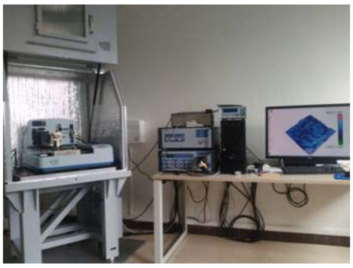


Fig.27. *Overview of the AMICE platform.*

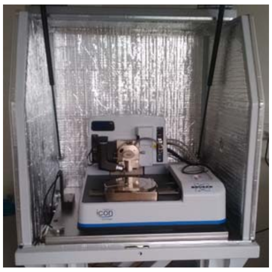


Fig.28. *The AFM-SECM platform.*

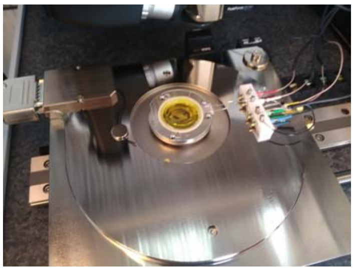


Fig.29. *Electrochemical cell for SECM measurements.*

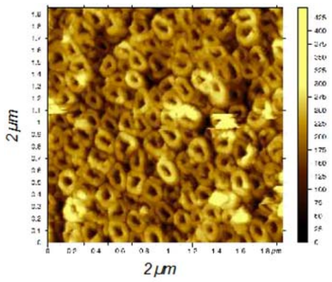


Fig.30. *TiO_2 nano-tubes (AFM).*

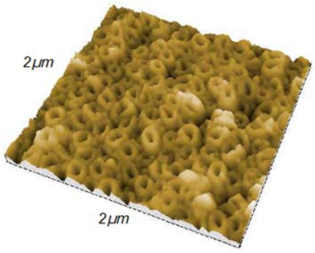


Fig.31. *TiO_2 nano-tubes (AFM).*

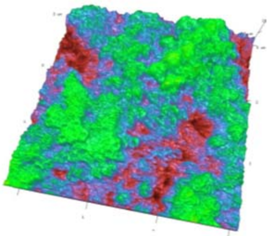


Fig.32. *TiO_2 nano-tubes (SECM).*

2. **GenHytech** platform: design and test of PEM water electrolysis stacks for pressurized H_2 production (cf. **Fig. 5**). The platform was the main deliverable of a former FP6 research project (GenHyPEM, 2005-2009) supported by the European Commission and managed by the team. It has been upgraded two times over the 2013-2018 period with the financial support of the Council of Essonne. It can be operated automatically and remotely on a 24h a day basis. It is used as a support in the frame of various research projects related to either water dissociation or carbon dioxide reduction.

Highlights

The domains of excellence of the Eriée team over the 2013-2018 period are:

1. Team members have been able to conduct fundamental research activities in material science and physical-chemistry: elaboration and characterization of nano-structured electrocatalytic interfaces for electrochemical and photo-electrochemical applications in the field of energy storage.
2. Various scientific collaborations have been initiated and developed at national and international levels, to perform complementary activities in electrocatalysis.
3. A strong partnership has been developed with the industry sector: the team is involved in innovation, prototype development, technology transfer and expertise activities.
4. A significant financial support has been obtained from the industry sector to purchase the new AFM characterization platform that will play a central role in the scientific activities of the Eriée team during the next contract.
5. Team members are significantly involved in student training (master, PhD and post-docs).
6. Key figures related to the scientific production are summarized in the next table :

Peer-reviewed papers (ACL)	46	Invited lectures (international conferences)	30
Books / Book chapters	20	Non-invited oral communications	49
Patents	1	Invited seminars	40
Mean team impact factor	**4.237**	**ACL/(ETPR/an)**	**3.47**

2- Organisation and life of the research team

Management, organisation and scientific animation

The team has only 5 Profs and Associate Profs (no technical support and no CNRS researcher). There is therefore a light management structure. The focus of periodical meetings is on scientific activities. Regular group meetings involving team members, PhD students and post docs are organized on a weekly basis (L. Assaud is the organizer). Most team funds come from research contracts: the budget received from the university and the CNRS is less than 10%, every year. University funds are used for day-to-day work and allocated using informal procedures, mainly upon student requests. Contract funds are directly managed by scientists in charge of these contracts. All the research equipment available within the team (in the lab and on the two platforms) has been purchased using research contract funds. Examples of specific scientific and technical equipments available for electrochemical and photo-electrochemical research are: potentiostats, gas chromatograph, light simulators and detectors, electrochemical and photo-electrochemical reactors of different shape and size, a catalytic ink printer, non-harmonic impedance equipment, battery characterization. More recently, the Amice platform (AFM-SECM) has been purchased likewise.

3- SWOT analysis

Strengths	Weaknesses
** strong involvement of team members in research despite the fact that none of them is full time researcher.* ** international visibility in research gained during the 2013-2018 period via several international collaborations.* ** a large portfolio of research contract (both academic and industry) has been successfully obtained.* ** over the 2013-2018 period, the team has been able to acquire several high level research equipments, in line with its scientific and technical objectives.* ** good (in terms of number and IF) scientific production in high quality peer-reviewed research journals.* ** a significant number of PhD and post-doc grants have been obtained over the 2013-2018 period.* ** significant involvement of team members in teaching and training management.*	** the size of the team is critically low.* ** in spite of its efforts, the team has failed to attract/obtain permanent staff from the CNRS and technical support from the university.* ** lack of appropriate technical support within the institute; need to rely on PhD students to develop and maintain technical equipments, and to sub-contract technical tasks.* ** lack of the necessary place to install new equipments and receive a larger number of research students to maintain a good level of scientific production.* ** there are other teams working on similar topics in the neighbourhood, outside the institute, but there are reduced interactions and lack of common strategy.*
Opportunities	**Threats**
** the research strategy of the team (focus on the manufacturing and characterization of electrochemical interfaces and devices) facilitate collaborations with international experts in material science (semiconductors and molecular catalysts) that would otherwise be competitors.* ** research topics of the team have a good visibility at national and international levels; this is facilitating collaborations and scientific networking.* ** possibility to interact at the local, regional, national and international scale with other research groups involved in complementary activities.*	** research activities of the team strongly depend on contracts, to purchase the necessary equipment and to hire the necessary non-permanent staff; considering the limited number of permanent staff in the team and their heavy teaching + management tasks, there is a risk of reduced activities if team leaders fail to obtain the appropriate resources.* ** lack of local technical support that will force the team, on the short term, to stop innovation and technology developments and to refocus its activities on basic science only.* ** no real perspective to recruit permanent staff despite the results obtained over the 2013-2018 and the positioning of the team on research topics of societal interest and large international visibility.*

4- Scientific strategy and projects

Fig. 33 provides an overview of the Eriee organization and objectives for the next period :

* the composition and organization of the team will remain identical for the next period; the team will continue to work on the same research topics, namely water electro- and photo-electro-dissociation, CO_2 electro- and photo-electro-reduction, batteries.

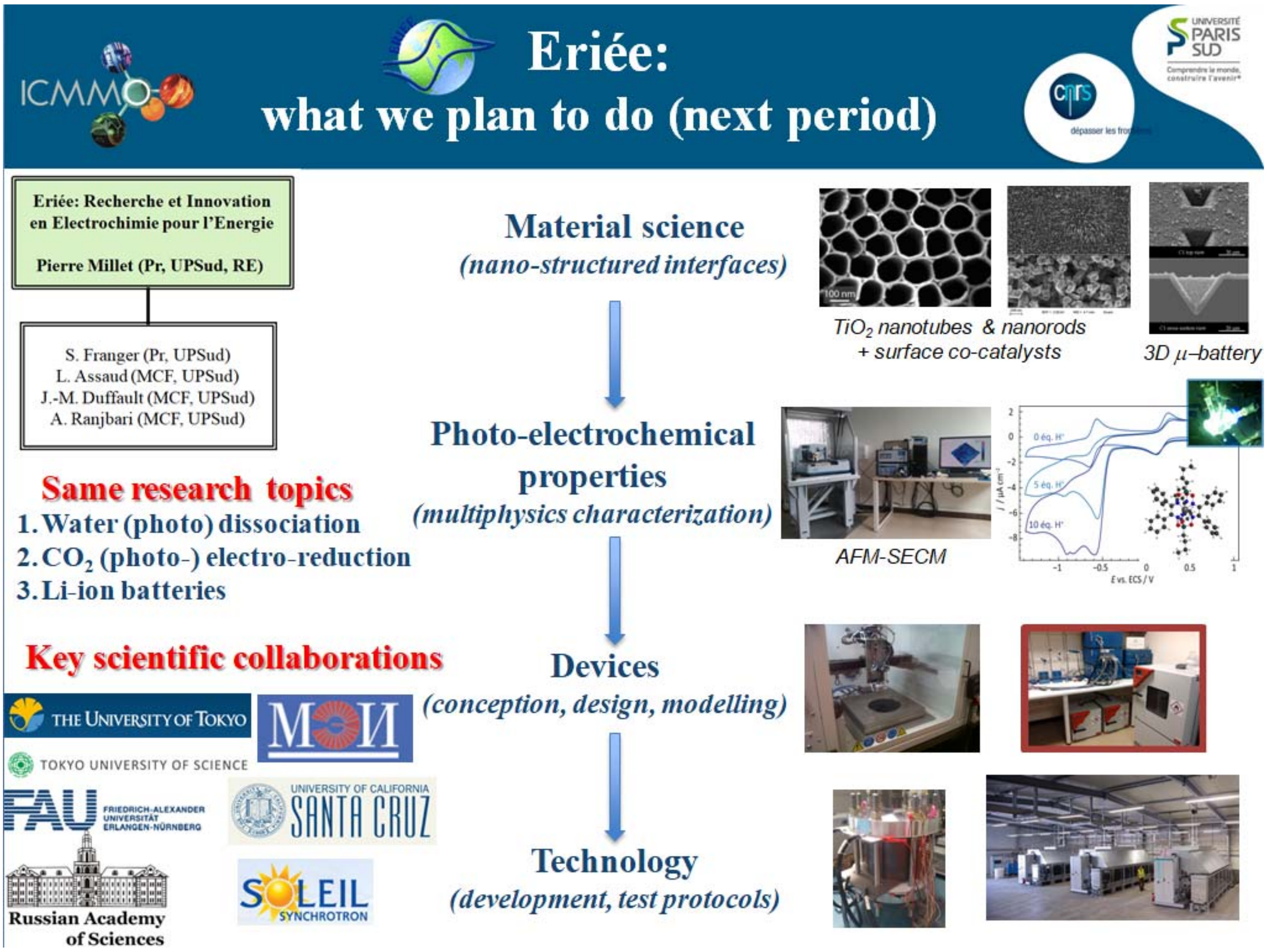
* the same strategy will prevail despite risks: (i) basic research in material science and physical-chemistry; (ii) technology developments and links with the industry sector. The necessary infrastructure will be available in the future building of the institute to continue these tasks.

* the new AFM equipment of the team will play a central scientific role; it will be used to perform extended structure/property characterization on interfaces of interest; in situ and local scale multi-physics characterization (e.g. QNM, KPFM, SECM, non-harmonic impedance spectroscopies) will be performed to analyze charge transfer phenomena and multi-step reaction paths at photo-electrochemical interfaces and to optimize systems of interest for target applications.

* local (UPSay) interactions with research groups working on similar research topics will be developed.

* international collaborations with existing partners in Europe, Japan, Russia, China, India and USA will be further developed; exchanges of PhD students are already scheduled.

* team members will continue their implication in the management of masters that can provide future PhD students to the team.



Eriée: what we plan to do (next period)

Eriée: Recherche et Innovation en Electrochimie pour l'Energie

Pierre Millet (Pr, UPSud, RE)

S. Franger (Pr, UPSud)
L. Assaud (MCF, UPSud)
J.-M. Duffault (MCF, UPSud)
A. Ranjbari (MCF, UPSud)

Same research topics

1. Water (photo) dissociation
2. CO_2 (photo-) electro-reduction
3. Li-ion batteries

Key scientific collaborations

The University of Tokyo
Tokyo University of Science
FAU Friedrich-Alexander Universität Erlangen-Nürnberg
Russian Academy of Sciences
University of California Santa Cruz
SOLEIL Synchrotron

Material science
(nano-structured interfaces)

Photo-electrochemical properties
(multiphysics characterization)

Devices
(conception, design, modelling)

Technology
(development, test protocols)

TiO_2 nanotubes & nanorods + surface co-catalysts

3D µ–battery

AFM-SECM

Fig.33. *Overview of the Eriée organization and objectives for the next period.*

APPENDICES

Appendix 1

EVALUATION CAMPAIGN 2018-2019
GROUP E

Contractual mission statement

ICMMO is not concerned by this.

Appendix 2

EVALUATION CAMPAIGN 2018-2019
GROUP E

Equipement, platforms

Appendix 2: Equipment, platforms

I- Instruments owned by the research unit.

NMR spectroscopy

Instrument Platform (PICMMO)

- Bruker 250 MHz spectrometer equipped with a QNP probe (^{1}H, ^{19}F, ^{31}P, ^{13}C) and an automatic sample changer
- Bruker 300 MHz spectrometer equipped with a BBO (^{1}H, X) probe and an automatic sample changer
- Bruker 360 MHz spectrometer equipped with a BBO (^{1}H, X) probe and an automatic sample changer
- 2 Bruker 400 MHz spectrometers with QXO, TBO (^{1}H, ^{31}P, X), TBI (^{1}H, ^{13}C, X) and BBI (^{1}H, X) probes
- Bruker 600 MHz spectrometer equipped with a proton/deuterium cryogenic probe

Mass spectrometry

PICMMO

- **Thermo scientific DSQ spectrometer, Electron Impact ionization or chemical ionization, quadrupole analyzer**
- **Thermo scientific TSQ spectrometer, Electrospray Ionization (ESI) or Atmospheric Pressure Chemical Ionization** (APCI), tandem triple quadrupole analyzer
- **Bruker MicrOTOFq spectrometer, Electrospray Ionization (ESI) or Atmospheric Pressure Chemical Ionization** (APCI), tandem quadrupole coupled to a Time-of-flight (Tof) analyzer

Microscopy and surface analysis

PICMMO

- Zeiss Supra 55 VP Variable pressure Scanning Electron Microscope with Field Emission Gun (SEM-FEG) equipped with Secondary Electron (SE), In-lens and Electron backscattered Electron (BSE) detectors, Energy Dispersive X-ray Spectroscopy (EDS), Electron BackScattered Diffraction (EBSD) and 2 heating plates (650°C EBSD compatible, 1000°C).
- Zeiss Sigma HD SEM-FEG equipped with Secondary Electron (SE), in-lens and Electron backscattered Electron (BSE) detectors, Energy Dispersive X-ray Spectroscopy (EDS), Electron BackScattered Diffraction (EBSD) and 600°C heating plate. A cathodoluminescence spectrum system is also present.
- Bruker DiInnova Atomic Force Microscope (AFM)
- Bruker Dimension Icon AFM. PeakForce Tapping mode. Measurement techniques: Atomic Force Microscopy (AFM), Quantitative Nanomechanical Mapping (QNM), Scanning Electrochemical Microscope (SECM), Kelvin Probe Force Microscope (KPFM). This microscope arrived in the ERIEE team in March 2018. It is currently undergoing a commissioning phase, after which it is expected to be accessible through the PICMMO Instrument Platform over defined time periods.
- Thermo Scientific K-Alpha X-ray Photoelectron Spectrometer (XPS) equipped with an Al K_α micro-focused X-ray source with variable spot sizes, an 180° double focusing hemispheric analyzer with 128 channels detector, a dual beam source and ultra-low energy electron beam for charge compensation, an ion gun for depth profiling, a tilt module for angle-resolved XPS depth-profiling (ARXPS) and a 4-axis stage for sample manipulation.

Instruments in research teams

- Bruker Dimension Icon AFM. PeakForce Tapping mode. Measurement techniques: Atomic Force Microscopy (AFM), Quantitative Nanomechanical Mapping (QNM), Scanning Electrochemical Microscope (SECM), Kelvin Probe Force Microscope (KPFM).
- DS100 Krüss goniometer for contact angle measurements
- Phase Shift Interferometer microscope MicroXam
- Olympus PMG-3 optical microscope
- Leica S9i Stereomicroscope
- Struers CitoPress mounting press

- Buehler, VibroMet vibratory polisher
- Struers LectroPol-5 electrolytic polisher

X-ray diffraction and scattering

PICMMO

- PANalytical X'Pert PRO Materials Research Diffractometer (MRD)
- PANalytical X'Pert PRO Multipurpose Powder Diffractometer (MPD), equipped with high temperature chamber (Anton Paar HTK1200) and with low temperature chamber (PHENIX, cryogenic system)
- Bruker PHOTON100 D8 Venture single crystal X-Ray Diffractometer (XRD) with four-circle goniometer equipped with a cryogenic system
- Bruker Kappa APEX II XRD with four-circle goniometer equipped with a cryogenic system
- Rotating anode Bruker Microstar Small Angle X-ray Scatterer

Research teams

- XRD equipped with high pressure cell (laboratory made)
- 2 Inel XRG 3000 X-ray generators with texture goniometers and CPS 120 detectors and Labotex software for texture analysis.
- XRD Stress analyser SET-X

Magnetic studies - Electronic, optical and vibrational spectroscopies

PICMMO

- Quantum Design MPMS 5 SQUID magnetometer equipped with an optical fiber, dc measurement
- Quantum Design XL7 SQUID magnetometer equipped with an optical fiber and He recondenser, dc and ac measurements.
- Bruker ELEXYS EPR spectrometer (X-band perpendicular and parallel modes, Q-band, ENDOR, variable temperature 4-300 K)
- Bruker Vertex 70 Infrared Fourier Transform Spectrometer equipped with several configurations for surface analysis

Research teams

- Quantum Design MPMS SQUID magnetometer
- Electronic absorption spectroscopy – Spectrophotometer Varian Cary 60 using a quartz cell with 1 cm optical path length.
- Stopped Flow SFM4000 (BioLogic) with 4 controlled syringes coupled to a Diode Array Spectrometer (256 pixels, integration time : 0.4ms to 10s, wavelength range 300-1100 nm, light path 1cm or 1 mm). Anaerobic and Organic solvent options. Freeze quench option with EPR and Mössbauer holders.
- Double-beam UV-Vis-NIR (180-3300 nm) spectrophotometer CARY 5000 (Agilent). Variable temperature measurements with a APD Cryogenics closed cycle helium cryogenic system including a DMX-1E cryostat and a DE-202 expander (temperature range 15-300 K).
- UV-Visible Spectrophotometer SPECORD 205 (Analytikjena)
- FT-IR spectrometer Spectrum Two (Pelkin Elmer) equipped with diamond-ATR and diffuse reflectance accessories
- FTIR spectrometer equipped with an IR microscope Nicolet
- Jasco J-815 Circular Dichroism Spectrometer equipped with auto-sampler and temperature controller (Peltier effect)

Femtosecond Laser

Research teams

- Femtosecond Laser (Satsuma, Amplitude Systèmes)

Thermal analyses

Research teams

- Thermal analysis platform (ATG, DSC) (Setaram Labsys, Setaram Setsys Evo, 2x Setaram TG92, Setaram Setsys, Laboratory-made Thermodeflection system)

Mass and size measurements

Research teams

- SEC-MALS20 (Malvern) for absolute molar mass characterization of polymers
- Zetasizer Nanoparticle size analyzer (nano-ZS, ZEN3500) from Malvern

Calculations

Research teams

- 3 nodes cluster Dell PowerEdge R910 (3 x 64 CPUs – 1 Go RAM/CPU – 11 To HD) + 2 workstations Dell PowerEdge R640 (2x48 CPUs – 2 Go RAM/CPU – 2x2,4 To HD)

Electrochemistry

Research teams

- GenHyTech platform : Production of pressurized hydrogen by polymer electrolyte water electrolysis. Electrochemical engineering, cell/stack design, system qualification, performance measurement and ageing
- Specific equipment for battery testing, cycling and ageing under thermostated conditions.
- Specific electrochemical equipment for carbon dioxide reduction and online product analysis by gas chromatography
- Specific photo-electrochemical equipment (light simulator, calibrators, quartz cells, low current potentiostat) for water photo-dissociation and carbon dioxide photo-reduction
- Electrochemical and photo-electrochemical Impedance Spectroscopy (EIS)
- Cyclic voltammetry, Metrohm potentiostat Autolab (PGSTAT 20).

Synthesis equipment (molecules, macromolecules, materials)

Research teams

- Photochemical synthesis platform, with wavelength modularity (mono or polychromatic) and 5 mL to 1 L scale
- Flow synthesis platform (Vapourtec)
- FlowSyn (Uniqsis), continuous flow reactor
- Jacomex BS531 glovebox equipped with a freezer and several other gloveboxes
- *ÄKTAprime* protein purification system – Purification of proteins
- Freezer -80 °C – Storage of biomolecules and cells (proteins, DNA…)
- *Real-Time qPCR* – Real-time quantitative polymerase chain reaction (for amplification of a targeted DNA).
- Discovery microwave from CEM equipped with coolmat
- Image furnaces (Crystal System FZ-T-4000-H-II-PP, Crystal System FZ-T-4000-H-VII-VPO-PC, NEC SC-N15HD)
- 2 Rolling mills (one with crenellated rollers)
- Sheet metal guillotine
- Heat treatment furnaces

Separative Technics

Research teams

- HPLC composed with a Jasco quaternary pump (PU2089), a column oven 6 positions Hitachi and two detectors: a UV single wavelength UV100 from Thermo Separation Product and a circular dichroism CD2095 Plus from Jasco.

- HPLC composed with a Jasco isocratic pump (PU4185), a column oven 3 positions Hitachi and a UV single wavelength detector UV100 from Thermo Separation Product.
- HPLC chain 1260 Infinity (Agilent) equipped with DAD, ELSD and fractions collector
- GC 2010 Plus from Shimadzu equipped with a split/splitless injector and a FID detector (3 systems). One of these is equipped with a second split/splitless detector and two other detectors: one FID and one FPD.
- GC-430 from Varian equipped with a split/splitless injector and a FID detector and an autosampler.
- SFC Thar Investigator hybrid system (analytical and semi preparative) equipped with an autosampler, a column oven, a PDA detection (Waters PDA2998) and a fraction collector (6 fractions).

Metallurgy

Research teams

- Shimadzu HMV-G-FA microhardness tester (Vickers and Knoop indentors)
- Leco M-400-H microhardness tester
- Zwick/roell Z010, tensile test machine
- 2 Creep test machines

II- Instruments used by the members of the research unit outside ICMMO.

National and international Instruments

- TGIR RMN
- Synchrotron facilities : Soleil Saint-Aubin, ESRF Grenoble
- Neutron diffusion and diffraction facilities : LLB, Orsay – ILL, Grenoble
- SIMS Kameca, Ile de France platform, Meudon
- Laboratoire National des Champs Magnétiques Intenses, Grenoble
- National High Magnetic Field Lab, Tallahassee-USA

Other Instruments

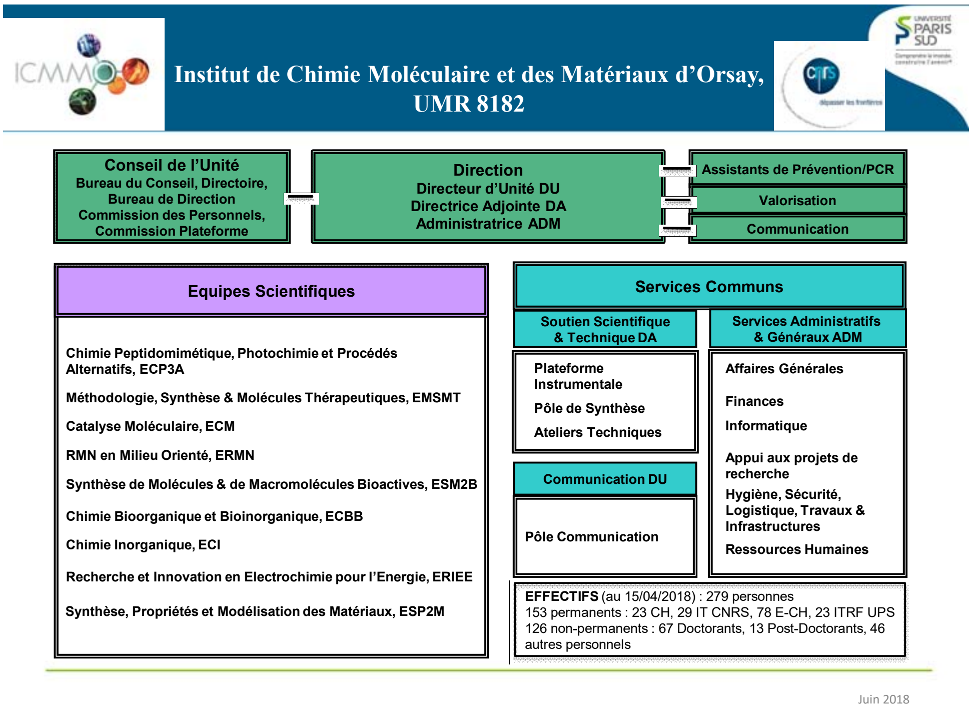
- Fluorescence spectroscopy – Corrected fluorescence spectra upon one-photon excitation (ENS, Paris, France) were recorded at 293 K with a Photon Technology International QuantaMaster QM-1 spectrofluorimeter (PTI, Monmouth Junction, NJ).
- Fluorescence microscopy – Epifluorescence imaging of the sample was achieved on a home built microscope (ENS, Paris, France). The setup incorporates three light sources. Epifluorescence illumination was performed using a FF505-606-Di01 (Semrock, Rocherster, NY) dichroic mirror and a 10× objective (Fluar, NA 0.5; Zeiss, Jena, Germany). The collected emitted fluorescence was filtered by a bi-band filter (FF524-628; Semrock) and the final image was reconstructed on a CCD camera chip (Luca-R; Andor Technology, Belfast, Northern Ireland).
- Matrix Assisted Laser Desorption Ionization – Time of Flight mass spectrometry (MALDI-TOF, protein analysis) - ICSN-CNRS, Gif-sur-Yvette, France.
- Multi Angle Light Scattering (MALS, protein molecular weight analysis) - ICSN-CNRS, Gif-sur-Yvette, France.
- **Isothermal Titration Calorimetry** (VP-ITC and ITC200 models, I2BC, Orsay, France) – principally dedicated to the study of molecular interactions. **ITC** is an equilibrium solution technic and is truly the only direct method to quantify Kd values without the use any label.
- **Differential scanning calorimetry** (VP-DSC model, I2BC, Orsay, France) – principally dedicated to the study of the thermal stability of macromolecules and their complexes.
- **Surface Plasmon Resonance (XPR36 Biorad, I2BC, Orsay, France) – The** technology allows real-time detection and monitoring of biomolecular binding events.
- **Oxygraph (LCP, Orsay, France) – Measurement of dissolved oxygen in solution or cellular oxygen comsumption in a closed-chamber system.**
- RAMAN microscopes (IPGP, Paris)
- Spark Plasma Sintering platform (ICMPE, Thiais)
- Physical measurement (PPMS) platform (LPS, Orsay)

Département d’évaluation
de la recherche

Appendix 3

EVALUATION CAMPAIGN 2018-2019
GROUP E

Organisational chart



Institut de Chimie Moléculaire et des Matériaux d’Orsay, UMR 8182

Conseil de l’Unité
Bureau du Conseil, Directoire,
Bureau de Direction
Commission des Personnels,
Commission Plateforme

Direction
Directeur d’Unité DU
Directrice Adjointe DA
Administratrice ADM

Assistants de Prévention/PCR

Valorisation

Communication

Equipes Scientifiques

- Chimie Peptidomimétique, Photochimie et Procédés Alternatifs, ECP3A
- Méthodologie, Synthèse & Molécules Thérapeutiques, EMSMT
- Catalyse Moléculaire, ECM
- RMN en Milieu Orienté, ERMN
- Synthèse de Molécules & de Macromolécules Bioactives, ESM2B
- Chimie Bioorganique et Bioinorganique, ECBB
- Chimie Inorganique, ECI
- Recherche et Innovation en Electrochimie pour l’Energie, ERIEE
- Synthèse, Propriétés et Modélisation des Matériaux, ESP2M

Services Communs

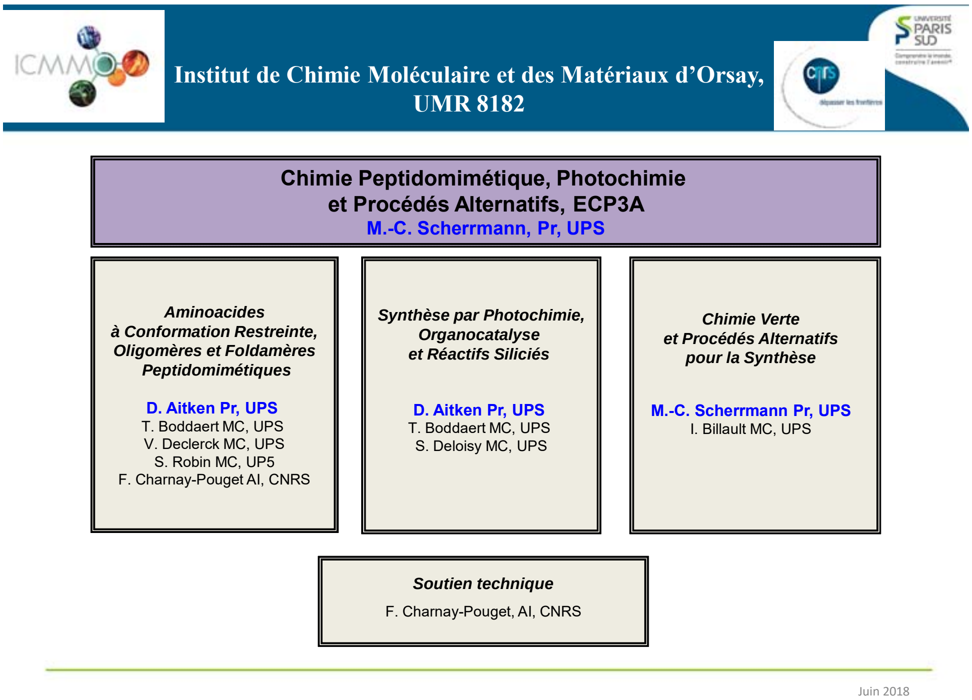
Soutien Scientifique & Technique DA
- Plateforme Instrumentale
- Pôle de Synthèse
- Ateliers Techniques

Communication DU
- Pôle Communication

Services Administratifs & Généraux ADM
- Affaires Générales
- Finances
- Informatique
- Appui aux projets de recherche
- Hygiène, Sécurité, Logistique, Travaux & Infrastructures
- Ressources Humaines

EFFECTIFS (au 15/04/2018) : 279 personnes
153 permanents : 23 CH, 29 IT CNRS, 78 E-CH, 23 ITRF UPS
126 non-permanents : 67 Doctorants, 13 Post-Doctorants, 46 autres personnels

Juin 2018



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Chimie Peptidomimétique, Photochimie et Procédés Alternatifs, ECP3A
M.-C. Scherrmann, Pr, UPS

Aminoacides à Conformation Restreinte, Oligomères et Foldamères Peptidomimétiques

D. Aitken Pr, UPS
T. Boddaert MC, UPS
V. Declerck MC, UPS
S. Robin MC, UP5
F. Charnay-Pouget AI, CNRS

Synthèse par Photochimie, Organocatalyse et Réactifs Siliciés

D. Aitken Pr, UPS
T. Boddaert MC, UPS
S. Deloisy MC, UPS

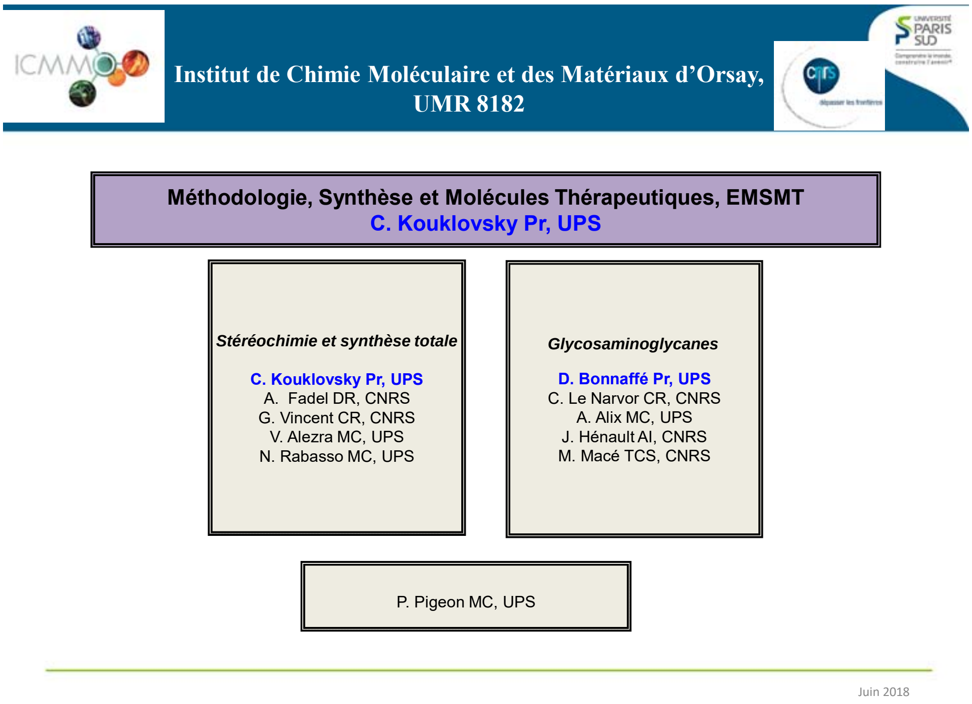
Chimie Verte et Procédés Alternatifs pour la Synthèse

M.-C. Scherrmann Pr, UPS
I. Billault MC, UPS

Soutien technique

F. Charnay-Pouget, AI, CNRS

Juin 2018



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Méthodologie, Synthèse et Molécules Thérapeutiques, EMSMT
C. Kouklovsky Pr, UPS

Stéréochimie et synthèse totale

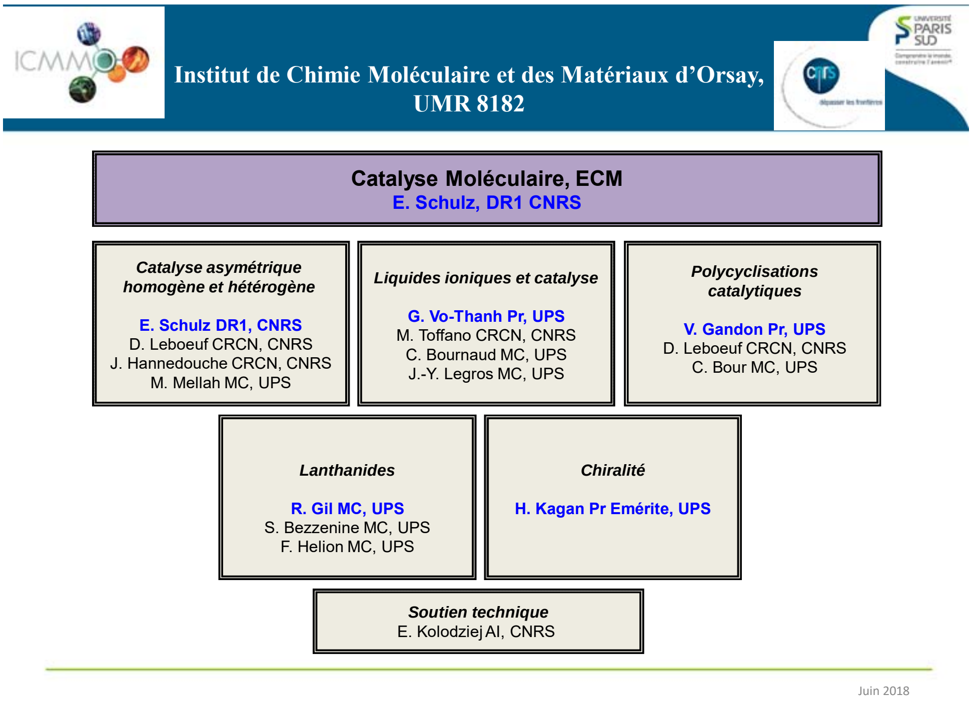
C. Kouklovsky Pr, UPS
A. Fadel DR, CNRS
G. Vincent CR, CNRS
V. Alezra MC, UPS
N. Rabasso MC, UPS

Glycosaminoglycanes

D. Bonnaffé Pr, UPS
C. Le Narvor CR, CNRS
A. Alix MC, UPS
J. Hénault AI, CNRS
M. Macé TCS, CNRS

P. Pigeon MC, UPS

Juin 2018



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Catalyse Moléculaire, ECM
E. Schulz, DR1 CNRS

Catalyse asymétrique homogène et hétérogène

E. Schulz DR1, CNRS
D. Leboeuf CRCN, CNRS
J. Hannedouche CRCN, CNRS
M. Mellah MC, UPS

Liquides ioniques et catalyse

G. Vo-Thanh Pr, UPS
M. Toffano CRCN, CNRS
C. Bournaud MC, UPS
J.-Y. Legros MC, UPS

Polycyclisations catalytiques

V. Gandon Pr, UPS
D. Leboeuf CRCN, CNRS
C. Bour MC, UPS

Lanthanides

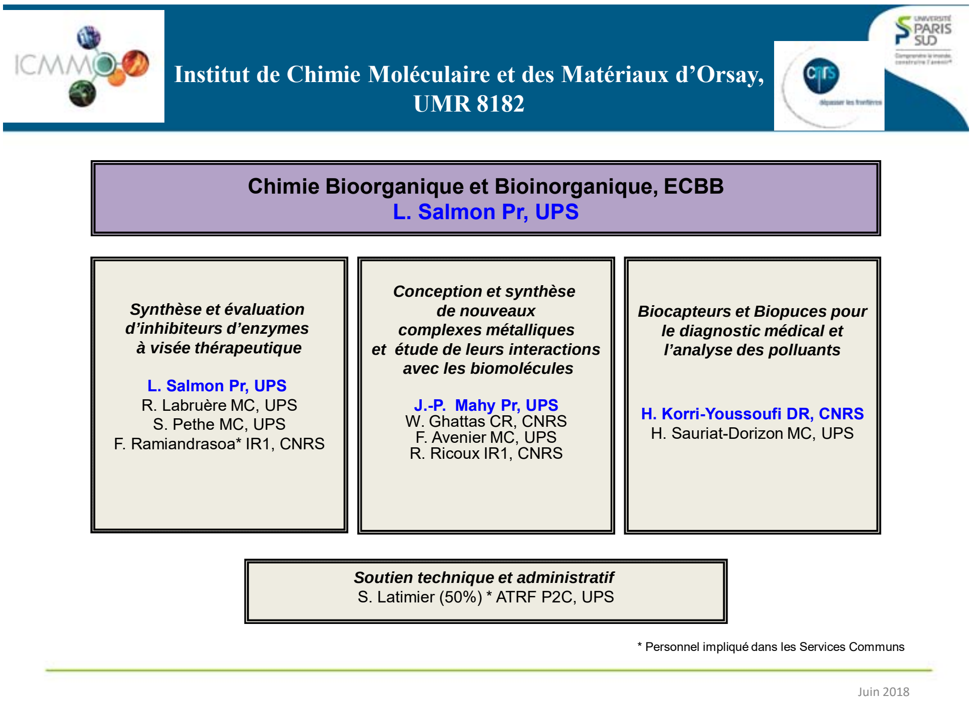
R. Gil MC, UPS
S. Bezzenine MC, UPS
F. Helion MC, UPS

Chiralité

H. Kagan Pr Emérite, UPS

Soutien technique
E. Kolodziej AI, CNRS

Juin 2018



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Chimie Bioorganique et Bioinorganique, ECBB
L. Salmon Pr, UPS

Synthèse et évaluation d’inhibiteurs d’enzymes à visée thérapeutique

L. Salmon Pr, UPS
R. Labruère MC, UPS
S. Pethe MC, UPS
F. Ramiandrasoa* IR1, CNRS

Conception et synthèse de nouveaux complexes métalliques et étude de leurs interactions avec les biomolécules

J.-P. Mahy Pr, UPS
W. Ghattas CR, CNRS
F. Avenier MC, UPS
R. Ricoux IR1, CNRS

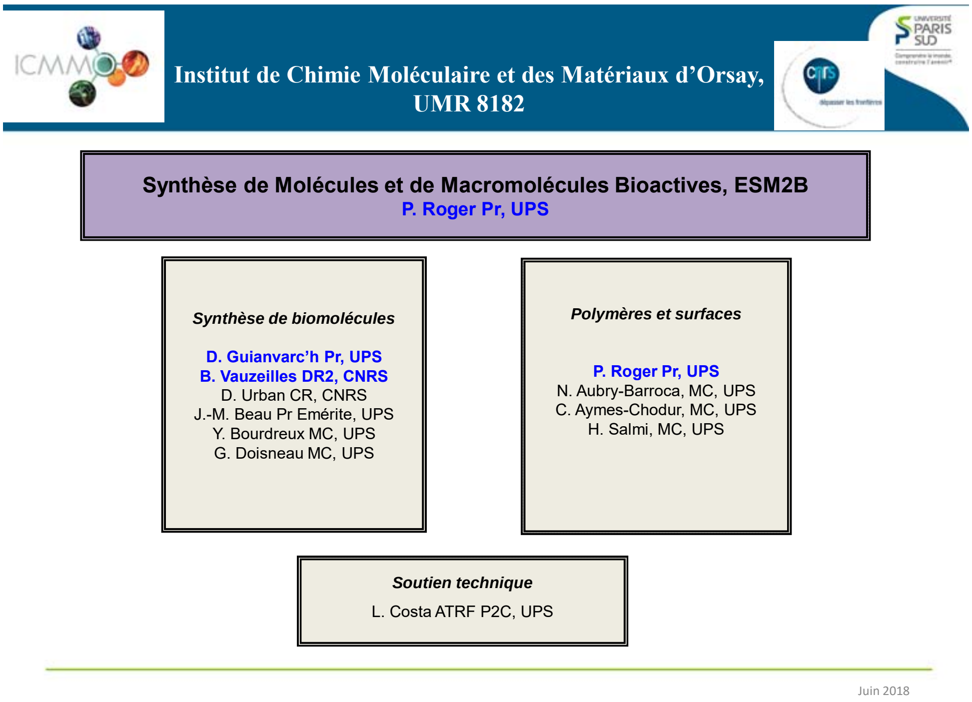
Biocapteurs et Biopuces pour le diagnostic médical et l’analyse des polluants

H. Korri-Youssoufi DR, CNRS
H. Sauriat-Dorizon MC, UPS

Soutien technique et administratif
S. Latimier (50%) * ATRF P2C, UPS

* Personnel impliqué dans les Services Communs

Juin 2018



Institut de Chimie Moléculaire et des Matériaux d’Orsay,
UMR 8182

Synthèse de Molécules et de Macromolécules Bioactives, ESM2B
P. Roger Pr, UPS

Synthèse de biomolécules

D. Guianvarc’h Pr, UPS
B. Vauzeilles DR2, CNRS
D. Urban CR, CNRS
J.-M. Beau Pr Emérite, UPS
Y. Bourdreux MC, UPS
G. Doisneau MC, UPS

Polymères et surfaces

P. Roger Pr, UPS
N. Aubry-Barroca, MC, UPS
C. Aymes-Chodur, MC, UPS
H. Salmi, MC, UPS

Soutien technique

L. Costa ATRF P2C, UPS

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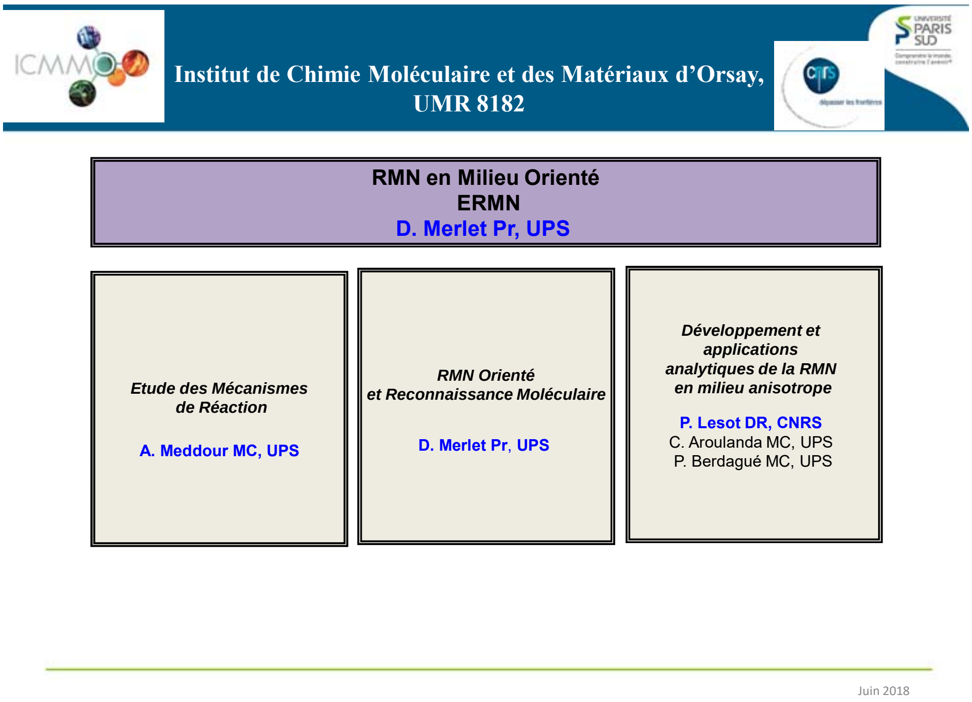


Institut de Chimie Moléculaire et des Matériaux d'Orsay, UMR 8182

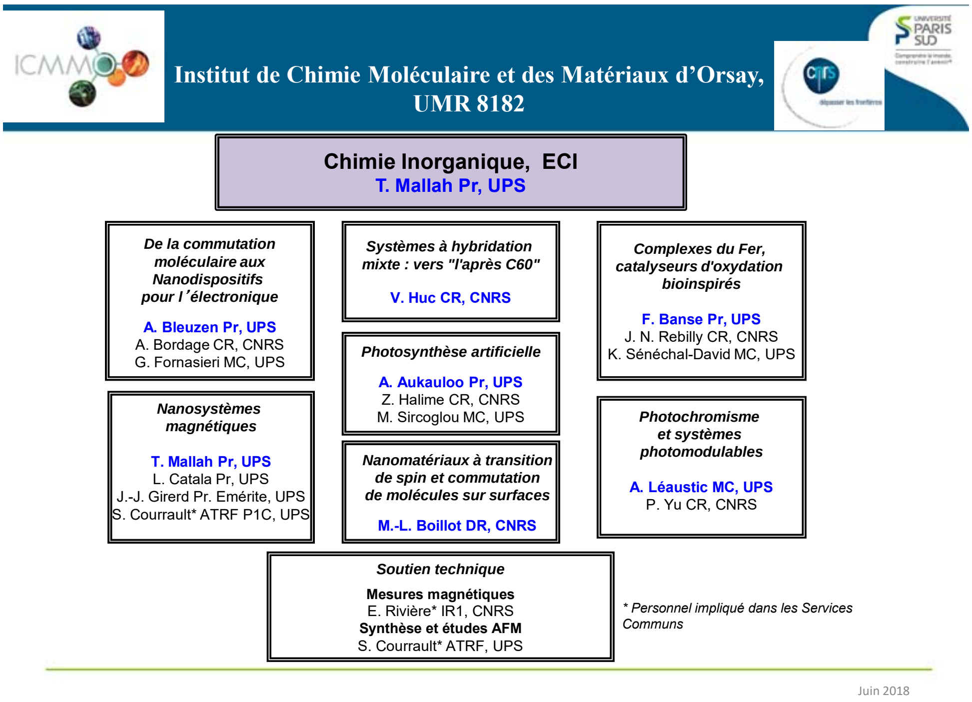
RMN en Milieu Orienté
ERMN
D. Merlet Pr, UPS

Etude des Mécanismes de Réaction
A. Meddour MC, UPS

RMN Orienté et Reconnaissance Moléculaire
D. Merlet Pr, UPS

Développement et applications analytiques de la RMN en milieu anisotrope
P. Lesot DR, CNRS
C. Aroulanda MC, UPS
P. Berdagué MC, UPS

Juin 2018



Institut de Chimie Moléculaire et des Matériaux d'Orsay, UMR 8182

Chimie Inorganique, ECI
T. Mallah Pr, UPS

De la commutation moléculaire aux Nanodispositifs pour l'électronique
A. Bleuzen Pr, UPS
A. Bordage CR, CNRS
G. Fornasieri MC, UPS

Nanosystèmes magnétiques
T. Mallah Pr, UPS
L. Catala Pr, UPS
J.-J. Girerd Pr. Emérite, UPS
S. Courrault* ATRF P1C, UPS

Systèmes à hybridation mixte : vers "l'après C60"
V. Huc CR, CNRS

Photosynthèse artificielle
A. Aukauloo Pr, UPS
Z. Halime CR, CNRS
M. Sircoglou MC, UPS

Nanomatériaux à transition de spin et commutation de molécules sur surfaces
M.-L. Boillot DR, CNRS

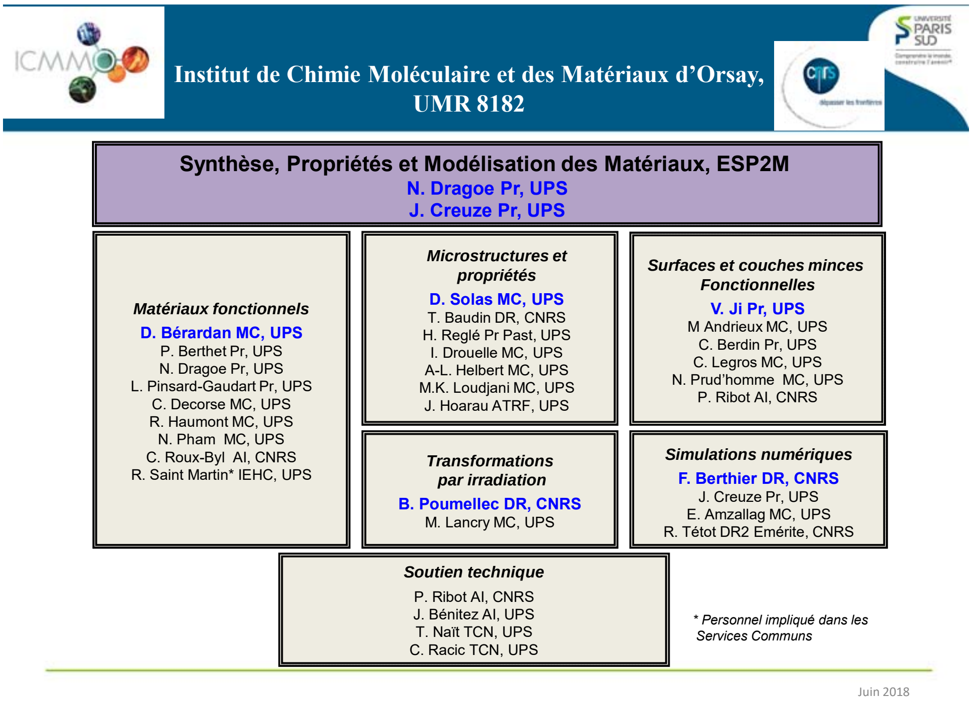
Complexes du Fer, catalyseurs d'oxydation bioinspirés
F. Banse Pr, UPS
J. N. Rebilly CR, CNRS
K. Sénéchal-David MC, UPS

Photochromisme et systèmes photomodulables
A. Léaustic MC, UPS
P. Yu CR, CNRS

Soutien technique
Mesures magnétiques
E. Rivière* IR1, CNRS
Synthèse et études AFM
S. Courrault* ATRF, UPS

** Personnel impliqué dans les Services Communs*

Juin 2018



Institut de Chimie Moléculaire et des Matériaux d'Orsay, UMR 8182

Synthèse, Propriétés et Modélisation des Matériaux, ESP2M
N. Dragoe Pr, UPS
J. Creuze Pr, UPS

Matériaux fonctionnels
D. Bérardan MC, UPS
P. Berthet Pr, UPS
N. Dragoe Pr, UPS
L. Pinsard-Gaudart Pr, UPS
C. Decorse MC, UPS
R. Haumont MC, UPS
N. Pham MC, UPS
C. Roux-Byl AI, CNRS
R. Saint Martin* IEHC, UPS

Microstructures et propriétés
D. Solas MC, UPS
T. Baudin DR, CNRS
H. Reglé Pr Past, UPS
I. Drouelle MC, UPS
A-L. Helbert MC, UPS
M.K. Loudjani MC, UPS
J. Hoarau ATRF, UPS

Surfaces et couches minces Fonctionnelles
V. Ji Pr, UPS
M Andrieux MC, UPS
C. Berdin Pr, UPS
C. Legros MC, UPS
N. Prud'homme MC, UPS
P. Ribot AI, CNRS

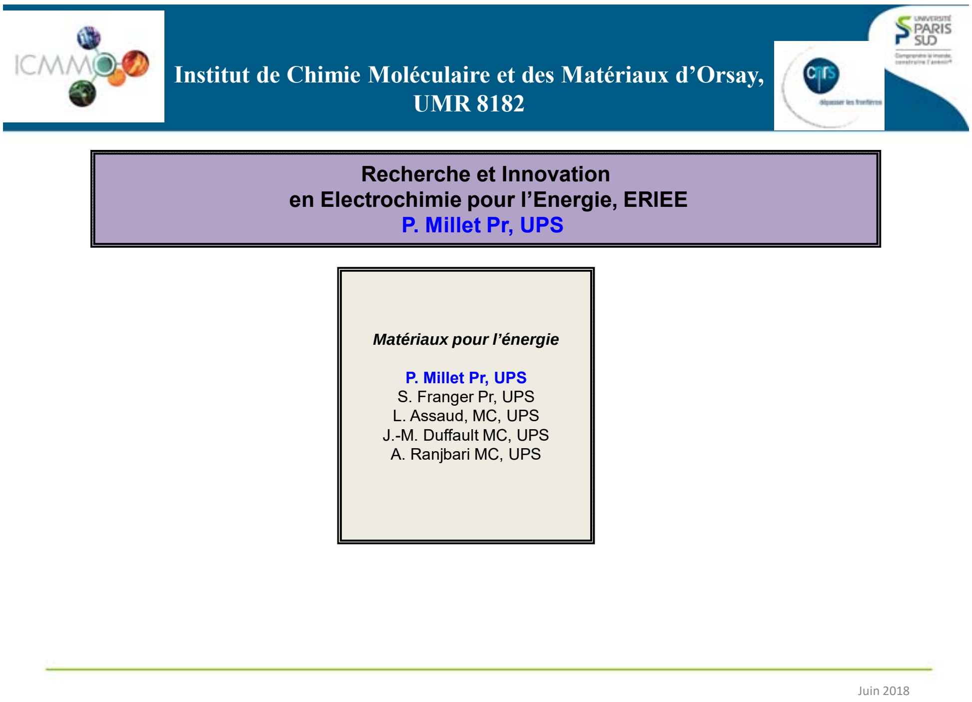
Transformations par irradiation
B. Poumellec DR, CNRS
M. Lancry MC, UPS

Simulations numériques
F. Berthier DR, CNRS
J. Creuze Pr, UPS
E. Amzallag MC, UPS
R. Tétot DR2 Emérite, CNRS

Soutien technique
P. Ribot AI, CNRS
J. Bénitez AI, UPS
T. Naït TCN, UPS
C. Racic TCN, UPS

** Personnel impliqué dans les Services Communs*

Juin 2018



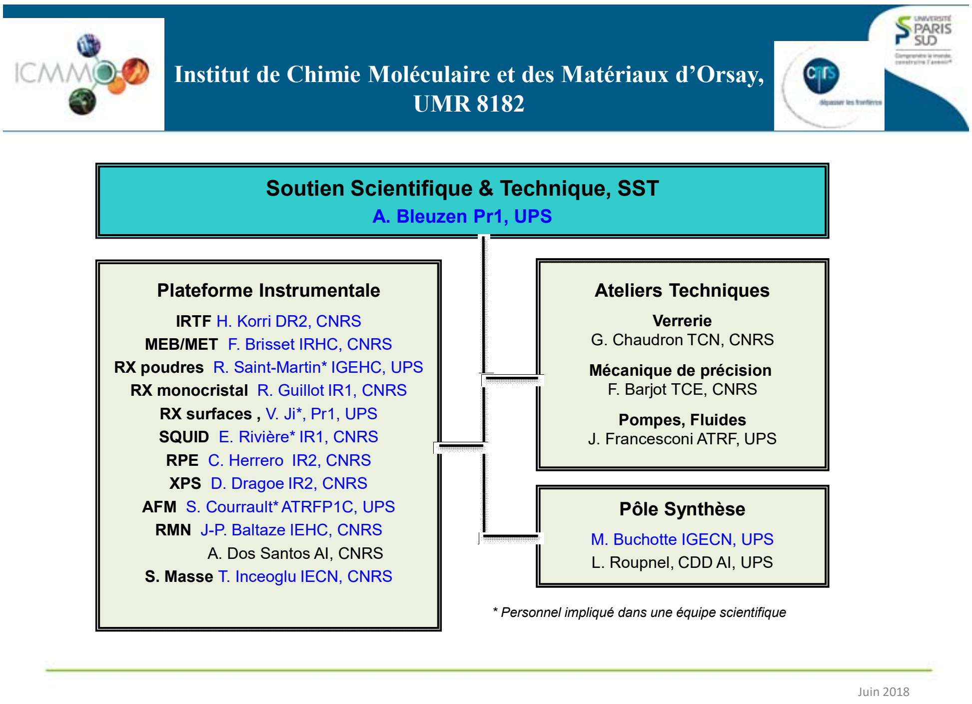
Institut de Chimie Moléculaire et des Matériaux d'Orsay, UMR 8182

Recherche et Innovation en Electrochimie pour l'Energie, ERIEE
P. Millet Pr, UPS

Matériaux pour l'énergie

P. Millet Pr, UPS
S. Franger Pr, UPS
L. Assaud, MC, UPS
J.-M. Duffault MC, UPS
A. Ranjbari MC, UPS

Juin 2018



Institut de Chimie Moléculaire et des Matériaux d'Orsay, UMR 8182

Soutien Scientifique & Technique, SST

A. Bleuzen Pr1, UPS

Plateforme Instrumentale

IRTF H. Korri DR2, CNRS
MEB/MET F. Brisset IRHC, CNRS
RX poudres R. Saint-Martin* IGEHC, UPS
RX monocristal R. Guillot IR1, CNRS
RX surfaces , V. Ji*, Pr1, UPS
SQUID E. Rivière* IR1, CNRS
RPE C. Herrero IR2, CNRS
XPS D. Dragoe IR2, CNRS
AFM S. Courrault* ATRFP1C, UPS
RMN J-P. Baltaze IEHC, CNRS
A. Dos Santos AI, CNRS
S. Masse T. Inceoglu IECN, CNRS

Ateliers Techniques

Verrerie
G. Chaudron TCN, CNRS

Mécanique de précision
F. Barjot TCE, CNRS

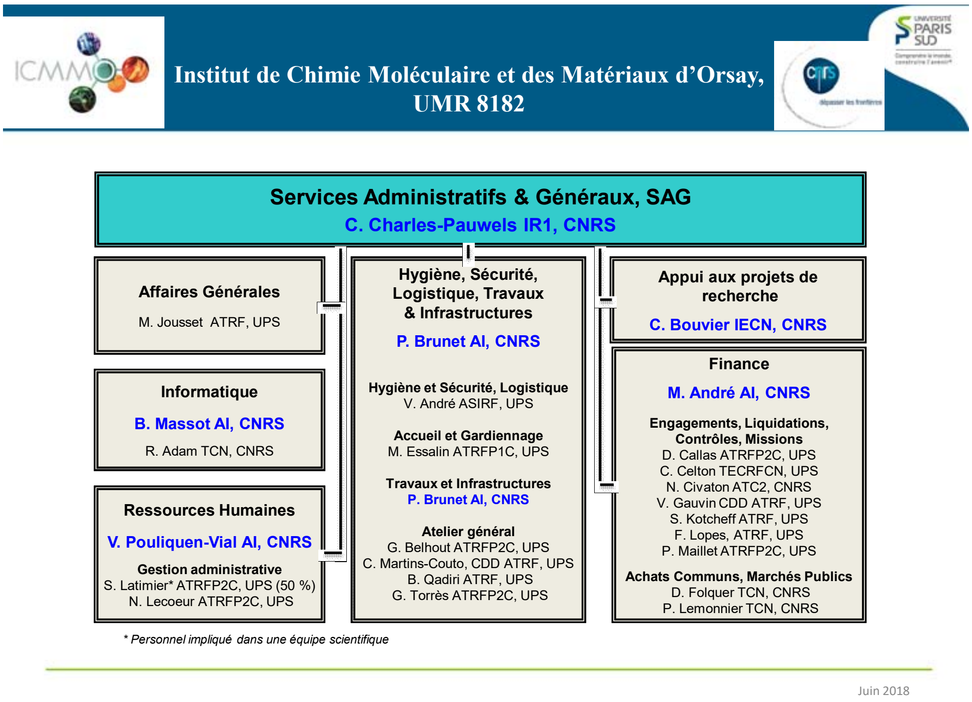
Pompes, Fluides
J. Francesconi ATRF, UPS

Pôle Synthèse

M. Buchotte IGECN, UPS
L. Roupnel, CDD AI, UPS

** Personnel impliqué dans une équipe scientifique*

Juin 2018



Institut de Chimie Moléculaire et des Matériaux d'Orsay, UMR 8182

Services Administratifs & Généraux, SAG

C. Charles-Pauwels IR1, CNRS

Affaires Générales

M. Jousset ATRF, UPS

Informatique

B. Massot AI, CNRS
R. Adam TCN, CNRS

Ressources Humaines

V. Pouliquen-Vial AI, CNRS

Gestion administrative
S. Latimier* ATRFP2C, UPS (50 %)
N. Lecoeur ATRFP2C, UPS

Hygiène, Sécurité, Logistique, Travaux & Infrastructures

P. Brunet AI, CNRS

Hygiène et Sécurité, Logistique
V. André ASIRF, UPS

Accueil et Gardiennage
M. Essalin ATRFP1C, UPS

Travaux et Infrastructures
P. Brunet AI, CNRS

Atelier général
G. Belhout ATRFP2C, UPS
C. Martins-Couto, CDD ATRF, UPS
B. Qadiri ATRF, UPS
G. Torrès ATRFP2C, UPS

Appui aux projets de recherche

C. Bouvier IECN, CNRS

Finance

M. André AI, CNRS

Engagements, Liquidations, Contrôles, Missions
D. Callas ATRFP2C, UPS
C. Celton TECRFCN, UPS
N. Civaton ATC2, CNRS
V. Gauvin CDD ATRF, UPS
S. Kotcheff ATRF, UPS
F. Lopes, ATRF, UPS
P. Maillet ATRFP2C, UPS

Achats Communs, Marchés Publics
D. Folquer TCN, CNRS
P. Lemonnier TCN, CNRS

** Personnel impliqué dans une équipe scientifique*

Juin 2018

Appendix 4

EVALUATION CAMPAIGN 2018-2019
GROUP E

Selected scientific production and activities

The ICMMO unit as a whole considers its selected scientific products and activities to be the collected contributions of each of the 9 research teams, to which is added the production of the Common Services, essentially from the Instrument Platform.

Appendix 4

Team 1- CP3A

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Chimie Peptidomimétique et Procédés Alternatifs**
Acronym:	**CP3A**
Director's name (current contract):	**Marie-Christine SCHERRMANN**
Director's name (future contract):	**Marie-Christine SCHERRMANN**

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

1- Articles

Scientific articles

1- *Stereoselective intermolecular [2+2]-photocycloaddition reactions of maleic anhydride: stereocontrolled and regiocontrolled access to 1,2,3-trifunctionalized cyclobutanes*. F. Hernvann, G. Rasore, V. Declerck, D. J. Aitken, *Org. Biomol. Chem.*, **2014**, *12*, 8212-8222

2- *Fine Tuning of β-Peptide Foldamers: a Single Atom Replacement Holds Back the Switch from an 8-Helix to a 12-Helix.* A. Altmayer-Henzien, V. Declerck, J. Farjon, D. Merlet, R. Guillot, D. J. Aitken, *Angew. Chem. Int. Ed.*, **2015**, *54*, 10807-10810

3- *Cupreine grafted onto silica as an enantioselective and recyclable catalyst for the 1,4-addition of malonate to trans-β-nitrostyrene*. I. Billault, R. Launez, M.-C. Scherrmann, *RSC Adv.*, **2015**, *5*, 29386-29390

4- *Synthesis of functionalized tryptamines by Brønsted acid catalysed cascade reactions.* N. Melis, F. Secci, T. Boddaert, D. J. Aitken, A. Frongia, *Chem. Commun.*, **2015**, *51*, 15272-15275

5- *13-Helix folding of a β/γ-peptide manifold designed from a "minimal-constraint" blueprint*. M. Grison, S. Robin, D. J. Aitken, *Chem. Commun.*, **2016**, *52*, 7802-7805

6- *Total synthesis of triazole-linked C-glycosyl flavonoids in alternative solvents and environmental assessment in terms of reaction, workup and purification.* F. Pessel, I. Billault, M.-C. Scherrmann, *Green Chem.*, **2016**, *18*, 5558-5568

7- *An α-Helix-Mimicking 12,13-Helix: Designed α/β/γ-Foldamers as Selective Inhibitors of Protein–Protein Interactions*. C. M. Grison, J. A. Miles, S. Robin, A. J. Wilson, D. J. Aitken, *Angew. Chem. Int. Ed.*, **2016**, *55*, 11096-11100

8- *Studies on cyclization reactions of 3-amino-2,4-dihydroxybutanoic acid derivatives*. M. Esgulian, V. Belot, R. Guillot, S. Deloisy, D. J. Aitken, *Org. Biomol. Chem.*, **2017**, *15*, 1453-1462

9- *Cooperative 5- and 10-membered ring interactions in the 10-helix folding of oxetin homo-oligomers*. S. S. Ragab, A. Kassir, R. Guillot, M.-C. Scherrmann, T. Boddaert, D. J. Aitken, *Chem. Commun.*, **2018**, *54*, 1968-1971

10- *Preparation of cyclobutene acetals and tricyclic oxetanes via photochemical tandem and cascade reactions*. J. Buendia, Z. Chang, H. Eijsberg, R. Guillot, A. Frongia, F. Secci, J. Xie, S. Robin, T. Boddaert, D. J. Aitken, *Angew. Chem. Int. Ed.*, **2018**, *57*, 6592-6596

Review articles

Other articles (professional journals, etc.)

2- Books

Scientific book edition

Book chapters

1- Electrochemical glycosylation, A. Marra, M.-C. Scherrmann, 40, 160-177, A. Pilar Rauter, T. Lindhorst, Y. Queneau, Royal Society of Chemistry, 2014, Specialist Periodical Reports - Carbohydrate Chemistry

3- Meetings

Meeting abstracts

4- Meeting and congress organisation

1- D. J. Aitken co-Chairman (with I. HUC, Bordeaux) of the international congress: "Paris Foldamers Symposium", Paris, April 10-12, 2013 (180 participants).

2- D. J. Aitken member of the Scientific Committee of the biennial conferences of the French Group of Peptides and Proteins (GFPP): "18th GFPP Congress", Sète, May 26-31, 2013; "19th GFPP Congress", Port Bail, May 17-22, 2015.; "20th GFPP Congress", Arcachon, May 26-30, 2017.

3- D. J. Aitken member of the Scientific Committee: "ICSN-UPSay Natural Substances Symposium", Gif-sur-Yvette, 29-30 June 2017.

5- Electronic tools and products

Softwares
Databases
Tools for decision-making

6- Instruments and methodology

Prototypes

- Laboratory-made flow synthesis platform equipped with in-line HPLC analysis

Platforms and observatories

- Photochemical synthesis platform, with wavelength modularity (mono or polychromatic) and 5 mL to 1 L scale
- Flow synthesis platform (Vapourtec)
- Jasco J-815 Circular Dichroism Spectrometer equipped with auto-sampler and temperature controller (Peltier effect)
- UV-Visible Spectrophotometer SPECORD 205 (Analytikjena)
- FT-IR spectrometer Spectrum Two (Pelkin Elmer) equipped with diamond-ATR and diffuse reflectance accessories
- HPLC chain 1260 Infinity (Agilent) equipped with DAD, ELSD and fractions collector
- Microwaves reactor (CEM Discover)

7- Other products

Artistic creations
Movie or theatre play creation
Movies

8- Editorial activities

Participation to journal editorial boards (books, collections)

1. C. Tomasini, I. Huc, D. J. Aitken, F. Fülöp, Guest Editor: special issue on foldamers, *Eur. J. Org. Chem*, 2013, Issue 17, pp. 3408-3596.
2. D. J. Aitken, Guest Editor: themed issue on foldamer chemistry, *New J. Chem.*, **2015**, *39*, Issue 5, pp. 3188-3189.

9- Peer reviewing activities

Reviewing of journal articles

The members of the team are regularly asked to evaluate submitted articles. The main journals are: *Nat. Chem., J. Am. Chem. Soc., Angew. Chem. Int. Ed., Chem. Commun., Chem. Eur. J., Org. Lett., OBC, J. Org. Chem., Eur. J. Org. Chem, Beilstein J. Org. Chem, Synthesis, Synlett, Peptide Sci., Green Chem., New J. Chem.,* and *C. R. Chim.* For this last journal, M.-C. Scherrmann obtained a certificate of « outstanding contribution in reviewing » awarded in october 2016.

Grant evaluation (public or charities)

Regional Programs:

- Research projects of regional interest (APR 2013) Région Centre (M.-C. Scherrmann)
- Aquit@ide Program, Aquitaine (2014, 2015; D. J. Aitken)
- Allocation Program, University of Reims Champagne-Ardenne (2016, D. J. Aitken)
- Research projects of regional interest (APR IR 2016) Région Centre Val de Loire (I. Billault)
- ARD 2020 Cosmetosciences program (2016, M.-C. Scherrmann)
- Doctoral Contracts Région Grand Est (2017, D. J. Aitken)
- Doctoral Contracts doctoral school “Agriculture Alimentation BIologie Environnement Santé” (2013, 2017, 2018, M.-C. Scherrmann)

National programs:

- ANR projects ("blanc" SIMI 7, JCJC SIMI 7, 2013, M.-C. Scherrmann; @RAction program, 2014, D. J. Aitken)
- CNRS, ITMM Challenge, Mission for Interdisciplinarity (2013, D. J. Aitken)

Foreign programs:

- Promotions Committee, University of Kent – UK (2014, D. J. Aitken)
- Promotions Committee, University of Newcastle – UK (2017, D. J. Aitken)
- FWO – Vlaanderen (2013, 2014, D. J. Aitken)
- NKFI-EPR, National Research Development & Innovation Office– Hongrie (2016, D. J. Aitken)
- Expert for the Research Quality Evaluation Committee of the Italian Universities for the period 2011-2014 "VQR 2011-2014" (2016, M.-C. Scherrmann)

Participation to lab site visit committees (Hceres etc.)

- CMS Expert Committee 2160003403 - LPM, Grenoble - Chair of the Committee (2014-2015, D. J. Aitken)
- CMS Expert Committee 2170004307 - ScanMAT & ISCR, Rennes (2015-16, D. J. Aitken)

Participation to institutional committees and juries (CNRS, INSERM, etc.)

The team members were part of various recruitment juries for ITA/BIATSS (1 Technical Assistant, 2 Assistant Engineers and 2 CNRS Technician; F. Charnay-Pouget) or teacher-researchers (6 Lecturers: D. J. Aitken (2), I. Billault (2), and M.-C. Scherrmann (2); 4 Professors: D. J. Aitken (1), M.-C. Scherrmann (3))

They are also members of various councils or committees:

- *Council of the department of Chemistry:* D. J. Aitken, elected member (2007-15), coopted member since 2015; I. Billault elected member since 2015; M.-C. Scherrmann, appointed member since 2015
- *Academic Council of Université Paris-Saclay:* D. J. Aitken, elected member since 2015
- *Academic Council of Université Paris-Sud and Research Commission:* M.-C. Scherrmann, elected member, appointed member of the Bureau
- *ICMMO Council:* D. J. Aitken (since 2013 as the Director of the Institute), I. Billault (appointed member, 2012-2015), T. Boddaert (elected member since 2015), F. Charnay-Pouget (elected member since 2015), V. Declerck (elected member 2013-2015), S. Deloisy (elected member since 2018), S. Robin (elected member 2015-2018), M.-C. Scherrmann (since 2013 as team manager)
- *National Council of Universities (Chemistry):* D. J. Aitken, elected reserve member (2011-2015 and since 2017)
- *Regional grading Committee (BAP B, Chemistry):* D. J. Aitken, (2014, 2015 and 2017)
- *Consultative Committee of Specialists for Chemistry (Paris-Sud University)*: V. Declerck (elected member since 2014), S. Deloisy (elected member 2010-2014), I. Billault (elected member 2010-2014), M.-C. Scherrmann (elected reserve member 2014-2015, member of the Bureau since 2015)

10- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

National public grants (ANR, PHRC, FUI, INCA, etc.)

- ANR - DFG Chemistry 2012-2015: CycloBeta-NPY: small-ring amino acids for the construction of analogues of Neuropeptide Y. (D. J. Aitken, V. Declerck)
- CNRS Interdisciplinary Collaborative Research Project " Défi instrumentation aux limites " 2013-2014: Real-time study of continuous flow reactions by MRI and NMR. (Coordinator D. Merlet, ERMN, ICMMO; I. Billault, M.-C. Scherrmann)
- ANR - PRC 2017-2020 - CP3A / IRAMIS-CEA / ISMO- Tuning foldamer building blocks using sulfur (D. J. Aitken, S. Robin, F. Charnay-Pouget)

Local grants ("collectivités territoriales")

PIA (Labex, Equipex etc.) grants

- InterLabEx PALM / CHARM3AT, D. J. Aitken, V. Declerck, CP3A / IRAMIS-CEA / ISMO, LaLiFold, 2013-2015
- LabEx CHARM3AT, I. Billault, Préparation de monolithes fonctionnalisés pour leur utilisation en catalyse et en conditions de flux, 2014-2015
- LabEx CHARM3AT, D. J. Aitken, S. Robin, CP3A / PPSM-ENS Cachan, CD-PhotoOrganoCat, 2015-2017
- Labex CHARM3AT, V. Declerck, L'Acide N-Aminoazétidine-2-carboxylique : Un Building Block pour la Construction de Nouvelles Architectures Moléculaires Pseudopeptidiques, 2016-2017
- LabEx CHARM3AT, D. J. Aitken, CP3A / ICSN, FoldaRho, 2017-2019
- Labex CHARM3AT, M.-C. Scherrmann, I. Billault, CP3A/ECHO, UVSQ, Multi-organocatalyse en flux continu, 2017-2018
- LabEx CHARM3AT, S. Robin, Développement de protocoles organocatalysés pour la synthèse énantiosélective de beta-aminoacides soufrés, 2017-2018
- LabEx CHARM3AT, M.-C. Scherrmann, Synthèse de composés antioxydants en flux continu, 2017-2018

Grants from foundations and charities (ARC, FMR, FRM, etc.)

11- Visiting senior scientists and post-doc

Post-docs

- Elisa PARADES, 2014-15 (6 months, Contractual post-doc - ANR)
- France BOYAUD, 2014-15 (18 months, Post-doc contract - ANR, then ATER University Paris-Sud)
- Sherif S. RAGAB, 2015-16 (9 months, STDF Fellowship - French Institute of Egypt)
- Julien BUENDIA, 2016-18 (24 months, Contractual post-doc - Labex Charm3at)
- Samad JAUFURALLY 2017-18 (12 months, Contractual post-doc - Labex Charm3at)

Publications which these post-docs have co-authored : *J. Org. Chem.,* **2016**, *81*, 9983-9991; *J. Org. Chem.*, **2017**, *82*, 9832-9836; *J. Org. Chem.*, **2018**, *83*, 527-534; *Chem. Commun*., **2018**, *54*, 1968-1971; *Angew. Chem. Int. Ed.*, **2018**, *57*, 6592-6596.

Visiting senior scientists

- Wantanee SITTIWONG, visiting academic from Thammasat University (Thailand) 2016 (3 months)
- Francesco SECCI, visiting academic from University of Cagliari (Italy) 2017 (2 months)
- Assia KENICHE, visiting academic from Maghnia University Centre – Tlemcen, Algeria 2017 (2 months) and 2018 (2 months)

The visit from Dr Secci was part of a long-standing collaboration with the University of Cagliari. 10 publications dealing with sustainable synthetic methodologies (7 on organocatalysis, 3 on photochemistry) have been jointly authored with the group of Dr Secci since 2013: *Tetrahedron Lett.*, **2013**, *54*, 2825-2827; *Adv. Synth. Catal.*, **2014**, *356*, 941-945; *Synlett*, **2015**, *26*, 123-126; *Eur. J. Org. Chem.*, **2015**, 4358-4366; *Chem. Commun.*, **2015**, *51*, 15272-15275; *Org. Biomol. Chem.*, **2016**, *14*, 3394-3403; *Eur. J. Org. Chem.*, **2017**, 5896-5902; *Org. Biomol. Chem.*, **2017**, *15*, 9779-9784; *Org. Biomol. Chem.*, **2017**, *15*, 10053-10063; *Angew. Chem. Int. Ed.*, **2018**, *57,* 6592-6596.

12- Scientific recognition

Prizes

C. M. Grison:

- Physicochemical Sciences PhD Prize of the National Academy of Pharmacy, 2016.
- Excellence in Organic Chemistry PhD Prize of the IdF Section - Société Chimique de France, 2017.

Distinctions

IUF members

Chair of learned and scientific societies

Invitations to meetings and symposia (out of France)

- *A bottom-up approach for peptidomimetic foldamer design.* 7th Annual World Protein and Peptide Conference, Dalian, Chine, 25-28 avril 2014. D. J. Aitken
- *The role of short-range interactions for peptide folding.* 3rd U.S. Workshop on Foldamers, New York City, Etas-Unis, 20-22 juin 2018. D. J. Aitken

Members' long-term visits abroad

D. J. Aitken:

- Module *Synthetic Organic Photochemistry*, Master 2 Molecular Chemistry, Lebanese University, Beirut. 12 h/year (2013, 2014, 2015, 2016, 2017, and 2018)
- Thematic schools: 1st Vietnam-France School in Pharmaceutical Chemistry, Đồ Sơn, Hải Phòng, Vietnam, 20-23 octobre 2014. *Organic photochemical methodology for the preparation of molecules and molecular scaffolds of biological and therapeutic interest. (3 × 2 h lectures). a) Organic photochemistry: theory and practice. b) Photooxygenation of organic molecules. c) [2+2] Photocycloaddition reactions.*
- 2nd Vietnam-France School in Pharmaceutical Chemistry, Ho Chi Minh City, Vietnam, 24-27 octobre 2016. *Photooxygenation as a tool for selective transformations of molecules of biological and therapeutic interest. (1 × 3 h lecture)*

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

1- Socio-economic interactions / Patents

Invention disclosures

Méthode de production et de purification du Fluoral-P.
S. Robin, D. J. Aitken, F. Charnay-Pouget, V. André
Enveloppe Soleau ref. 463913, pli cacheté valable jusqu'au 03/12/2017.

Filed patents

Nouveaux composés, compositions et méthodes pour le traitement de la résistance à l'insuline
T. Issad, A.-F. Burnol, A. Gondoin, M. Miteva, B. Villoutreix, D. J. Aitken
Patent FR-1752287 (57 pp), 20/03/2017

Accepted patents

Nouveaux composés, compositions et méthodes pour le traitement de la résistance à l'insuline
T. Issad, A.-F. Burnol, A. Gondoin, M. Miteva, B. Villoutreix, D. J. Aitken
International Extension PCT/EP2018/056931 (73 pp) 20/03/2018

Licenced patents

2- Socio-economic interactions

Industrial and R&D contracts

Acros Organics, 2013-2014, Synthesis of small ring intermediates, D. J. Aitken, F. Charnay-Pouget, J. Ollivier

Cifre fellowships
Creation of labs with private-public partnerships
Networks and mixed units *(Science and technology only)*
Start-ups

3- Expertise

Consulting

Participation in expert committees (ANSES etc.)

Specialized Expert Committee (CES) "Chemicals covered by the REACh and CLP Regulations", since September 2017, I. Billault

Legal expertise

4- Expert and standardization reports

5- Public outreach

Radio broadcasts, TV shows, magazines
Journal articles, interviews, book edition, videos, etc.

Other popularization outputs

F. Charnay-Pouget has been actively involved in the organization and animation of science festival workshops ("Fête de la Science") since 2013. She is also involved in the events of the University Paris Sud "Make science" for high school and college students as a member of the jury. Since inauguration in 2018, she also runs a "Molecules and Aromas" workshop at the House of Initiation and Awareness of Sciences (MISS : a project supported by public funds, in collaboration with the Diagonale Paris-Saclay, Université Paris-Sud and the CNRS whose goal is to receive children from 8 to 14 years with their teachers to experience the scientific approach in all areas of the daily life.)

Debates on science and society

Conferences for the general public:

- Vers une chimie plus éco-compatible. M.-C. Scherrmann, Centre d'Alembert, 23 mars 2017, Orsay, France (https://www.youtube.com/watch?v=b6S99nyCBP0)
- Développement durable : vers quelle chimie? M.-C. Scherrmann, Palais de la découverte, 19 avril 2017, Paris, France (http://www.cite-sciences.fr/fr/ressources/conferences-en-ligne/saison-2016-2017/la-recherche-a-lhorizon-2037/)

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

1- Educational outputs

Books

Chimie verte. Concepts et applications, J. Augé, M.-C. Scherrmann, edp sciences, CNRS éditions, 2016, Savoirs actuels

The goal of this book, published by the CNRS in the well-known Savoirs Actuels collection and intended for students of Grandes Ecoles, Master, PhD students, researchers and teachers is to make understand the concepts and objectives of green chemistry, the indicators adopted for evaluating the greenness of a product or a process, to raise awareness of recent advances in all areas of chemistry.

E-learning, MOOCs, multimedia lessons, etc.

2- For humanities only, published PhD theses

3- Quality of PhD student supervision

8 students prepared and defended their theses during the reporting period. The average duration of the theses was 37 months. Thesis supervisors, supervisors and sources of funding are given in the following table.

Name	Thesis director(s) supervisor	Financial support	Duration (month)	PhD defence
ALTMAYER-HENZIEN Amandine	D. J. Aitken V. Declerck	Specific allocation for "Normalien"	37	29/10/2013
PESSEL Freddy	I. Billault - M.-C. Scherrmann	MESR	36	4/11/2013
AWADA Hawraà	D. J. Aitken - A Hachem S. Robin	Association Azm & Saade / Eiffel Joint-diploma thesis - Lebanese University	37	5/12/2014
GRISON Claire M.	D. J. Aitken S. Robin	MESR	37	23/11/2015
HERNVANN Florian	D. J. Aitken	ANR	37	30/11/2015

	V. Declerck			
LAUNEZ Remy	I. Billault	MESR	38	16/12/2015
ESGULIAN Mathieu	D. J. Aitken S. Deloisy	MESR	37	17/11/2017
KASSIR Ahmad	M.-C. Scherrmann - D. J. Aitken T. Boddaert	Ministry of the Interior / Municipality of Tyre, Lebanon	38	21/03/2018

In addition to these PhD Students, others students registered in a foreign University spent short periods under our supervision in our laboratory: Thailand (6 months), Italy (9 months) and Tunisia (4 months).

4- Students’ follow up in association with doctoral schools

Postdoc or career opportunities are reported to our students who are strongly encouraged to anticipate their future at the end of the thesis. The team keeps in touch with them by regularly inviting them to the traditional end-of-year meals and the summer barbecue.
The current situation of former doctoral students is given below:

Name	Position, company
ALTMAYER-HENZIEN Amandine	Teacher in “classes préparatoires”, Lycée Victor Hugo, Besançon
PESSEL Freddy	Research engineer, SurfactGreen, Rennes
AWADA Hawraà	Production Engineer, Capgemini
HERNVANN Florian	Postdoctoral Research Scientist, Université de Rouen
LAUNEZ Remy	Operating Analyst / Infrastructure Consultant, Sogeti, Bois-d’Arcy
GRISON Claire M.	Postdoctoral Research Scientist, Institut de Génomique Fonctionnelle, Montpellier
ESGULIAN Mathieu	Postdoctoral Research Scientist, Université Aix Marseille
KASSIR Ahmad	Recently returned to Lebanon

5- Participation to international training programs (e. g. Erasmus Mondus)

6- PhD student participation to scientific animation and unit/team life

PhD students are strongly involved in the scientific animation of the team. They are asked to present their work during seminars, encouraged to present the results of their research in the form of oral communication or poster at conferences. Research products from theses are summarized in the following table.

Name	ref. (IF)	Average IF	Oral/Posters Communications
ALTMAYER-HENZIEN Amandine	1. Tetrahedron Lett., 2013, 54, 802 (2.347) 2. Org. Biomol. Chem., 2013, 11, 7611 (3.559) 3. J. Org. Chem., 2013, 78, 6031 (4.785) 4. Angew. Chem. Int. Ed., 2015, 54, 10807 (11.709)	5.600	5/7
PESSEL Freddy	1. New J. Chem., 2015, 39, 1986 (3.277) 2. Green Chem., 2016, 18, 5558 (8.506) 3. Beilstein J. Org. Chem., 2016, 12, 2351 (2.697)	4.827	1/1
AWADA Hawraà	1. Tetrahedron, 2013, 69, 3571 (2.645) 2. Eur J. Org. Chem. 2014, 7148 (3.902) 3. J. Org. Chem., 2017, 82, 4819 (4.785)	3.777	0/3
HERNVANN Florian	1. Org. Biomol. Chem., 2014, 12, 8212 (3.559)	3.559	1/4
LAUNEZ Remy	1. RSC Adv., 2015, 5, 29386 (3.289)	3.289	0/2
GRISON Claire M.	1. New J. Chem., 2015, 39, 3270 (3.277) 2. Chem Commun, 2015, 51, 7939 (6.567) 3. Chem. Commun., 2015, 51, 16233 (6.567) 4. Chem. Commun., 2016, 52, 7802 (6.567) 5. Angew. Chem. Int. Ed., 2016, 55, 11096 (11.709) 6. J. Org. Chem., 2017, 82, 4819 (4.785)	6.579	1/6
ESGULIAN Mathieu	1. Org. Biomol. Chem., 2017, 15, 1453 (3.559)	3.559	1/2
KASSIR Ahmad	1. J. Org. Chem., 2016, 81, 9983 (4.785)	5.676	2/5

	2. Chem. Commun., 2018, 54, 1968 (6.567)		

On average, each thesis results in 2.3 articles and the average impact factor of these articles is 4.6.
These thesis students, as well as all trainees, are also fully involved in the life of the team whether for group tasks or for the moments of conviviality organized regularly.

7- Participation of team members in setting up Master courses

- Billault is responsible for the analytical chemistry platform in master 1- University Paris-Saclay
- M.-C. Scherrmann is co-responsible for professional M2 Instrumentation and Methods of Molecular Analysis - University Paris-Saclay
- D. J. Aitken is responsible of the teaching module "photons and radicals" - Research Master in Organic Chemistry - University Paris -Saclay

Département d’évaluation de la recherche

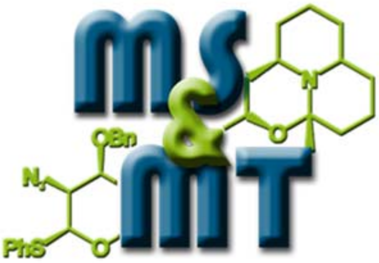
Appendix 4

Team 2 - MSMT

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Méthodologie, Synthèse & Molécules Thérapeutiques**
Acronym:	**MSMT**
Director's name (current contract):	**Cyrille KOUKLOVSKY**
Director's name (future contract):	**Cyrille KOUKLOVSKY**



I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

1- Articles

Scientific articles

1. *Bioinspired Oxidative Cyclization of the Geissoschizine Skeleton for the Total Synthesis of (-)-17-nor-Excelsinidine*. M. Jarret, A. Tap, C. Kouklovsky, E. Poupon, L. Evanno, G. Vincent, *Angew. Chem. Int. Ed.*, **2018**, 10.1002/anie.201802610.
2. *Base mediated fragmentation of bicyclic dihydro-3,6-oxazines: transformation of nitroso Diels-Alder cycloadducts*. R. Campagne, F. Schäkel, R. Guillot, V. Alezra, C. Kouklovsky, *Org. Lett.*, **2018**, *20*, 1884-1887.
3. *Frozen Chirality of Tertiary Aromatic Amides :Access to Enantioenriched Tertiary alpha-Amino Acid or Amino Alcohol without Chiral Reagent*. T. T. Mai, B. Viswambharan, D. Gori, R. Guillot, J.-V. Naubron, C. Kouklovsky, V. Alezra, *Chem. Eur. J.*, **2017**, *23*, 5787-5798.
4. *Unified biomimetic assembly of voacalgine A and bipleiophylline via divergent oxidative couplings*. D. Lachkar, N. Denizot, G. Bernadat, K. Ahamada, M. A. Beniddir, V. Dumontet, J.-F. Gallard, R. Guillot, K. Leblanc, E. O. N'Nang, V. Turpin, C. Kouklovsky, E. Poupon, L. Evanno, G. Vincent, *Nature Chemistry*, **2017**, *9*, 793-798 FI 27.893
5. *Efficient synthesis of both diastereomers of β,γ-diamino acids from phenylalanine and tryptophan*. N. Auberger, A. Stanovych, S. Thétiot-Laurent, R. Guillot, C. Kouklovsky, S. Cote Des Combes, C. Pacaud, I. Devillers, V. Alezra, *Amino Acids*, **2016**, *48(9)*, 2237-2242 FI 3.196
6. *Cerium(iv) ammonium nitrate mediated 5-endo-dig cyclization of α-amino allenylphosphonates to spirodienones*. P. Adler, A. Fadel, N. Rabasso, *Chem. Commun.*, **2015**, *51*, 3612-3615 FI 6.567.
7. *Synthesis of 5-Phosphonoisoxazoline N-Oxides by Selective O-Alkylation of Nitronate Anions*. V. Perez, N. Rabasso, A. Fadel, *Eur. J. Org. Chem.*, **2016**, 320-324
8. *Repairing the Thiol-Ene Coupling Reaction*.G. Povie, A.-T. Tran, D. Bonnaffe, J. Habegger, Z. Hu, C. Le Narvor, P. Renaud, *Angew. Chem. Int. Ed.*, **2014**, *53*, 3894-3898.
9. *Characterization of Glycosaminoglycan (GAG) Sulfatases from the Human Gut Symbiont Bacteroides thetaiotaomicron Reveals the First GAG-specific Bacterial Endosulfatase*. J. E. Ulmer, E. M. Vilen, R. B. Namburi, A. Benjdia, J. Beneteau, A. Malleron, D. Bonnaffe, P.-A. Driguez, K. Descroix, G. Lassalle, C. Le Narvor, C. Sandstrom, D. Spillmann, O. Berteau, *J. Biol. Chem.*, **2014**, *289*, 24289-24303.
10. *Direct Oxidative Coupling of N-Acetyl Indoles and Phenols for the Synthesis of Benzofuroindolines Related to Phalarine* T. Tomakinian, R. Guillot, C. Kouklovsky, G. Vincent, *Angew. Chem. Int. Ed.*, **2014**, *53*, 11881-11885

Scientific articles with last authorship *(Biology only)*

Review articles

Other articles (professional journals, etc.)

Clinical articles

2- Books

Scientific book edition

Book chapters

1. *Stereoselective Synthesis of Drugs and Natural Products,* G. Vincent, 41, V. Andrushko and N. Andrushko (editors), John Wiley and Son, Cycloadditions with Stereoselective C-N Bond Formation in Total Syntheses, 2013, 1ère edition
2. *Comprehensive Organic Synthesis, 2nd edition.* G. Vincent, C. Kouklovsky, Vol. 8: Reduction (editor J. Clayden), P. Knochel, G. A. Molander (editors in chiefs), Elsevier, Reduction of N=N, N-N, N-O and O-O bonds, 2014
3. *Topics in Heterocyclic Chemistry,* G. Vincent, Synthesis of Heterocycles by Metathesis Reactions, 115-190, J. Prunet (editor), Springer, Synthesis of Lactams by Metathesis Reactions, 2015

3- Meetings

Meeting abstracts

1. *Landscapes of taste.* L.-A. Garcon, G. Genua, Y. Hou, A. Buhot, R. Calemczuk, D. Bonnaffe, H. Lortat-Jacob, T. Livache, Y. Hou, 24th Annual Meeting of the European Chemoreception Research Organization (ECRO 2014), 10-13 septembre 2014, 244-245, Dijon, France
2. *Mini CD4-heparan Sulfate Mimetic Conjugates Display Sub Nanomolar Anti-HIV-1 Activity and Protect Macaques against a SHIV162P3 Vaginal Route Challenge.* F. Baleux, K. Arien, D. Desjardins, J. Michiels, Y.-M. Coic, B. J. Connell, D. Bonnaffe, K. Bouchemal, L. G. Le Grand, G. Vanham, N. Dereuddre-Bosquet, H. Lortat-Jacob, HIV Research for Prevention 2014, 28-31 octobre 2014, A 262, Cape Town, Afrique du Sud

4- Meeting and congress organisation

- As secretary (2013-2015), then President (2015-2018) of the Organic Chemistry Division of the French Chemical Society, C. Kouklovsky has co-organized 10 international symposia including 2 three day symposia (JCO 2013 and JCO 2016) with 600 registered persons. He was president of organizing committee for all symposia between 2015 and 2018.
- G. Vincent has co-organized the 7$^{\text{ème}}$ Symposium Français de Synthèse Totale in 2017 (Orsay).
- D. Bonnaffé, C. Le Narvor and A. Alix have organized the « 25$^{\text{èmes}}$ Journées du Groupe Français des Glycosciences » in 2014 (Paris).

5- Electronic tools and products

Softwares

Databases

N. Rabasso created and developed the ChemProducts software which is a database that stores all the chemicals present at ICMMO to easily locate them. Due to the merger of ICMMO and BIOCIS institutes in a single building in 2022 (BPC Project), the need for the development of a new version of this software that takes into account the whole university labs led to a new version that has been installed in April 2018.

Tools for decision-making

Cohorts *(Biology only)*

Solver competition tools *(Science and technology only)*

6- Instruments and methodology

Please, highlight the most selective.

Prototypes

Platforms and observatories

7- Other products

Artistic creations

Movie or theatre play creation

Movies

P. Adler (PhD student under the supervision of N. Rabasso) has recorded at the ACS meeting in San Diego (March 2016) a short video (3 min.) summarizing her research. This video, in English, is available on the Youtube plateform (https://youtu.be/XTJ51jZyOgY) and on the ACS website.

8- Editorial activities

Participation to journal editorial boards (books, collections)

9- Peer reviewing activities

Reviewing of journal articles

All permanent team members are regular reviewers for principal international journals (ACS, Wiley, Elsevier, ChemPubSoc Europe, RSC, Thieme, etc.)

Grant evaluation (public or charities)

All permanent team members are regular referees for national and international grant applications (ANR, LABEX, etc.)

Participation to lab site visit committees (Hceres etc.)

V. Alezra: expert for HCERES formation evaluation (Master of Chemistry, Licence of Chemistry, Licence in Chemistry and Physics)-2016

Participation to institutional committees and juries (CNRS, INSERM, etc.)

10- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

1. Marie Curie Fellowship DYNAMAX (V. Alezra 2013-2015)
2. Marie Curie Fellowship ELECTROINDOLE (G. Vincent) 2015-2017

National public grants (ANR, PHRC, FUI, INCA, etc.)

1. ANR Sulf@as (D. Bonnaffé, C. Le Narvor 2018-2022)
2. ANR ArDCo (G. Vincent 2017-2020)
3. ANR Mount Indole (G. Vincent 2015-2020)
4. ANR Hépaféron (D. Bonnaffé, C. Le Narvor 2013-2014)
5. Fondation pour le développement de la Chimie des Substances Naturelles 2012-2015 (PhD, Coord. G. Vincent)

Local grants ("collectivités territoriales")

PIA (Labex, Equipex etc.) grants

The name of the team member is underlined in the following list.

1. LabEx LERMIT 2012-2014 (Lermit T2, 132 k€ with S. Lesieur, C. Sizun, F. Bachelerie, Coord: D. Bonnaffe and K. Balabanian);
2. LabEx LERMIT 2015-2017 (Lermit T2, 129 k€ with S. Lesieur, C. Sizun, F. Bachelerie, Coord: D. Bonnaffe and K. Balabanian);
3. Prématuration IdEx Paris-Saclay 2016-2017 (6TMATIC, 42 k€ ,Coord. D. Bonnaffé);
4. IdEx Paris-Saclay (Départements SdV et Chimie) 2017 (D. Bonnaffé ; 5 k€ with S. Lesieur, C. Sizun,);

5. LabEx LERMIT 2018-2019 (Lermit T2, 10 k€ with S. Lesieur, C. Sizun, F. Bachelerie, Coord: D. Bonnaffe and K. Balabanian);
6. Labex LERMIT Emergence 2018-2019 (Sulf@mark, 15 k€ with S. Cohen-Kaminsky, R. Daniel, Coord: C. Le Narvor);
7. LabEx CHARM3AT 2015-2018 (G. Vincent; PhD with X. Moreau and I. Chataigner)
8. Inter-LabEx CHARM3AT/SYNORG 2017-2018 (V. Alezra; 1 year post-doc + 10 k€, with M. Sebban)

Grants from foundations and charities (ARC, FMR, FRM, etc.)

11- Visiting senior scientists and post-doc

Post-docs

The team has recruited 7 postdoctoral fellows during the 2013-2018 period, with various funding resources: ANR, LABEX, Europe (Marie Curie Fellowships) and industrial collaborations; except for the Marie Curie Fellowships, the average duration for postdocs is one year. The funding distribution is as follows:

Name	Funding	Current Position
Baby Wiswambharan	Marie Curie Fellowship	Academic position abroad
Radj K. Nandi	Marie Curie Fellowship	International postdoc
Aurélien Tap	ANR	Industry career
Nicolas Auberger	Industrial	Academic position France
Sophie Thétiot-Laurent	Industrial	Academic position France
Ennaji Najahi	LabEx CHARMMMAT/SYNORG	Currently in the group
Stéphane Laval	ANR	Industry career
Karunakar Bonepally	ANR	International postdoc

In the following publication list, the names of postdoctoral fellows are underlined

1. *Bioinspired Oxidative Cyclization of the Geissoschizine Skeleton for the Total Synthesis of (-)-17-nor-Excelsinidine.* M. Jarret, A. Tap, C. Kouklovsky, E. Poupon, L. Evanno, G. Vincent, *Angew. Chem. Int. Ed.*, **2018**, 10.1002/anie.201802610
2. *Dearomative Diallylation of N-Acylindoles Mediated by FeCl₃.* J. Wu, R. K. Nandi, R. Guillot, C. Kouklovsky, G. Vincent, *Org. Lett.*, **2018**, *20*, 1845-1848
3. *Frozen Chirality of Tertiary Aromatic Amides :Access to Enantioenriched Tertiary alpha-Amino Acid or Amino Alcohol without Chiral Reagent.* T. T. Mai, B. Viswambharan, D. Gori, R. Guillot, J.-V. Naubron, C. Kouklovsky, V. Alezra, *Chem. Eur. J.*, **2017**, *23*, 5787-5798
4. *Efficient synthesis of both diastereomers of β,γ-diamino acids from phenylalanine and tryptophan.* N. Auberger, A. Stanovych, S. Thétiot-Laurent, R. Guillot, C. Kouklovsky, S. Cote Des Combes, C. Pacaud, I. Devillers, V. Alezra, *Amino Acids*, **2016**, *48(9)*, 2237-224

Visiting senior scientists

12- Scientific recognition

Prizes

Distinctions

- G. Vincent was selected to be the French Representative at the EUCHEMS Young Investigator Workshop (2014, Cyprus)

- C. Kouklovsky was elected as President of the Organic Chemistry Division of the French Chemical Society (2015)

IUF members

Chair of learned and scientific societies

- C. Kouklovsky: Secretary (2013-2015) then President (2015-2018) of the Organic Chemistry Division of the French Chemical Society; member of the executive board of the SCF.
- David Bonnaffé: Elected French representative at the European Carbohydrate Organization
- Aurélien Alix: Member of the local (Ile-de-France) network of the French Chemical Society

Invitations to meetings and symposia (out of France)

1. *Combinatorial surfaces mimicking heparan sulfate biological activities: unexpected application to new electronic tongue devices.* D. Bonnaffe, 17th European Carbohydrate Symposium, 7-11 juillet 2013, Tel-Aviv, Israel
2. *From Memory of Chirality to Frozen Chirality: original methods for the enantioselective synthesis of amino acids.* V. Alezra, 10th International Symposium on Carbanion Chemistry (ISCC-10), 23-26 septembre 2013, Kyoto, Japan
3. *The Quest for a Bio-Inspired Oxidative Coupling of Indoles and Phenols to Access Benzofuroindolines Containing Natural Products.* G. Vincent, 6th Young Investigator Workshop of EuCheMs – Organic Division, 28-30 août 2014, Larnaca, Cyprus
4. *Synthesis of New Amino Acids; Applications in Peptide Synthesis.* C. Kouklovsky, Congrès de la Société Chimique Tunisienne, 18-21 décembre 2016, Hammamett, Tunisia

Members' long-term visits abroad

- V. Alezra: Visiting Professor at Kyoto University, Japan (3 months in 2014-2015)
- A. Mambrini (PhD student under the supervision of V. Alezra) spent 4 months (2x2 months) in Kyoto University in the group of Prof. K. Yoshida, in a collaborative research project.
- P. Adler (Ph. D. Student working under the supervision of N. Rabasso) spent 3 months in Glasgow University in the group of Joëlle Prunet from Apr. to July 2015 for a doctoral internship.
- N. Rabasso was invited to give a series of lectures at Adam Mickiewicz University at Poznan, Poland (May 2018)
- D. Bonnaffé was visiting Professor in Taiwan University, Taiwan (23-29 March 2014)

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

Please, highlight the most selective.

1- Socio-economic interactions / Patents

Invention disclosures

Filed patents

Accepted patents

Conjugated molecules comprising a peptide derived from the CD4 receptor coupled to an anionic polypeptide for the treatment of AIDS. F. Baleux, H. Lortat-Jacob, D. Bonnaffe, Y.-M. Coïc, CNRS, Université Paris-Sud, CEA, 23 octobre 2015, PCT/EP2015/074598, 23 octobre 2015, WO2016/062854 (A1) ; Publié le 28 avril 2016

Licenced patents

Licence taken by Aryballe Technologies on patent : Capteurs de nez ou de langue électroniques. D. Bonnaffe, Y. Hou-Broutin, A. Buhot, T. Livache, CNRS, Université Paris-Sud, CEA, 13 octobre 2014, FR 12 51579, 13 octobre 2014, WO2013124810 (A1) publié le 29 août 2013 - Licence taken by Aryballe Technologies 13 october 2014

2- Socio-economic interactions

Industrial and R&D contracts

1. D. Bonnaffé, Sanofi (P. Trouilleux, P.-A. Driguez), 2013-2016
2. V. Alezra, Sanofi (I. Devillers), 2012-2014

Cifre fellowships

Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*

G. Vincent is member of the COST "Natural Products" network

Start-ups

Clinical trials *(Biology only)*

3- Expertise

Consulting

Participation in expert committees (ANSES etc.)

Legal expertise

4- Expert and standardization reports

5- Public outreach

Radio broadcasts, TV shows, magazines

Journal articles, interviews, book edition, videos, etc.

Other popularization outputs

V. Alezra is regularly involved in the " Fête de la Science", where she performs chemical experiences for the general public

Debates on science and society

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

1- Educational outputs

Books

Ouvrages

- V. Alezra is currently writing a book entitled « Toute la chimie pour bien commencer sa licence », ed : De Boeck Supérieur (available in stores at the end of August 2018).

- N. Rabasso has a long history of publishing famous text books in organic chemistry, for both bachelor and master students. In Sept. 2014, he published his 7th book in the series entitled « chimie organique des hétéroélements », for master students (Ed. De Boeck). His latest book, intended for undergraduate students titled "Chimie Organique" (Ed. De Boeck) will be available in stores in May 2018

E-learning, MOOCs, multimedia lessons, etc.

2- For humanities only, published PhD theses

3- Quality of PhD student supervision

During the 2013-2018 period, 23 PhD students have been working in the team (13 recruited since october 2013); the funding distribution is listed below (ASN: Allocation Spéciale pour Normalien):

The average duration for PhD is 38 months, except for 2 CSC students (48 months)

Name	Period	Funding
Z. Hu	2010-2013	Sidaction
M. Jouanneau	2010-2013	ANR
R. Beaud	2011-2014	MESRI
V. Ivashchenko	2011-2014	MESRI
A. Stanovych	2011-2014	MESRI
W. Liu	2011-2015	CSC
L. Tang	2012-2015	LabEx LERMIT
T. Tomakinian	2012-2015	ANR
N. Denizot	2012-2015	French Academy of Sciences
P. Adler	2013-2016	ASN
A. Rousseau	2013-2016	MESRI
Y. Lu	2012-2016	CSC
V. Perez	2014-2017	MESRI
M. Mock-Joubert	2014-2017	LabEx LERMIT
Y. Wan	2014-2017	CSC
R. Campagne	2014-2017	ASN
A. Mambrini	2015-2018	MESRI
J. Ma	2015-2018	CSC
D. Ryzhakov	2016-2019	MESRI
J. Wu	2016-2019	CSC
M. Jarret	2016-2019	ANR
P. Quellier	2017-2020	MESRI
Y. Dou	2017-2020	CSC

8 Students funded by MESRI
2 Students funded by ASN
6 Students funded by CSC
3 Students funded by ANR
2 Students funded by LABEX LERMIT
1 Student funded by the Fondation pour le Développement des Substances Naturelles (French Academy of Sciences)
1 Student funded by Sidaction

4- Students' follow up in association with doctoral schools

All students from the team are sent to international symposia in order to increase their scientific visibility and their integration with the scientific community.

The team as always been very careful with the future of PhD students and contribute, in association with the doctoral school to help them in their career prospects.

-7 students have been recruited as postdocs in international groups
-7 Students are currently undergoing careers in industry
-3 Students have started an academic career

5- Participation to international training programs (e. g. Erasmus Mondus)

- N. Rabasso is co-responsible of the SERp-CHEM Master course which was labelled Erasmus Mundus from 2010 to 2015. In sept 2017, the SERP+ Master (evolution from the previous version of the SERP-Chem taking into consideration the new challenges in chemistry) received the Erasmus+ label for 3 years.
- The team has hosted two ERASMUS Students (M2 level) for research internships: F. Rastch (University of Cologne, 2015-2016, 6 months internship); F. Schäkel (University of Hannover, 2016-2017, 6 months internship).

6- PhD student participation to scientific animation and unit/team life

7- Participation of team members in setting up Master courses

- N. Rabasso is responsible for the M2 SERP+ International Master course.
- D. Bonnaffé (2013-2015) and C. Kouklovsky (2015-2018) are responsible for the M2 Paris-Saclay in Organic Chemistry
- Alix is responsible for the “Chemistry-Biology” course in the M1 Chemistry Paris –Saclay
- Alix and D. Bonnaffé have been widely involved in the constitution of the Master in Chemistry at Paris-Saclay (creation of new courses, common courses between different specialities).

8- Student publications (for Biology only)

Appendix 4

Team 3 - ECM

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Catalyse Moléculaire**
Acronym:	**ECM**
Director's name (current contract):	**Emmanuelle SCHULZ**
Director's name (future contract):	**Giang VO-THAN**

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

13- Articles

Scientific articles

Copper Salts as Additives in Gold(I)-Catalyzed Reactions. Guérinot, A.; Fang, W.; Sircoglou, M.; Bour, C.; Bezzenine-Lafollée, S.; Gandon, V. *Angew. Chem. Int. Ed.* **2013**, *52*, 5848**-**5852.
https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201300600

Calcium(II)-catalyzed Aza-Piancatelli Reaction. Lebœuf, D.; Schulz, E.; Gandon, V. *Org. Lett*. **2014**, *16*, 6464**-**6467.
https://pubs.acs.org/doi/abs/10.1021/ol5032987

Gallium-Assisted Transfer Hydrogenation of Alkenes. Michelet, B.; Bour, C.; Gandon, V. *Chem. Eur. J.* **2014**, *20*, 14488-14492.
https://onlinelibrary.wiley.com/doi/abs/10.1002/chem.201404139

Transition Metal-Free Tunable Chemoselective N-Functionalization of Indoles with Ynamides. Hentz, A.; Retailleau, P.; Gandon, V.; Cariou, K.; Dodd, R. H. *Angew. Chem. Int. Ed.* **2014**, *53*, 8333**-**8337.
https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201402767

Well-Defined Four-coordinate Iron(II) Complexes for Intramolecular Catalytic Hydroamination of Primary Aliphatic Alkenylamines. Bernoud, E.; Oulié, P.; Guillot, R.; Mellah, M.; Hannedouche, J. *Angew. Chem. Int. Ed.* **2014**, *53*, 4930-4934.
https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201402089

Heterobimetallic Dual-Catalysts Systems for the Hydrolytic Kinetic Resolution of Terminal Epoxides. Hong, X.; Mellah, M.; Schulz, E. *Catal. Sci. Technol.* **2014**, *4*, 2608-2617.
http://pubs.rsc.org/en/content/articlelanding/2014/cy/c4cy00235k#!divAbstract

Direct immobilization of Ru-based catalysts on silica through hydrogen bond as non-covalent interaction for recycling in metathesis reactions. Nasrallah, H.; Dragoe, D.; Magnier, C.; Crévisy, C.; Mauduit, M.; Schulz, E. *ChemCatChem*. **2015**, *7*, 2493-2500.
https://onlinelibrary.wiley.com/doi/abs/10.1002/cctc.201500261

***P*-Aryl-Diphenylphospholanes and their Phospholaniums Salts as Efficient Monodentate Ligands for Asymmetric Rhodium-Catalyzed Hydrogenation.** Dobrota, C.; Fiaud, J.-C.; Toffano, M. *Chem. Cat. Chem.* **2015**, *7*, 144.
https://onlinelibrary.wiley.com/doi/abs/10.1002/cctc.201402687

Dibromoindium(III) Cation as π-Lewis Acid: Characterization of $[\mathrm{IPr{\bullet}InBr_2}][\mathrm{SbF_6}]$ and Catalytic Activity Towards Alkynes and Alkenes. Michelet, B.; Colard-Itté, J.-R.; Thiery, G.; Guillot, R.; Bour, C.; Gandon, V. *Chem. Commun*. **2015**, *51*, 7401**-**7404.
https://onlinelibrary.wiley.com/doi/abs/10.1002/cctc.201402687

Gallium(III)- and Calcium(II)-Catalyzed Meyer-Schuster Rearrangements Followed by Intramolecular Aldol Condensation or *endo*-Michael Addition. Presset, M.; Michelet, B.; Guillot, R.; Bour, C.; Bezzenine-Lafollée, S.; Gandon, V. *Chem. Commun*. **2015**, *51*, 5318**-**5321.
http://pubs.rsc.org/en/content/articlelanding/2015/cc/c4cc09514f#!divAbstract

Biosourced Ligands from Isosorbide for Ethylation of Aldehydes or Alkynylation of Imines. Huynh, K.-D.; Ibrahim, H.; Bouchardy, L.; Bournaud, C.; Kolodziej, E.; Toffano, M.; Vo-Thanh, G. *Asian J. Org. Chem.* **2016**, *5*, 1242-1246
http://dx.doi.org/10.1002/ajoc.201600291

***S*-Trifluoromethyl Sulfoximine as directing group in *ortho*-Lithiation reaction. Towards structural complexity**. Le, T.-N.; Diter, P.; Pégot, B.; Bournaud, C.; Toffano, M.; Guillot, R.; Vo-Thanh, G.; Magnier, E. *Organic Letters*, **2016**, 18, 5102-5105.
http://dx.doi.org/10.1021/acs.orglett.6b02548

Phosphine-Thiourea-Organocatalyzed Asymmetric C-N and C-S Bond Formation Reactions. Ngo, T.-T.-D.; Nguyen, T.-H.; Bournaud, C.; Guillot, R.; Toffano, M.; Vo-Thanh, G. *Asian J. Org. Chem.* **2016**, *5*, 895-899. http://dx.doi.org/10.1002/ajoc.201600212

Synthesis of Cyclooctatetraenes through an Unprecedented Palladium-Catalyzed Cascade Reaction. Blouin, S.; Gandon, V.; Blond, G.; Suffert, J. *Angew. Chem. Int. Ed*. **2016**, *55*, 7208–7211 ***(SYNFACTS)***.
https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201602586

Asymmetric Assisted Tandem Catalysis: Hydroamination followed by Asymmetric Friedel–Crafts Reaction from a Single Chiral N,N,N',N'-Tetradentate Pyridylmethylamine-Based Ligand. Aillerie, A.; Rodriguez-Ruiz, V.; Carlino, R.; Bourdreux, F.; Guillot, R.; Bezzenine-Lafollée, S.; Gil, R.; Prim, D.; Hannedouche, J. *ChemCatChem* **2016**, *8*, 2455 – 2460.
https://onlinelibrary.wiley.com/doi/abs/10.1002/cctc.201600604

Lithium-Catalyzed anti-Markovnikov Intermolecular Hydroamination Reactions of Vinylarenes and Simple Secondary Amines. Germain, S.; Lecocq, M.; Schulz, E.; Hannedouche, J. *ChemCatChem* **2017**, *9*,1749–1753.
https://onlinelibrary.wiley.com/doi/abs/10.1002/cctc.201700043

Revealing the Activity of π-Acid Catalysts Using a 7-Alkynyl Cycloheptatriene. Vayer, M.; Guillot, R.; Bour, C.; Gandon, V. *Chem. Eur. J*. **2017**, *23*, 13901-13905.
https://onlinelibrary.wiley.com/doi/abs/10.1002/chem.201703817

One-Pot Assembly of Highly Functionalized Cyclopenta[b]pyrroles via a Calcium(II)- and Copper(II)-Catalyzed Reaction Sequence. Marin, L.; Gandon, V.; Schulz, E.; Leboeuf, D. *Adv. Synth. Catal.* **2017**, *359*, 1157-1163.
https://onlinelibrary.wiley.com/doi/abs/10.1002/adsc.201601301

Convenient Electrocatalytic Synthesis of Azobenzenes from Nitroaromatic Derivatives Using SmI_2, Zhang, Y.-F.; Mellah, M. *ACS Catal.* **2017**, *7*, 8480-8486.
https://pubs.acs.org/doi/abs/10.1021/acscatal.7b02940

Well-Defined -Diketiminatocobalt(II) Complexes for Alkene Cyclohydroamination of Primary Amines. Lepori, C.; Gómez-Orellana, P.; Ouharzoune, A.; Guillot, R.; Lledós, A.; Ujaque, G.; Hannedouche, J. *ACS Catal.*, **2018**, *8*, 4446-4451.
https://onlinelibrary.wiley.com/doi/pdf/10.1002/ange.201402089

Iron-Catalyzed Reductive Ethylation of Imines Using Ethanol. Vayer, M.; Morcillo, S. P.; Dupont, J.; Gandon, V.; Bour, C. *Angew. Chem. Int. Ed.* **2018**, 57, 3228-3232.
https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201800328

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Catalytic Use of Low-Valent Cationic Gallium(I) Complexes as π-Acids. Li, Z.; Thiery, G.; Lichtenthaler, M. R.; Guillot, R.; Krossing, I.; Gandon, V.; Bour, C. *Adv. Synth. Catal.* **2018**, *360*, 544-549. https://onlinelibrary.wiley.com/doi/abs/10.1002/adsc.201701081

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Well-Defined Organo-Gallium Complexes as Lewis Acids for Molecular Catalysis: Structure-Stability-Activity Relationships. Bour, C.; Gandon, V. *Coord. Chem. Rev*. **2014**, *279*, 43.
https://www.sciencedirect.com/science/article/pii/S0010854514002021

Recent developments in alkene hydrofunctionalisation promoted by homogeneous catalysts based on earth abundant elements: formation of C–N, C–O and C–P bond. Rodriguez-Ruiz, V.; Carlino, R.; Bezzenine-Lafollée, S.; Gil, R.; Prim, D.; Schulz, E.; Hannedouche, J. *Dalton Trans.*, **2015**, *44*, 12029–12059.
http://pubs.rsc.org/en/content/articlelanding/2015/dt/c5dt00280j#!divAbstract

Carbon-Carbon and Carbon-Heteroatom Bond-Forming Transformations Catalyzed by Calcium(II) Triflimide. Leboeuf, D.; Gandon, V. *Synthesis* **2017**, *49*, 1500-1508.
https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0036-1588406

Other articles (professional journals, etc.)

''Procédés catalytiques non-métalliques : Construction facile de molécules chirales hautement fonctionnalisées ayant une utilisation potentielle en chimie médicinale''. G. Vo-Thanh, La France au Japon, published by the French Embassy in Tokyo; January 2018
https://jp.ambafrance.org/Procedes-catalytiques-non-metalliques

« L'éthanol, candidat sérieux pour la fabrication de molécules bioactives, » C. Bour, V. Gandon En direct des laboratoires of the Institute of Chemistry, CNRS, April 2018
http://www.cnrs.fr/inc/communication/direct_labos/bour.htm

14- Books

Scientific book edition

Book chapters

"**Computational Studies on the Reactivity of Transition Metal Complexes Featuring N-Heterocyclic Carbene Ligands**" In RSC Catalysis Series, 2016, Chap 4, 120-177. Leboeuf, D.; Gandon, V.

15- Meetings

Meeting abstracts

255th ACS National Meeting in New Orleans (Etats-Unis), 18-22 mars 2018, *Low-Valent Cationic Gallium(I) Complexes as π-Acid Catalysts.* C. Bour

16- Meeting and congress organisation

The members of the ECM group participated in the organization of 12 scientific events over the period. Among these, worthy of note:

Co-organization of two Franco-Vietnamese schools in Hanoi (20-23 October 2014) and Ho Chi Minh City (24-28 October 2016). G. Vo-Thanh

Co-organization of theJournée des Terres Rares Paris Saclay, Ecole Polytechnique 11 June 2015. (2 guest speakers, 100 participants). Co-organizers: S. Bezzenine, Gr. Nocton, A. Auffrant, J.C. Berthet, T. Cantat.

Co-organization of the GECO 56 in Nant in Aveyron, from 23 to 28 August 2015 (12 guest speakers, 75 participants), President P. Dauban, co-organizer, E. Schulz, S. Piguel.

Co-organization of GECOM-CONCOORD in Forges-les-Eaux 15-18 May 2018. C. Bour, V. Gandon

Co-organization of the SECO 2016 (co-organizer G. Thierry), SECO 2017 (Treasurer C. Lepori), 2018 (President, M. Vayer)

17- Electronic tools and products

Softwares
Databases
Tools for decision-making

18- Instruments and methodology

Prototypes
Platforms and observatories

19- Other products

Artistic creations
Movie or theatre play creation
Movies

20- Editorial activities

Participation to journal editorial boards (books, collections)

Wiley-VCH - Vietnam Journal of Chemistry. Member of Editorial Board (2018-2023). G. Vo-Thanh

Member of Editorial Board of the journal published by ISTE OpenScience Ltd (Grande-Bretagne) : Catalysis by Transition Metals since 2016. V. Gandon

21- Peer reviewing activities

Reviewing of journal articles

We have regular referral activities for ACS, Wiley, RSC, Elsevier, Thieme ... journals with an average of about 90 articles referred by the team, per year. One of us (D. Leboeuf) is part of the crowd reviewing experience that was set up by Benjamin List (https://www.nature.com/news/crowd-based-peer-review-can-be-good-and-fast-1.22072).

Grant evaluation (public or charities)

The team members are regularly asked to evaluate research projects from various national (ANR, LabEx, CIFRE, CRITT...) and international (FNRS, ACS Petroleum Research Fund, CEFIPRA, Research Council K.U Leuven, JSPS, Nafosted, FWF, Academies of Science, DFG ....). This represents about 55 expertises over the period for the team.

Participation to lab site visit committees (Hceres etc.)

Member of the HCERES Evaluation Committee of the Institut de Chimie Radicalaire de Marseille, UMR 7273, in January 2017. E. Schulz

Expert member of the HCERES Evaluation Committee, Europe and International Department, since 2018. G. Vo-Thanh

Participation to institutional committees and juries (CNRS, INSERM, etc.)

Scientific Advisor of the Ministry of Science and Technology (MOST) of Viet Nam since 2012. G. Vo-Thanh

Vice-President of the Evaluation Committee of the ANR Programs Blanc, JCJC, Blanc International SIMI 7, 2013. E. Schulz

Expert Member of DAAD, German Academic Exchange Office, since 2015. Mr Mellah

Full Member appointed to the CNU (Section 32), College A since December 2015. E. Schulz

22- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

Core-to-Core Program Japan-Europe 2013-2018. G. Vo-Thanh, french coordinator

Project 'Chimie-Santé' 2012-2015. G. Vo-Thanh, coordinator (2 thesis grants funded by the Vietnamese Government).

National public grants (ANR, PHRC, FUI, INCA, etc.)

The laboratory was awarded 7 fundings by the ANR during the period; three of them were managed by permanent staff of the team. The overall funding allocated to the team is 1025.5 k€. Two of these fundings are specified below :

ANR JCJC (ANR-11-JS07-012-01) « Développement de catalyseurs d'HydroAMination à base de FER pour la cyclisation des amines aliphatiques primaires et secondaires » (DHAMFER) (2011-2014) J. Hannedouche (166 k)

ANR JCJC (ANR-JCJC 2016) «Elaboration of supramolecular assemblies of organometallic complexes by π-anion interactions and application in asymmetric catalysis» (OREO) (2017-2020) D. Leboeuf (160 k€)).

Local grants ("collectivités territoriales")

PIA (Labex, Equipex etc.) grants

ANR Labex Research Contracts CHARMMMAT (ANR-11-LABEX-0039)
Over the period, the team got
- As PI, 10 post-doctoral contracts
- As a partner, 5 postdoctoral contracts
- As PI, 1 valuation contract
- As a partner, 1 doctoral contract
- Financial support for 9 M2 internship

In partnership with ILV, ICSN, Ecole Polytechnique and LabEx SynOrg.

ANR IdEx Research Contract
As PI, 1 support for a prematuration contract (2017-2018)

Grants from foundations and charities (ARC, FMR, FRM, etc.)

23- Visiting senior scientists and post-doc

Post-docs

DUPRE, Nathalie; RODRIGUEZ-RUIZ, Violeta ; PRESSET, Marc ; BERNOUD, Elise ; PAREDES-GANDON, Elisa ; PAREEK, Manish; MARETS, Nicolas
With ILV: ZABOROVA, Elena ; MORCILLO MARTINEZ, Sara Patricia ; AILLERIE, Alexandre ; PERATO, Serge; PRIETO Alexis ; AWADA Mohamed
With ICSN: MAURY, Julien; PANTAINE, Loic; HAMDOUN Ghanem; CASTANHEIRO Thomas
With Ecole Polytechnique: LE DUC, Gaëtan ; ALVARADO BELTRAN, Maria Isabel
With ECI, ICMMO; ABDELLAH, Ibrahim

With LabEx Synorg, Cobra; WITTMANN, Stéphane

Visiting senior scientists

The team received Pr. Ernesto Mata in 2014 and Dr. Carina del Piccolo in 2015 in the context of a collaboration with Argentina (V. Gandon, C. Bour) financed by the program ECOS SUD. Ass. Prof. Shinobu Takizawa, from Osaka University, Japan, was received in the Lab in October 2016 for one month thanks to a Core-to-Core Program (G. Vo-Thanh). Pr. Thierry Ollevier (Laval University in Quebec City) was present for a one-month stay as a guest professor (LabEx funding) in November 2017 (E. Schulz).

12. Scientific recognition

Prizes

Pr V. Gandon received from the DCO-SCF in December 2017, the Jean-Marie Lehn Prize.

Distinctions

Pr V. Gandon has been named Junior Distinguished Member of the SCF in October 2014 for a period of 5 years.

IUF members

Pr V. Gandon has been named Junior Member of the IUF in October 2012 for a period of 5 years.

Chair of learned and scientific societies

V. Gandon has been a member of the Bureau of the Ile-de-France section of the Société Chimique de France from 2012 to 2015. E. Schulz is a member of the Bureau of the Organic Chemistry Division of the Société Chimique de France since March 2018.

Invitations to meetings and symposia (out of France)

IX International School of Organometallic Chemistry (ISOC 2013), Camerino, August 30-September 3, 2013, Italy. E. Schulz

46th Heyrovský Discussion on Molecular Electrochemistry In Organometallic Science, 22-27 juin 2013, Castle Třešť, Czech Republic, M. Mellah

XVIth International Conference on Organometallic Chemistry (ICOMC, Sapporo, Japon), 13-18 juillet 2014. V. Gandon

JSP Program- 50ème Bürgenstock Stereochemistry Brünnen Switzerland, Avril 2015, C. Bour

Kansen International Symposium, December 15-16, 2016, Osaka, Japan, G. Vo-Thanh

Members' long-term visits abroad

The team has strong long-term international collaborations, and in this context, some of its members have had the opportunity to stay in these universities several times.

East China Normal University, Shanghai, Chine. October 2013, Vietnam Academy of Science and Technology, Hanoi, Viet Nam. October 2014, Osaka University, Osaka, Japon. October 2015, University of Technology Petronas, Iskanda, Malaisie. February 2017. G. Vo-Thanh

Osaka University, Osaka, Japon. December 2015. M. Toffano

Visiting Professor at the University of Rosario (Argentina) from August 1st to 14th 2014 (25 h of organometallic chemistry courses at Master 2 level). V. Gandon

Instituto Quimica de Rosario, Argentina December 1-18, 2017 C. Bour

Queen Mary, London, summer 2018, 2 months visit as guest researcher, D. Leboeuf

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

6- Socio-economic interactions / Patents

Invention disclosures

Filed patents

Catalyseurs supportés cycliques, Vincent Huc, Cyril Martini, Ibrahim Abdellah, Emmanuelle Schulz, Dépôt PCT/FR2017/052980, 27 octobre 2017, WO2018078304.

Nouveau procédé de synthèse d'amines tertiaires dissymétriques. Bour, C.; Vayer, M.; Gandon, V. (Fr. Demande initiale n° 17/59117 (2017)

Accepted patents
Licenced patents

7- Socio-economic interactions

Industrial and R&D contracts

Roquette company 2017-2018: 'Valorisation of biomass'. G. Vo-Thanh, coordinator (Funding of a post-doc, 65 k€)

EDF 2012-2013 : Contract N° 8610-4300300624 (UPSud/SAIC91340) "Détection de composés soufrés dans les huiles de transformateurs électriques", M. Mellah, coordinator 15 k€

Cifre fellowships
Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*

GDRI CNRS-RAS « Catalyse Homogène pour le Développement Durable » (CH2D) (2012-2015) (PI Prof. R. Poli (UPR 8241) E. Schulz and J. Hannedouche with C. Bruneau and J.F. Carpentier (UMR 6226), F. Lamaty (UMR 5247), E. Shubina and S. Osipov (Nesmeyanov Institute, Russia), A. Trifonov (Razuvaev Institute, Russie), I. Beletskaya (Moscou University, Russia), G. Giambastiani and M. Peruzzini (ICCOM, Italy).

GDR CNRS « Phosphore » (2017-2021) Director M. Lecouvey (UMR 7244). Member list - Section : 12, 14, 15, 16.: D. Virieux (UMR 5253), M. Toffano (UMR8182), K.Miqueu (UMR5254), N. Mezailles, A. Baceiredo, D. Bourissou (UMR5069), A-C. Gaumont (UMR6507), P-A. Jaffrès, F. Acher (UMR6521), S. Peyrottes (UMR5247), B. Bujoli (UMR6230), F. Leroux (7509), M. Hissler, F. Paul, J-F. Halet, C. Darcel (UMR6226), A. Marinetti, A. Voituriez, J. F. Betzer, X. Guinchard (UPR2301), A-M. Caminade (UPR8241)

GDR-LIPS « Liquides Ioniques et Polymères » (2013-2020) Director Margarida COSTA GOMES (UMR 6296) and Jannick DUCHET-RUMEAU (UMR 5223), .G. Vo-Thanh (UMR 81812)

Start-ups

Stakeholder with V. Huc (ECI) of the Novecal Company created by C. Martini last spring

8- Expertise

Consulting

Expert Member 'FRANCE L'Oréal-UNESCO Scholarships for Women and Science' since 2011. G. Vo-Thanh

Expert for the Directorate General of Armaments (DGA) since 2018. V. Gandon

Participation in expert committees (ANSES etc.)

Legal expertise

9- Expert and standardization reports

10- Public outreach

Radio broadcasts, TV shows, magazines

Journal articles, interviews, book edition, videos, etc.

Other popularization outputs

Some of us have participated very frequently in scientific outreach efforts through interventions in schools to moderate scientific workshops. (C. Bour, V. Gandon, C. Bournaud, M. Mellah)

Debates on science and society

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

9- Educational outputs

Books

Synthèses en chimie organique – Exercices corrigés, R. Gil, N. Lubin-Germain, J. Uziel, Dunod, 2016, 2nde édition

E-learning, MOOCs, multimedia lessons, etc.

Participation in the creation of videos on MOODLE platform of Organic Chemistry for the L1 of Biology (AAP- e-learning). 4 videos made, C Bour.

10- For humanities only, published PhD theses

11- Quality of PhD student supervision

There was no thesis interruption in the team. The funding obtained comes mainly from the Doctoral School, CSC, LabEx, ANR, other foreign funding (Vietnamese government, for example ...). The duration of theses on average is 38 months.

12- Students' follow up in association with doctoral schools

The policy followed by the team in this area is the same as that of the Doctoral School. We support our PhD students to direct them towards postdoctoral contracts and also put them in touch with all our private sector contacts for those who wish.

13- Participation to international training programs (e. g. Erasmus Mondus)

In 2013, the team received an Italian student, Filippo Moscatelli, as an Erasmus trainee for three months, in collaboration with Prof. F. Ragaini, University of Milan. He prepared yttrium catalysts bearing reduced Ar-BIANH$_2$ ligands and used them efficiently in olefin hydroamination reactions. This common work resulted in the publication of one paper in New. J. Chem. (2016, E. Schulz, J. Hannedouche)

14- PhD student participation to scientific animation and unit/team life

The team organizes weekly internal scientific seminars with all of its members of approximately one hour. A student or a permanent begins by presenting an article from the very recent bibliography for about fifteen minutes. The second part of the seminar is devoted exclusively to the intervention of PhD students who can deal with a topic of research (deepening a subject using the bibliography) or summarize their work in progress. These different presentations are followed by discussions.

Students participate actively in the life of the team to achieve many collective tasks that are not performed due to lack of permanent staff: fluids control, responsibility for different equipment and appliances, sorting and disposal of waste, etc.

15- Participation of team members in setting up Master courses

R. Gil manages the 1st year Master's degree entitled "Chemical Pollutions and Environmental Management" and the Organic Chemistry platform of the Master 1 Chemistry. He is actively participating in the implementation of the organization of these formations in the new courses of the University Paris-Saclay since September 2015. Furthermore, and since 2014 he is co-organizer of a chemistry competition “challenge de chimie” for 3rd year chemistry students tethering 5 universities in the Paris region.

G. Vo-Thanh is pedagogical manager of MIC 2018, which features exchange of teacher-researchers and students (master, PhD student) between Paris-Sud University and Vietnamese universities.

16- Student publications (for Biology only)

Département d'évaluation
de la recherche

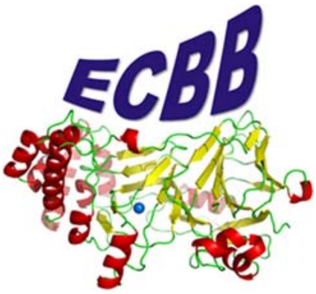
Appendix 4

Team 4 - ECBB

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Chimie Bioorganique et Bioinorganique**
Acronym:	**ECBB**
Director's name (current contract):	**Laurent SALMON**
Director's name (future contract):	**Laurent SALMON**



I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

1- Articles

Scientific articles

1. Photoassisted Generation of a Dinuclear Iron(III) Peroxo Species and Oxygen-Atom Transfer. F. Avenier, C. Herrero, W. Leibl, A. Desbois, R. Guillot, J.-P. Mahy, A. Aukauloo, *Angew. Chem. Intern. Ed.* **2013**, *52*, 3634-3637.
2. Direct electrochemical detection of PB1-F2 protein of influenza A virus in infected cells. A. Miodek, H. Sauriat-Dorizon, C. Chevalier, B. Delmas, J. Vidic, H. Korri-Youssoufi, *Biosens. Bioelectron.* **2014**, *59*, 6-13.
3. Bio-inspired electron-delivering system for reductive activation of dioxygen at metal centres towards artificial flavoenzymes. Y. Roux, R. Ricoux, F. Avenier, J.-P. Mahy, *Nat. Commun.* **2015**, *6*, 8509.
4. E-DNA Sensor of Mycobacterium tuberculosis Based on Electrochemical Assembly of Nanomaterials (MWCNTs/PPy/PAMAM). A. Miodek, N. Omrani Mejri, M. Gomgnimbou, C. Sola, H. Korri-Youssoufi, *Anal. Chem.* **2015**, *87*, 9257-9264.
5. Large area graphene nanomesh: an artificial platform for edge-electrochemical biosensing at the sub-attomolar level. B. Zribi, J.-M. Castro-Arias, D. Decanini, N. Gogneau, D. Dragoe, A. Cattoni, A. Ouerghi, H. Korri-Youssoufi, A.-M. Haghiri-Gosnet, *Nanoscale* **2016**, *8*, 15479-15485.
6. Artificial Metalloenzymes with the Neocarzinostatin Scaffold: Toward a Biocatalyst for the Diels–Alder Reaction. W. Ghattas, L. Cotchico-Alonso, J.-D. Maréchal, A. Urvoas, M. Rousseau, J.-P. Mahy, R. Ricoux, *ChemBioChem* **2016**, *17*, 433-440.
7. Carbohydrate-based electrochemical biosensor for detection of a cancer biomarker in human plasma. M. Devillers, L. Ahmad, H. Korri-Youssoufi, L. Salmon, *Biosens. Bioelectron.* **2017**, *96*, 178-185.
8. Metal–organic frameworks: a novel host platform for enzymatic catalysis and detection. E. Gkaniatsou, C. Sicard, R. Ricoux, J.-P. Mahy, N. Steunou, C. Serre, *Mater. Horiz.* **2017**, *4*, 55-63.
9. αRep A3: A versatile artificial scaffold for metalloenzyme design. T. Di Meo, W. Ghattas, C. Herrero, C. Velours, P. Minard, J.-P. Mahy, R. Ricoux, A. Urvoas, *Chem. Eur. J.* **2017**, *23*, 10156-10166.
10. Direct electrochemical DNA biosensor based on reduced graphene oxide and metalloporphyrin nanocomposite. Y. Wang, H. Sauriat-Dorizon, H. Korri-Youssoufi, *Sens. Actuators B-Chem.*, **2017**, *251*, 40-48.
11. Synthesis and antikinetoplastid evaluation of bis(benzyl)spermidine derivatives. E. Jagu, S. Pomel, A. Diez-Martinez, E. Rascol, S. Pethe, P. M. Loiseau, R. Labruère, *Eur. J. Med. Chem.* **2018**, *150*, 655-666.

Review articles

Other articles (professional journals, etc)

2- Books

Scientific book edition

Book chapters

1. *Biosensors for security and bioterrorism applications*, H. Korri-Youssoufi, A. Miodek, W. Ghattas, 161-180, Nikolelis, Dimitrios P. & Nikoleli, Georgia-Paraskevi, Springer, Electrochemical DNA biosensors for bioterrorism prevention, **2016**, ISBN: 978-3-319-28924-3

3- Meetings

Meeting abstracts

1. *Artificial Flavoreductase for the Reductive Activation of Dioxygen at Metal Centers in Water.* F. Avenier, Y. Roux, K. Cheiab, A. Naim, R. Ricoux, J.-P. Mahy, 18th International Congress of Bioinorganic Chemistry ICBIC 18, July 31-August 4, **2017**, Florianopolis, Brazil, *J. Biol. Inorg. Chem.* **2017**, *22*, S237-S237.

4- Meeting and congress organisation

- International conferences:

1. 16th International Conference in Bio-Inorganic Chemistry, ICBIC16, Grenoble, 21-25 July **2013** (J.-P. Mahy, SC).
2. 28th European Conference on Solid-State Transducers, Euro Sensors 2014, Brescia (Italy), 7-10 September **2014** (H. Korri-Youssoufi, SC).
3. 42nd International Conference on Coordination Chemistry, ICCC 2016, Brest 3-8 July **2016** (J.-P. Mahy, SC).
4. 1st International Symposium of Paris-Saclay University on Drug Discovery and New Therapeutics, Orsay, 9-11 April **2018** (J.-P. Mahy, CS).
5. **The Copper Bioinorganic Chemistry Symposium** (CuBICS 2018), Marseille (France), 21-24 May **2018** (J-P Mahy, SC and OC).

- National Conferences:

6. Journées d'électrochimie 2013, Paris, 8-11 July **2013** (H. Korri-Youssoufi, OC).
7. Journée ICMMO Chimie et Santé, Orsay, 8 February **2013** (L. Salmon, OC/SC).
8. 15ème Rencontres de Chimie Organique Biologique, RECOB 15, Aussois, 23-27 March **2014** (C. Blonski, OC/SC).
9. 16ème Rencontres de Chimie Organique Biologique, RECOB 16, Aussois, 13-17 March **2016** (C. Blonski, OC/SC).

5- Electronic tools and products

Softwares
Databases
Tools for decision-making
Solver competition tools *(Science and technology only)*

6- Instruments and methodology

Prototypes

1. Prototype for detection of *Brettanomyces* yeast in wine (S. Chebil, N. Mejri-Omrani, H. Korru-Youssoufi).

Platforms and observatories

7- Other products

Structure deposition

1. RCSB PDB **5NW7**: *Crystal structure of candida albicans phosphomannose isomerase in complex with inhibitor*. I. Li de la Sierra-Gallay, L. Ahmad, S. Plancqueel, H. van Tilbeurgh, L. Salmon, May, 9th. **2018**.

Artistic creations
Movie or theatre play creation
Movies

8- Editorial activities

Participation to journal editorial boards (books, collections)

1. Journal of Colloid Science and Biotechnology, H. Korri-Youssoufi, Member of Editorial Board, **2013-2016**.
2. Biosensors Guest Editors Special Issue "Electrochemical DNA/RNA Biosensors", **2018**.

Collection and series management

9- Peer reviewing activities

Reviewing of journal articles

Members of the team were asked to evaluate more than 100 submitted articles for the following journals: *ACS Nano, Adv. Mater., Adv. Synth. Catal., Anal. Bioanal. Chem., Anal. Chim. Acta, Anal. Biochem., Anal. Chem., Angew. Chem. Intern. Ed., Appl. Catal. A, Arab. J. Chem., Bioelectrochemistry, Bioorg. Med. Chem., Bioorg. Med. Chem. Lett., Biosens. Bioelectron., Carbon, Cat. Commun., Catalyst, Chem. Rev., ChemBioChem, ChemCatChem, Chemistry, ChemPlusChem, Colloids Surf. B., Dalton Trans., Electroanalysis, Eur. J. Inorg. Chem., Eur. J. Med. Chem., Eur. J. Org. Chem., FEBS J., Heterocycl. Chem., Inorg. Chem., Inorg. Chim. Acta, Isr. J. Chem., J. Am. Chem. Soc., J. Biol. Inorg. Chem., J. Chem. Soc. Chem. Commun., J. Enz. In. Med. Chem., J. Inorg. Biochem., J. Med. Chem., J. Mol. Catal. A: Chem., Lab on chip, Mat. Sci. Eng. C, Med. Chem., Molecules, NanoLetters, New J. Chem., Polyhedron, Sens. Act, SynLett, Talanta, Tetrahedron, Tetrahedron Lett.*.

Grant evaluation (public or charities)

1. Region (2) : L. Salmon, H. Korri-Youssoufi
2. ANR (14) : F. Avenier (2), R. Ricoux (3), H. Horri-Youssoufi (9)

Participation to lab site visit committees (Hceres etc.)

1. LCBM, Chemistry and Biology of Metals Laboratory, Biosciences and Biotechnology Institute of Grenoble, CEA-INSERM-CNRS-Univ. Grenoble Alpes UMR5249, 01/**2015** (J.-P. Mahy, Hcéres)
2. URCOM, Research Unit of Organic and Macromolecular Chemistry, Univ. du Havre, 11/**2015** (J.-P. Mahy, Hcéres)
3. Fédération des Recherches en Environnement, Univ. Blaise Pascal, UBP/CNRS FR 3467/INRA, Clermont-Ferrand, 01/**2016** (J.-P. Mahy, Hcéres)
4. Institut de Chimie de Clermont-Ferrand (ICCF), 01/**2016** (J.-P. Mahy, Hcéres)
5. Project IBITECS-I2BM CEA, 06/**2016** (J.-P. Mahy, Hcéres)
6. National Fundation for Petroleum Research, USA (J.-P. Mahy)
7. Swiss national Science Fundation, Switzerland (J.-P. Mahy)
8. Netherlands Organisation for Scientific Researh, The Netherlands (J.-P. Mahy)
9. Lab. Archéologie Moléculaire et Structurale (LAMS) UMR UPMC-CNRS 8220, 01/**2018** (J.-P. Mahy, Hcéres)
10. Lab. of Chemistry of Biological Processes (LCPB), UMR Collège de France-UPMC-CNRS 8229, 12/**2017** (J.-P. Mahy, Hcéres)

Participation to institutional committees and juries (CNRS, INSERM, etc)

1. Department of Chemistry of Paris-Saclay University (J.-P. Mahy, director & scientific committee)
2. CNU 32, National Council of Universities, organic, mineral and industrial chemistry section [J.-P. Mahy (vice-president) and S. Pethe (member of section B)]
3. CCSU (advisory committee of university specialists), Univ. Paris-Sud, Orsay (F. Avenier and H. Korri-Youssoufi)
4. ED 2MIB, Doctoral school of Chemical Sciences: Molecules, Materials, Instrumentation and Biosystems, Univ. Paris-Sud, Orsay (F. Avenier)
5. Council of the Chemistry Department, Univ. Paris-Sud (H. Dorizon, R. Ricoux and L. Salmon)

6. Council of ICMMO, Orsay Institute of Molecular Chemistry and Materials, Univ. Paris-Sud (R. Labruère and L. Salmon)
7. Staff Commission of ICMMO (L. Salmon)
8. PhD juries: J.-P. Mahy (23), H. Korri-Youssoufi (20, including 8 international), L. Salmon (6), C. Blonski (1), W. Ghattas (1), F. Avenier (3), R. Labruère (2), R. Ricoux (2)
9. HDR juries: J.-P. Mahy (5), L. Salmon (3), H. Korri-Youssoufi (1)

10- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

1. Franco-Quebec cooperation agreement, Samuel Champlain program, R. Ricoux, J.-P. Mahy, N. Doucet (INRS-Institut Armand-Frappier, Laval, Canada), *Design and development of new generations of hemozymes for industrial applications*, **2013-2014**
2. JPIAMR, Joint Programming Initiative on Antimicrobial Resistance, T. Naas (APHP Univ. Paris-Sud, France), Y. Glupzynski (UCL Belgique), B. Iorga (ICSN-CNRS Gif-sur-Yvette, France), M. Jaskolski (Poznam, Pologne), S. Pethe, R. Labruère, L. Salmon, C. Blonski, DesInMBL: *Structure-guided design of pan inhibitors of metallo-beta-lactamases*, **2016-2018**
3. PHC Maghreb, Partenariat Hubert Curien France-Maghreb (3 ans), H. Korri-Youssoufi, **2018**-2021

National public grants (ANR, PHRC, FUI, INCA, etc.)

4. ANR, Retour post-doctorant (RPDOC), W. Ghattas, REBAR: *Receptor-based multipotent artzymes*, 2012-**2015**
5. ANR, J.-P. Mahy, R. Ricoux, F. Banse, F. Avenier, H. van Tilbeurgh (I2BC, Univ. Paris-Sud), D. Mandon (ULP Strasbourg), B. Schollorn (LEM, Paris 7), CATHYMETOXY: *New hybrid metalloprotein catalysts for selective oxidation by dioxygen*, 2012-**2015**
6. ANR, F. Avenier, R. Ricoux, C. Aroulanda, BIOXICAT : Bio-inspired oxidation catalysts for a more environmentally friendly chemistry, **2013-2015**
7. CNRS, Interdisciplinary Challenges: Instrumentation to the limits, A.-M. Haghiri-Gosnet (CNRS C2N UPSud), L. Salmon, H. Korri-Youssoufi, FLUTRACE: *Microfluidic sensors for in vitro direct detection of ultra-traces of biomarkers*, **2014**
8. ANR, R. Labruère, EDIFIS: *Ecodesign of drugs incorporating a self-immolating structure*, **2016**-2019
9. ANR, F. Avenier, J.-P. Mahy, J.-P. Goddard, D. Le Nouen, LCOB, ENSC Mulhouse, ARTENOSYN*: Artificial enzymes in the world of organic synthesis*, **2016**-2020
10. ANR, J.-P. Mahy, R. Ricoux, F. Avenier, W. Ghattas, O. Berteau (INRA Jouy-en-Josas, Synchrotron Soleil, CEA Saclay), CARB2ZYME: *Unprecedented chemistry for carbon-carbon bond formation by an emerging class of metallo-enzymes*, **2017**-2020

Local grants ("collectivités territoriales")

11. DIM R2DS Ile-de-France, PhD fellowship (Y. Roux), *Development of bio-inspired catalysts for a more environmentally friendly chemistry*, F. Avenier, **2013-2015**
12. Univ. Paris-Sud, Attractivity fellowship, R. Labruère, **2015**
13. SATT Paris-Saclay, Maturation project, H. Korri-Youssoufi, N. Mejri-Omrani, S. Chebil, PATTOX: *Analytical devices for the detection of pathogens and toxins*, **2017-2018**

PIA (Labex, Equipex etc.) grants

14. LabEx LERMIT, Laboratory of Excellence in Research on Medication and Innovative Therapeutics, T. Naas, B. Iorga, C. Blonski, L. Salmon, R. Labruère, S. Pethe, F. Ramiandrasoa; post-doctoral fellowships: M. Gayral and A. Diez-Martinez, *Targeting carbapenemases for fighting antibiotic-resistant Gram-negative bacteria*, 2012-**2018**
15. IDEX Paris-Saclay, PhD fellowship (T. Di Meo), R. Ricoux, J.-P. Mahy, A. Urvoas, Ph Minard (I2BC, Univ. Paris-sud): *Artificial metalloenzymes engineering*, **2014-2016**
16. LaBex CHARMMMAT, Laboratory of Excellence in Chemistry of multifunctional molecular architectures and materials, J.-P. Mahy (Director), F. Ozanam, D. Prim, B. Ploumellec (UPSud, UVSQ, CNRS, Ecole

Polytechnique, ENS Cachan, Centrale-Supélec, CEA, UEVE (2012-2019); post-doctoral fellowship (C. Herrero), F. Banse, F. Avenier, J.-P. Mahy : *Photoactivation of peroxidic intermediates*, **2014**

17. LaBex CHARMMMAT, post-doctoral fellowship (J. Buendia), A. Aukauloo, J.-P. Mahy, R. Ricoux, Ph. Dauban (ICSN-CNRS, Gif-sur-Yvette): *Photoactivation for iron-catalyzed intermolecular C(sp3)-H amination reaction*, **2014-2015**
18. LaBex CHARMMMAT, PhD fellowship (E. Gkaniatsou), N. Steunou, R. Ricoux, J.-P. Mahy: *Design of new enzymatic immobilisation matrices based on Metal Organic Frameworks (MOF) for the catalytic degradation of environmental pollutants*, **2015-2018**
19. Labex CHARMMMAT, post-doctoral fellowship (A. Naim), F. Avenier, P. Mialane (UVSQ), **2016-2017**
20. LabEx CHARMMMAT, W. Ghattas, J.-P. Mahy, Pierre-Yves Renard, Cyrille Sabot/COBRA-Rouen, SynOrg: *Screening methods for the rapid identification of catalytic systems for Diels–Alder reactions*, **2017-2018**
21. LaSISP-IRS BME, C.-T. Nguyen, A.-M. Haghiri-Gosnet, H. Korri-Youssoufi, LPQM CNRS-ENSPS, C2N CNRS-UPS, ICMMO CNRS-UPS, POFADIAG: *Analytical microfluidic platforms for the diagnosis of pathogenic diseases*, **2018**-2019

Grants from foundations and charities (ARC, FMR, FRM, etc.)

22. Ligue Nationale contre le Cancer, R. Labruère, *Synthesis and physicochemical evaluation of benzeneboronate prodrugs with antitumor aim*, **2016-2018**
23. Fondation ARC pour la Recherche sur le Cancer, R. Labruère, *Tool for the optimal administration of several antitumor drugs*, **2017**-2020

11- Visiting senior scientists and post-doc

Post-docs

1. W. Ghattas, *ANR REBAR* (1/12/2012-30/6/**2016**)
2. M. Gayral, *LabEx LERMIT* (1/1/**2013**-31/12/**2015**)
3. F. Hammerer, *ANR CATHYMETOXY* (1/3/**2013**-28/2/**2014**)
4. K. Cheaib, *ANR BIOXICAT* (1/2/**2014**-31/3/**2016**)
5. V. Dubosclard, *ANR REBAR* (1/7/**2014**-30/6/**2016**)
6. S. Serra, *Ligue contre le Cancer* (1/1/**2016**-31/12/**2017**)
7. A. Diez-Martinez, *LabEx LERMIT* (1/2/**2016**-30/9/**2016**) + *JPIAMR* (1/10/**2016**-14/2/**2017**)
8. A. Naim, *LabEx CHARMMMAT* (9/1/**2017**-8/1/**2018**)
9. E. Rascol, *ANR EDIFIS* (1/4/**2017**-30/9/**2018**)
10. M. Abellan Flos, *JPIAMR* (1/6/**2017**-31/7/**2018**)
11. C. Skarbek, *Fondation ARC* (1/10/**2017**-30/9/2020)

Publications which these post-docs have co-authored: *Dalton Trans.* **2014**, *43*, 8344-8354; *Bioorg. Med. Chem.* **2014**, *22*, 5678-5686; *Dalton Trans.* **2014**, *43*, 7708-7711; *Dalton Trans.* **2015**, *44*, 5966-5968; *ChemBioChem* **2016**, *17*, 433-440; *Catalysts* **2016**, *6*, 202; *Dalton Trans.* **2016**, *45*, 18098-18101; *Bioorg. Med. Chem.* **2017**, *25*, 84-90; *Eur. J. Inorg. Chem.* **2017**, 3884-3891; *FEBS Lett.* **2018**, *592*, 1667-1680; *Chem. Commun.* **2018**, DOI 10.1039/C8CC03253J; *Eur. J. Med. Chem.* **2018**, *150*, 655-666.

Visiting senior scientists

1. M. Marrakchi, MCF Faculté de Médecine Tunis, high-level scientific stay, **2015**, 15 days
2. A. Mars, MCF Univ. El Manar, Tunis, bourse de haute étude, ambassade de France, **2016**, 15 days
3. N. Raouafi, Prof. Université de Tunis El Manar, high-level scientific stay, mai **2016**, 15 days
4. R. Mlika, Prof. Faculté des Sciences de Monastir, scientific stay

Publications which these visiting scientists have co-authored: *Anal. Chim. Acta* **2016**, *920*, 37-46; *Sens. Actuators B: Chem.* **2016**, *226*, 370-380; *Electroanalysis* **2016**, *28*, 2533-2542; *Anal. Chim. Acta* **2017**, *994*, 10-18; *Talanta* **2018**, *184*, 475-483.

12- Scientific recognition

Prizes

1. S. Serra, Prix Georges Calothy, Ligue Nationale contre le Cancer, Comité de l'Essonne, 15 septembre **2017**

Distinctions

IUF members

Chair of learned and scientific societies

Invitations to meetings and symposia (out of France)

1. H. Korri-Youssoufi, Recent Advances in Micro/Nano Sensors for Mono- and Multi-Target Assays, 20-22/5/**2013**, Kiev, Ukraine
2. H. Korri-Youssoufi, Sample Prep 2013, 9-10/5/**2013**, San Diego, USA
3. J.-P. Mahy, 8th International Conf. on Porphyrins and Phtalocyanins, ICPP 8, 22-27/6/**2014**, Istanbul, Turkey
4. 26ème Forum international des sciences biologiques et de biotechnologie, 23-26/3/**2015**, Monastir, Tunisie
5. J.-P. Mahy, 227th ElectroChemical Society Meeting, 26-29/5/**2015**, Chicago, USA
6. J.-P. Mahy, Workshop 'Chimie Pharmaceutique et Chimie de Substances Naturelles', 24-28/10/**2016**, Ho Chi Minh Ville, Viet Nam
7. H. Korri-Youssoufi, The 2nd Energy Engineering Alliance Forum, 17/11/**2016**, Ho Chi Minh Ville, Vietnam
8. H. Korri-Youssoufi, 2nd International Conference on Genomic Medecine, 26-28/02/**2018**, Houston, USA

Members' long-term visits abroad

1. R. Ricoux, Projet de coopération franco-québecoise, Institut Armand Frappier, INRS, Montréal (Canada) : 2013-2014 (1 month)
2. J.-P. Mahy, Projet de coopération franco-québecoise, Institut Armand Frappier, INRS, Montréal (Canada) : 2013-2014

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

1- Socio-economic interactions / Patents

Invention disclosures

Filed patents

Accepted patents

1. *Methods of increasing the cytotoxicity of chemotherapeutic agents with multisubstrate inhibitors of histone, protein-Lys, polyamine acetylation, and polyamine metabolism.* J. Parello, K. Bandyopadhyay, J.-L. Baneres, C. Blonski, R. A. Gjerset, A. Martin, 18 August **2015**, US 9,107,879 B
2. *Système de détection électrochimique de molécules d'intérêt.* H. Korri-Youssoufi, A. Miodek, N. Mejri-Omrani, Université Paris-Sud/CNRS, 13 November **2015** (FR15 60917), extension internationale 14 novembre **2016** (PCT/EP2016/077564), Application 18 May **2017** (WO2017081315A1)

Licenced patents

2- Socio-economic interactions

Industrial and R&D contracts

Cifre fellowships

Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*

1. COST CM1003 (J.–P. Mahy, F. Avenier, R. Ricoux)
2. French BIC (J.–P. Mahy, F. Avenier, W. Ghattas, R. Ricoux)
3. GDR 3429 "BioMatPro" CNRS/INRA, Resp. J. Barrault/CNRS et A. Buleon/INRA (R. Ricoux)

4. Club Bioconversions, CBSO, L. Hecquet coordinatrice (J.–P. Mahy, R. Ricoux)

Start-ups

1. Maturation project PATTOX: *Analytical devices for the detection of pathogens and toxins*, SATT Paris-Saclay, H. Korri-Youssoufi, N. Mejri-Omrani, S. Chebil, **2017-2018**

3- Expertise

Consulting
Participation in expert committees (ANSES etc.)
Legal expertise

4- Expert and standardization reports

5- Public outreach

Radio broadcasts, TV shows, magazines

1. *Une approche biomimétique pour oxyder plus proprement,* F. Avenier, C. Herrero, W. Leibl, R. Guillot, J.-P. Mahy, A. Aukauloo, A. Desbois, Site web du CNRS / En direct des laboratoires de l'institut de chimie, 28 February **2013**.
2. *CHARMMMAT met les matériaux au coeur des recherches,* J.-P. Mahy, Interview par Aurélie Dureuil, 24, Formule verte, 2 November **2015**.
3. *Les matériaux au coeur des projets de CHARMMMAT,* J.-P. Mahy, Interview par Aurélie Dureuil, 534, Infochimie Magazine, P 44-45, 1 December **2015**.

Journal articles, interviews, book edition, videos, etc.

1. *Powerfull tools for biocatalysis,* W. Ghattas, 162, 104-106 (**2014**), International Innovation, Emerald Publishing Limited, Bingley, UK

Other popularization outputs

1. Participation annuelle à la fête de la science (avec le concours de doctorants et post-doctorants)

Debates on science and society

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

1- Educational outputs

Books
E-learning, MOOCs, multimedia lessons, etc.

2- Quality of PhD student supervision

The 13 ECBB's PhD students were financially supported for 3 years by national grants from MESRI (6) and DIM Ile-de-France (2), and by international grants from Tunisia (2), China (1) and Lebanon (1). No withdrawal was recorded.

First Name	Name	Financial support	Thesis director(s) and supervisor	PhD defence
Stéphanie	Courtiol-Legourd	MESRI	L. Salmon	05/04/2013
Anna	Miodek	MESRI	H. Korri-Youssoufi	11/12/2013
Alexandre	Trehoux	MESRI	J.-P. Mahy-F. Avenier (sup.)	23/10/2015
Yoann	Roux	DIM IdF	J.-P. Mahy-F. Avenier (sup.)	27/11/2015
Marion	Devillers	MESRI	L. Salmon-H. Korri-Youssoufi	18/02/2016
Bacem	Zribi	France/Tunisia	H. Korri-Youssoufi	26/02/2016
Nawel	Mejri-Omrani	Europe	H. Korri-Youssoufi-J.-L. Marty	21/03/2016
Salma	Bizid	France/Tunisia	H. Korri-Youssoufi	26/06/2016
Elodie	Jagu	DIM IdF	C. Blonski-P. Loiseau-R. Labruère (sup.)	25/11/2016
Thibault	Di Méo	MESRI	R. Ricoux-P. Minard	19/01/2017
Yaqiong	Wang	China (CSC)	H. Korri-Youssoufi-H. Dorizon (sup.)	09/10/2017
Lama	Ahmad	MESRI	L. Salmon	01/12/2017
Rabih	Khoder	Lebanon	H. Korri-Youssoufi	11/04/2018

In addition to these PhD Students, others students registered in a foreign University spent short periods under our supervision in our laboratory: N. Kleczewska (supervisor S. Pethe), PhD internship, Erasmus, **2014**, 9 months ; M. Haddaoui (dir. H. Korri-Youssoufi), PhD internship, Univ. de Tunis, Tunisie, **2015**, 3 months.

3- Students' follow up in association with doctoral schools

In order to facilitate their future professional integration, PhD students are invited to present their work in various national congresses and in at least one international congress. At the end of their thesis, the majority of them pursue a post-doc contract in France or abroad. Others fit directly into the private sector.

First Name	Name	PhD defence	Current situation	Society
Stéphanie	Courtiol-Legourd	05/04/2013	Head of Time Managt & Activities	Sopra HR software
Anna	Miodek	11/12/2013	Researcher	Boston (USA)
Alexandre	Trehoux	23/10/2015	CAPES preparation	Cergy-Pontoise
Yoann	Roux	27/11/2015	Post-doctoral position	Lyon ; Paris
Marion	Devillers	18/02/2016	Teacher	MESRI
Bacem	Zribi	26/02/2016	Post-doctoral position	Paris
Nawel	Mejri-Omrani	21/03/2016	CDD Engineer « PATTOX »	SATT Paris-Saclay
Salma	Bizid	26/06/2016	ATER	Monastir (Morocco)
Elodie	Jagu	25/11/2016	Post-doctoral position	Birmingham (UK)
Thibault	Di Méo	19/01/2017	Post-doctoral position	Paris
Yaqiong	Wang	09/10/2017	Post-doctoral position	Beijing (China)
Lama	Ahmad	01/12/2017	Unemployed	-
Rabih	Khoder	11/04/2018	Unemployed	-

4- Participation to international training programs (e. g. Erasmus Mondus)

1. Convention Univ. Paris-Sud/Tomsk Polytechnic Univ. (Russie) for Master 2 Pollutions Chimiques et Gestion Environnementale (PCGE) in double diploma (L. Salmon).

5- PhD student participation to scientific animation and unit/team life

The follow-up of PhD students in the conduct of their research and in their professionalization is carried out on several levels: 1) within the team during laboratory seminars (average 2 per year for each PhD student), 2) at the level of the institute during the PhD Students Day of ICMMO, 3) during the day of the doctoral school of attachment. 41 publications (articles + reviews) are based on 13 theses, giving an average of 3.15 publications per student. The average 2015 impact factor for these 41 publications is 4.95.

First Name	Name	Nb of publi.	Publications	Average IF 2015
Stéphanie	Courtiol-Legourd	2	*J. Phys. Chem.* **2011**, *115*, 8304-8316 ; *Bioorg. Med. Chem.* **2012**, *20*, 1511-1520	3.055
Anna	Miodek	10	*Anal. Chem.* **2013**, *85*, 7704-7712; *Anal. Bioanal. Chem.* **2013**, *405*, 2505-2514; *Sens. Actuators B: Chem.* **2013**, *185*, 762-770; *Anal. Chem.* **2014**, *86*, 9098-9105; *Biosens. Bioelectron.* **2014**, *56*, 104-111; *Biosens. Bioelectron.* **2014**, *59*, 6-13 ; *Anal. Chem.* **2015**, *87*, 9257-9264; *Anal. Chim. Acta* **2016**, *920*, 37-46; *Electroanalysis* **2016**, *28*, 1824-1832 ; *Talanta* **2016**, *154*, 446-454	5.171
Alexandre	Trehoux	4	*J. Mol. Catal. A: Chem.* **2015**, *396*, 40-46; *Dalton Trans.* **2016**, *45*, 706-710; *Dalton Trans.* **2016**, *45*, 18098-18101; *Coord. Chem. Rev.* **2016**, *322*, 142-158	6.327
Yoann	Roux	4	*J. Mol. Catal. A: Chem.* **2015**, *396*, 40-46; *Nat. Commun.* **2015**, *6*, 8509; *Dalton Trans.* **2015**, *44*, 5966-5968; *Dalton Trans.* **2016**, *45*, 18098-18101	5.910
Marion	Devillers	1	*Biosens. Bioelectron.* **2017**, *96*, 178-185	7.476
Bacem	Zribi	3	*Biomicrofluidics* **2016**, *10*, 014115; *Anal. Chim. Acta* **2016**, *920*, 37-46; *Nanoscale* **2016**, *8*, 15479-15485	5.060
Nawel	Mejri-Omrani	4	*Anal. Chem.* **2015**, *87*, 9257-9264; *Biomicrofluidics* **2016**, *10*, 014115; *Anal. Chim. Acta* **2016**, *920*, 37-46; *Talanta* **2016**, *154*, 446-454	4.335
Salma	Bizid	4	*Sens. Actuators B: Chem.* **2016**, *226*, 370-380; *Electroanalysis* **2016**, *28*, 2533-2542; *Anal. Chim. Acta* **2017**, *994*, 10-18; *Talanta* **2018**, *184*, 475-483	4.026
Elodie	Jagu	4	*Bioorg. Med. Chem. Lett.* **2015**, 25, 207-209; *Eur. J. Med. Chem.* **2017**, 139, 982-1015; *Bioorg. Med. Chem.* **2017**, 25, 84-90; *Eur. J. Med. Chem.* **2018**, 150, 655-666	3.612
Thibault	Di Méo	1	*Chem. Eur. J.* **2017**, *23*, 10156-10166	5.771
Yaqiong	Wang	1	*Sens. Actuators B-Chem.* **2017**, *251*, 40-48	4.758
Lama	Ahmad	2	*Biosens. Bioelectron.* **2017**, *96*, 178-185; *FEBS Lett.* **2018**, *592*, 1667-1680	5.550
Rabih	Khoder	1	*Talanta* **2016**, *154*, 446-454	4.035
TOTAL		***41***		
Average/PhD student		***3.15***		***4.95***

6- Participation of team members in setting up Master courses

1. Liability and coordination of licenses and masters : M2 Pollutions Chimiques et Gestion Environnementale (PCGE, L. Salmon), L3P Chimie Organique et Bioorganique (S. Pethe), PACES (F. Avenier), L2 Chimie, Biologie-Chimie et Physique-Chimie (H. Dorizon), L3 Biologie-Chimie (H. Dorizon).
2. Coordination of Teaching Units : M2 PCGE (L. Salmon), M2 ICBM/M2 chimie organique (L. Salmon), L3 chimie-biologie (L. Salmon), PACES (F. Avenier).
3. Courses-conferences in Viet-Nam for Master 2 students (J.-P. Mahy, Franco-vietnamese Workshop).
4. Annual participation in the Open Days of the Paris-Sud and Paris-Saclay Universities.

Appendix 4

Team 5 – SM2B

EVALUATION CAMPAIGN 2018-2019

GROUP E

INFORMATION

Team name:	**Synthèse de Molécules et Macromolécules Bioactives**
Acronym:	**SM2B**
Director's name (current contract):	**Philippe ROGER**
Director's name (future contract):	**Philippe ROGER**

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

13- Articles

Scientific articles

1. "A Tin-Free Regioselective Radical De-*O*-benzylation by an Intramolecular Hydrogen Atom Transfer on Carbohydrate Templates" Attouche A., Urban D., Beau J.-M., Angew. Chem., *Int. Ed. Engl*. **2013**, *52*, 9572–9575.
2. "Synthesis of a *Mycobacterium tuberculosis* Tetra-Acylated Sulfolipid Analogue and Characterization of the Chiral Acyl Chains Using Anisotropic NAD 2D-NMR Spectroscopy" Lemétais A., Bourdreux Y., Lesot P., Farjon J., Beau J.-M., J. Org. Chem. **2013**, *78*, 7648-7657.
3. "One-Pot Synthesis of D-Glucosamine and Chitobiosyl Building Blocks Catalyzed by Triflic Acid on Molecular Sieves" Despras G., Urban D., Vauzeilles B., Beau J.-M., Chem. Comm. **2014**, *50*, 1067-1069.
4. "Direct Umpolung of Glycals Including 2,3-Unsaturated N-Acetylneuraminic Acid Derivatives Using Samarium Diodide" Le X. T., Papin C., Doisneau G., Beau J.-M., Angew. Chem. Int. Ed. **2014**, *53*, 6184-6187.
5. "From Chitin to Bioactive Chitooligosaccharides and Conjugates: Access to Lipochitooligosaccharides and the TMG-chitotriomycin" Despras G., Alix A., Urban D., Vauzeilles B., Beau J.-M., Angew. Chem. Int. Ed. **2014**, *53*, 11912-11916.
6. "Identification of Living Legionella pneumophila Using Species-Specific Metabolic Lipopolysaccharide Labeling" Mas Pons J., Dumont A., Sautejeau G., Fugier E., Baron A., Dukan S., Vauzeilles B., Angew. Chem. Int. Ed. **2014**, *53*, 1275-1278.
7. "Antibacterial Poly(Ethylene terephthalate) Surfaces Obtained From Thymyl Methacrylate Polymerization" Bedel S., Lepoittevin B., Costa L., Leroy O., Dragoe D., Bruzaud J., Herry J.-M., Guilbaud M., Bellon-Fontaine M.-N., Roger P., J. Polym. Sci. Polym. Chem., 2015, 53, 1975-1985.
8. "Plant cell wall imaging by metabolic click-mediated labelling of rhamnogalacturonan II using azido 3-deoxy-D-manno-oct-2-ulosonic acid" Dumont M., Lehner A., Vauzeilles B., Malassis J., Marchant A., Smyth K., Linclau B., Baron A., Mas Pons J., Anderson C. T., Schapman D., Galas L., Mollet J.-C., Lerouge P., Plant J. **2016**, *85*, 437–447.
9. "Catalytic Iron(III) Chloride Mediates Site-selective Protection of Mono- and Disaccharides and one Trisacchairde." Gouasmat A., Lemetais A., Solles J., Bourdreux Y., Beau J.-M., Eur. J. Org. Chem. **2017**, 3355-3361.
10. "Poly(ethylene terephthalate) films modified by UV-induced surface graft polymerization of vanillin derived monomer for antibacterial activity" Salmi-Mani H., Terreros G., Barroca-Aubry N., Aymes-Chodur C., Regeard C., Roger P., Eur. Polym. J., 2018, 103, 51-58.

Review articles

Other articles (professional journals, etc.)

1. "Couplage chimique de biomolécules in cellulo et in vivo" Clerc F., Commerçon A., Vauzeilles B., *Actualité Chimique*, **2015**, *393-394*, 24-30.
2. "Neoglycoconjugates Derived from Deoxynojirimycin as Possible Therapeutic Agents for Cystic Fibrosis Lung Disease, by Modulation of the Sphingolipid Metabolism" Munari S., Loberto N., Aureli M., Vauzeilles B., Baron A., Guisot N., Schiumarini D., Bassi R., Tironi M., Giri M. G., Tamanini A., Lippi G., Cabrini G., Sonnino S., Dechecchi M. C., *JSM Genet. Genomics* **2016**, 3, 1015.
3. "Biomodification Strategies for the Development of Antimicrobial Urinary Catheters: Overview and Advances" S. Anjum, S. Singh, B. Lepoittevin, P. Roger, M. Panigrahi, B. Gupta, *Global Challenges*, **2018**, 2, 1700068.

Clinical articles

14- Books

Scientific book edition

Book chapters

1. Jean-Marie Beau, Yann Bourdreux, François-Didier Boyer, Stéphanie Norsikian, Dominique Urban, Gilles Doisneau, Boris Vauzeilles, Alexandra Gouasmat, Aurélie Lemétais, Aurélie Mathieu, Jean-François Soulé, Arnaud Stevenin, Amandine Xolin: Recent Results in Synthetic Glycochemistry with Iron Salts, *Carbohydr. Chem*. **2014**, *40*, 118-139. DOI: 10.1039/9781849739986-00118.

2. *Yann Le Guen, Guillaume Le Heiget, Dominique Urban, Pierre Chassagne, Laurence A. Mulard:* Allyl 4,6-O-benzylidene-2-deoxy-2-trichloroacetamido-β-D-glucopyranoside in *Carbohydrate Chemistry: Proven Synthetic Methods*, C. Vogel, P. Murphy, Eds, CRC Press, **2017**, Vol. 4, Chapitre 39

3. Jean-Marie Beau, Yann Bourdreux, Guillaume Despras, Alexandra Gouasmat, Géraldine San Jose, Dominique Urban and Boris Vauzeilles : One-pot multi-step regioselective protection of carbohydrates catalyzed by acids in *Protecting Groups – Strategies and Applications in Carbohydrate Chemistry*, S. Vidal, Wiley-VCH, **2018**, ISBN: 978-3-527-34010-1.

15- Meetings

Meeting abstracts

16- Meeting and congress organisation

Please, highlight the most selective.
- Co-organizer – XIIIème Symposium de l'ICSN [ICSN-XIII] – Gif-sur-Yvette – 13-14/06/2013 – 200 participants (BV)
- Organizer – Colloque Pluridisciplinaire de l'UFR Sciences de l'UPSud – Les multiples facettes de la Cristallographie – Orsay – 13/03/2014 (PR)
- Co-organizer – Colloque International « Biomaterials 2014 », New Delhi (Inde) du 27-30/10/2014, coordinateur de la session VII « Antimicrobial Chemistry and Infection Control » (PR)
- Co-organizer – PhysChemCell 2015 - Physical Chemistry of the Cell – Orsay – 4-6/11/2015 – 100 participants (BV)
- Organizer – Colloque Pluridisciplinaire de l'UFR Sciences de l'UPSud – Les machines moléculaires autour du Prix Nobel de Chimie 2016 – Orsay – 16/03/2017 (PR)
- Co-organizer – Colloque Bioadh 2017, Domaine de Frémigny, Bouray-sur-Juine, 15-16/11/2017 (PR)
- Co-organizer – PhysChemCell 2017 - Physical Chemistry of the Cell – Orsay – 15-17/11/2017 – 100 participants (BV)
- Co-organizer – Journée d'automne de la Société de Chimie Thérapeutique - Chemical Biology – Paris – 7/12/2017 - 150 participants (BV)

17- Electronic tools and products

Softwares
Databases
Tools for decision-making
Cohorts *(Biology only)*
Solver competition tools *(Science and technology only)*

18- Instruments and methodology

Prototypes
Platforms and observatories

19- Other products

Artistic creations
Movie or theatre play creation
Movies

20- Editorial activities

Participation to journal editorial boards (books, collections)

Rédacteur en chef − Revue Glycosciences et sciences de la vie − ISTE OpenScience (BV)

21- Peer reviewing activities

Reviewing of journal articles

- Reviewing of journal articles in most journals of organic or bioorganic or polymer chemistry : Angew. Chem. Int. Ed., ACS Chem. Biol., ChemBioChem, Chem. Eur. J., Biochem., Eur. J. Org. Chem., J. Med. Chem., J. Org. Chem., Tetrahedron, Tetrahedron Lett., Synlett, Chem. Commun, J. Am. Chem. Soc., Org. Lett., J. Org. Chem., Carbohydr. Res., Sensors, Polymer, Langmuir, European Polymer Journal, Biomacromolecules, Carbohydrate Research, Reactive and Functional Polymer, Macromolecular Bioscience et Journal of Applied Polymer Science …

Grant evaluation (public or charities)

- Member of the contest researcher of CEA Saclay since 2013 (JMB)
- Evaluation of FRC (Frontier Research in Chemistry) projects : Strasbourg since 2013 (JMB, BV)
- Evaluation of international projects (Europa, USA) (JMB)
- Evaluation of ANR projects (DG, BV)
- Evaluation of CIFRE projects (PR)
- Chairman Committee of Experts : FRM (Fondation pour la Recherche Médicale) – 2018 (BV)

Participation to lab site visit committees (Hceres etc.)

- President of AERES/HCERES committees : Toulouse, Amiens (JMB)
- Member of HCERES committees : Amiens (2016), Nice (2016), Curie-Paris (2017), Bobigny (2018) - (BV)
- Member of CNRS visiting committees, Amiens (2013 et 2015) - (BV)
- Member of evaluation committees of European laboratories (eg, audit of the chemistry department of the University of Namur) (JMB)

Participation to institutional committees and juries (CNRS, INSERM, etc.)

- Jury president « Chaires Idex de l'Université de Bordeaux », 2017, 2018 (JMB)
- Member of CoNRS Section 16 (2012-2016, BV)
- President of CoNRS Section 16 (2016-2021, BV)

- Vice-President Research of Department of Chemistry, Univ Paris Sud (2012-2018, PR)

- Members of Professor and Assistant Professor recruiting committees: Lille, Poitiers, Reims, Cergy-Pontoise, Rouen, Bobigny, Caen, Evry, Châtenay-Malabry, Jussieu, Montpellier, Orsay,…
- Panel member of an ANR evaluation committee (ANR 2018, DG)

- Member of Paris Saclay Academic council (since 2015, DU)

- Member of Chemistry Department of Paris Saclay University (since 2016, DU)

- President, External Recruiting Committee - Group Leader and Future Unit Director position – Institut Curie Orsay, February 2018 (BV)

- President, Selection committee – Doctoral School 2MIB Doctoral Grants – Concours Chimie Organique et Biomoléculaire, 2018 (BV)

- Members of PhD (National and International) and HDR Defense Committees: 10-12 per year

- Members of PhD monitoring committees: Université de Lille, Université Pierre et Marie Curie, Paris, Institut Curie, Orsay, Institut Curie, Paris, Unversité de Nantes, Université Paris-Saclay …

22- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

National public grants (ANR, PHRC, FUI, INCA, etc.)

1. Contrat ANR SIALIFLU "Nouvelles chimies de l'acide sialique ciblant le virus de la grippe" (2010-2014) Coordinateur : Jean-Marie Beau
2. Contrat ANR BioCOS "Innovative Access to Biomass-Based Chitooligosaccharides and their Derivatives for Agrochemical Applications" (2010-2014) Coordinateur : Boris Vauzeilles
3. Partenaire (Resp. Scient. Ph. Roger) de l'ANR SANBACT (2010-2015) "Conception de nouvelles surfaces à propriétés antibactériennes par une approche multidisciplinaire et multiéchelle"
4. Contrat ANR ROSAS "Une collection de sondes fluorescentes pour étudier la production de Formes Réactives de l'Oxygène au niveau de la cellule unique" (2012-2016) Coordinateur : Boris Vauzeilles
5. Partenaire (Resp. Scient. B. Vauzeilles) de l'ANR AuxiWall (2011-2015) Régulation par l'Auxine du métabolisme des Xyloglucanes de la paroi.
6. Partenaire (Resp. Scient. A. Aukauloo) de l'ANR TECH'BIOHYP (2010-2015) Towards Efficient and CHeap BIOinspired cells for Photoelectrochemical HYdrogen Production.
7. Partenaire (Resp. Scient. E. Roulland) de l'ANR Syntia (2014-2019) Tiacumicin B, a new Antibacterial Natural Product Lead Acting on a Novel Druggable Target (JMB).
8. Partenaire (Resp. Scient. Ph. Roger) de l'ANR GASP (2016-2020) "Polymères biosourcés hautement barrière aux gaz et vapeurs pour l'emballage"
9. Partenaire (Resp. Scient. D. Guianvarc'h) de l'ANR AMetHist (2018-2021) Identifying non-histone substrates of the lysine methyltransferase EZH2 with chemically designed orthogonal enzyme-cofactor pairs
10. Contrat CNRS-Mission pour l'Interdisciplinarité – Défi Imag'In - Imagerie tridimensionnelle super−résolue de glycanes de la surface bactérienne et de cellules tumorales. Coordinateur B. Vauzeilles
11. Contrat ANR IngeniOse "Metabolic polysaccharide functionalization for industrial applications – Proof of concept with a cholera vaccine " (2018-2020) Coordinateur : Boris Vauzeilles

Local grants ("collectivités territoriales")

1. Contrat de maturation Declick 1, Société d'Accélération du Transfert de Technologie SATT Sud Est, Marquage de bactéries, Resp. scient B. Vauzeilles, 2013
2. Contrat de maturation Declick 2, Société d'Accélération du Transfert de Technologie SATT Sud Est, Marquage de bactérie, Resp. scient B. Vauzeilles, 2014-2015
3. Contrat de Prématuration MicroTag, IDEX Paris-Saclay, Marquage de microorganismes, Resp. scient B. Vauzeilles, 2016-2017

PIA (Labex, Equipex etc.) grants

1. Partenaire (Resp. Scient. Ph. Roger) du contrat Interdisciplinaire « DtacheBiofilm » financé par le Triangle de la Physique(2014-2016) sur le Détachement de biofilm bactérien en collaboration avec E. Raspaud (LPS, porteur) et C. Regeard (I2BC).
2. Contrat LabEx Charmmmat Formation M2R (2015-2016), porteur : D. Urban, Développement de procédés par « catalyse tandem assistée » Financement d'un M2R de Kévin Muru (6 mois).
3. Initiative de Recherche Stratégique Bioprobe – IDEX Paris-Scalay – Département de Chimie - In vivo metabolic labeling of glycans – Resp. scientif. B. Vauzeilles
4. Contrat France Life Imaging (FLI) – Amorce à collaboration – GRAMM : Ima**G**erie TEP de l'infection b**A**ctérienne par **M**arquage **M**étabolique du lipopolysaccharide – Co-resp. Scientifique B. Vauzeilles

Grants from foundations and charities (ARC, FMR, FRM, etc.)

1. Contrat FRM "Marquage métabolique de bactéries Gram négatives : diagnostic et approches thérapeutiques" (2013-2016) Coordinateur : Boris Vauzeilles

23- Visiting senior scientists and post-doc

Post-docs

Guillaume Despras (January 2011-December 2013) : ANR funding
Scientific output : 4 articles and 1 book chapter

1. "One-Pot Synthesis of D-Glucosamine and Chitobiosyl Building Blocks Catalyzed by Triflic Acid on Molecular Sieves" Despras Guillaume, Urban Dominique, Vauzeilles Boris, Beau Jean-Marie, *Chem. Comm.* **2014**, *50*, 1067-1069.
2. "From Chitin to Bioactive Chitooligosaccharides and Conjugates: Access to Lipochitooligosaccharides and the TMG-chitotriomycin" Despras Guillaume, Alix Aurélien, Urban Dominique, Vauzeilles Boris, Beau Jean-Marie, *Angew. Chem. Int. Ed.* **2014**, *53*, 11912-11916.
3. "Enzymatic remodelling of chitin for agrochemical applications" Chambon Rémi, Despras Guillaume, Urban Dominique, Vauzeilles Boris, Beau Jean-Marie, Fort Sébastien, Armand Sylvie, Cottaz Sylvain, *New Biotechnology* **2014**, *31*, S16-S16.
4. "Efficient chemoenzymatic synthesis of lipo-chitinoligosaccharides plant growth promotors" Chambon Rémi, Despras Guillaume, Brossay Antoine, Vauzeilles Boris, Urban Dominique, Beau Jean-Marie, Armand Sylvie, Cottaz Sylvain, Fort Sébastien, *Green Chem.* **2015**, *17*, 3923-3930.
5. Jean-Marie Beau, Yann Bourdreux, Guillaume Despras, Alexandra Gouasmat, Géraldine San Jose, Dominique Urban and Boris Vauzeilles : One-pot multi-step regioselective protection of carbohydrates catalyzed by acids in *Protecting Groups – Strategies and Applications in Carbohydrate Chemistry*, S. Vidal, Wiley-VCH, **2018**, ISBN: 978-3-527-34010-1.

Visiting senior scientists

Bhuvanesh Gupta (ITT New Delhi, Inde) May 2016 : Charmmmat funding
Scientific output : 1 article

1. "Biomodification Strategies for the Development of Antimicrobial Urinary Catheters: Overview and Advances" S. Anjum, S. Singh, B. Lepoittevin, P. Roger, M. Panigrahi, B. Gupta, *Global Challenges*, **2018**, *2*, 1700068.

24- Scientific recognition

Prizes

- Prix La Recherche 2015 (mention Chimie) : BV
- « APA distinguished award 2016 » by the Scientific Committee of the Asian Polymer Association : PR

Distinctions

IUF members

Senior member of IUF until 2014 (JMB)

Chair of learned and scientific societies

Member of the Scientific Council - Société de Chimie Thérapeutique – since 2016 (BV)

Invitations to meetings and symposia (out of France)

1. B. Vauzeilles : Click-labeling of living bacteria, *8th Indo French Conference in Organic Synthesis,* April 1-3, **2013**, Goa, India.
2. J.-M. Beau: Cascade modifications of carbohydrates in one pot, *27th International Carbohydrate Symposium,* January 12-17, **2014**, Bangalore, India.
3. J.-M. Beau: Opportunities for Exploiting Glycoconjugates and Mimics in Applied Biology: The Example of Plant Growth Stimulation, *International Conference on Challenges in Chemistry and Biology of Carbohydrates (CARBO 28)*, January 20-22, **2014**, Dehradun, India.
4. J.-M. Beau: Boron, iron and samarium for the transformation of carbohydrates, *Meeting of the Hungarian Academy of Sciences: Carbohydrates, Nucleic Acids and Antibiotics*, May 21–23, **2014**, Mátraháza, Hungary.
5. B. Vauzeilles : Detecting Living Pathogens, *New Trends in Chemistry and Chemical Biology - Indo-French Conference,* November 9-12, **2014**, Puducherry, India.
6. J.-M. Beau: Chemistry of the sialic acids, *Glycosciences at CAU*, June 15-17, **2016**, Kiel, Germany.
7. B. Vauzeilles : *Explorations in Chemical Biology*, Twenty-Fifth French- Japanese Symposium on Medicinal and Fine Chemistry (FJS 2016), May 15-18, **2016**, Tokyo, Japan.
8. P. Roger: Polymer obtained from biomolecules with promising antibacterial properties *Conférence Asian Polymer Association-2016*, 5-7 septembre **2016**, Flic-en-Flac, Ile Maurice.
9. B. Vauzeilles : Identification of living Legionella pneumophila using species-specific metabolic lipopolysaccharide Labeling, Annual Meeting of NARILIS Infectiology Research Pole, UNamur, November 24, 2017, Namur, Belgium.

Members' long-term visits abroad

1. P. Roger: Invitation in the framework of the international Cedre program by the Lebanon Atomic Energy Commission (LAEC), April 17-22, **2018**, Beyrouth, Liban.

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

6- Socio-economic interactions / Patents

Invention disclosures

Filed patents

1. *A method for specifically detecting living bacteria*, Application EP12151622.3, January 18, **2012** (CNRS-Univ. Paris-Sud). Sam Dukan, Audrey Dumont, Annie Malleron, Monzer Awwad, Boris Vauzeilles. International extension (PCT) PCT/EP2013/050712, January 16, **2013**.
2. *A method for labeling specifically living bacteria comprising the use of modified monosaccharide compounds, Application EP13190794.1, October 30,* ***2013*** *(CNRS-Aix Marseille Université). Aurélie Baron, Sam Dukan, Jordi Mas Pons, Boris Vauzeilles.* International extension (PCT) PCT/EP2014/073252, October 29, **2014**.
3. *A method for labeling specifically living microorganisms comprising the use of modified monosaccharide compounds, Application EP15166249.1, May 4,* ***2015*** *(CNRS-Aix Marseille Université-Univ. Paris-Sud). Sam Dukan, Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron*. International extension (PCT) PCT/EP2016/059864, May 3, **2016**.
4. *A method for labeling specifically living bacteria comprising the use of modified non endogenous monosaccharide compounds, Application EP15166250.9, May 4,* ***2015*** *(CNRS-Aix Marseille*

Université). Sam Dukan, Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron. International extension (PCT) PCT/EP2016/059880, May 3, **2016**.

5. *New 5-azido-5-deoxy-2 :3-isopropylidene-d-arabinose compounds ; their method of manufacture and their use for the synthesis of Ara-N3, Kdo-N3 And 4eKdo-N3, Application EP15306824.2, November 17,* ***2015*** *(CNRS). Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron.* International extension (PCT) PCT/EP2016/077900, November 16, **2016**.
6. *Method of preparation of 6-azido-2,4-diacetamido-2,4,6-trideoxy-D-mannose, Application EP15306825.9, November 17,* ***2015*** *(CNRS). Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron, Laura Fourmois.* International extension (PCT) PCT/EP2016/077901, November 16, **2016**
7. *Nouveaux polymères, leurs procédés de préparation, et leurs utilisations notamment pour le captage de métaux.* M. Maaz, T. Elzein, B. Nsouli, P. Roger, N. Barroca-Aubry, B. Lepoittevin, Université Paris-Sud, 2 octobre 2017, PCT / FR 2017 / 052705, October 2**, 2017**
8. *Nouveaux polymères greffés, leurs procédés de préparation, et leurs utilisations notamment pour le captage de métaux.* M. Maaz, T. Elzein, B. Nsouli, P. Roger, N. Barroca-Aubry, B. Lepoittevin, CNRS, Université Paris-Sud, 2 octobre 2017, PCT / FR 2017 / 052706, October 2**, 2017**

Accepted patents

Licenced patents

1. *A method for specifically detecting living bacteria*, Application EP12151622.3, January 18, **2012** (CNRS-Univ. Paris-Sud). Sam Dukan, Audrey Dumont, Annie Malleron, Monzer Awwad, Boris Vauzeilles. International extension (PCT) PCT/EP2013/050712, January 16, **2013**.

2. *A method for labeling specifically living bacteria comprising the use of modified monosaccharide compounds, Application EP13190794.1, October 30,* ***2013*** *(CNRS-Aix Marseille Université). Aurélie Baron, Sam Dukan, Jordi Mas Pons, Boris Vauzeilles.* International extension (PCT) PCT/EP2014/073252, October 29, **2014**.

3. *A method for labeling specifically living microorganisms comprising the use of modified monosaccharide compounds, Application EP15166249.1, May 4,* ***2015*** *(CNRS-Aix Marseille Université-Univ. Paris-Sud). Sam Dukan, Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron*. International extension (PCT) PCT/EP2016/059864, May 3, **2016**.

4. *A method for labeling specifically living bacteria comprising the use of modified non endogenous monosaccharide compounds, Application EP15166250.9, May 4,* ***2015*** *(CNRS-Aix Marseille Université). Sam Dukan, Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron.* International extension (PCT) PCT/EP2016/059880, May 3, **2016**.

5. *New 5-azido-5-deoxy-2 :3-isopropylidene-d-arabinose compounds ; their method of manufacture and their use for the synthesis of Ara-N3, Kdo-N3 And 4eKdo-N3, Application EP15306824.2, November 17,* ***2015*** *(CNRS). Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron.* International extension (PCT) PCT/EP2016/077900, November 16, **2016**.

6. *Method of preparation of 6-azido-2,4-diacetamido-2,4,6-trideoxy-D-mannose, Application EP15306825.9, November 17,* ***2015*** *(CNRS). Boris Vauzeilles, Jordi Mas Pons, Aurélie Baron, Laura Fourmois.* International extension (PCT) PCT/EP2016/077901, November 16, **2016**.

7- Socio-economic interactions

Industrial and R&D contracts

- Research Collaborative Contracts (scient. leader : PhR) with the start-up Ethera (Crolles, 38) in 2013-2014 and in 2016-2017 for a total amount of € 27,000 sur « la synthèse par voie enzymatique de fractions d'amylose pour une application capteur ».
- Scientific partner (NBA, CAC, HSM, PR) of a Research Collaborative Contract (Project leader : V. Huc, ECI, ICMMO) with Vernet (2017-2018), amount of funding: 35 k€, confidential.
- Scientific partner (PhR) of a Research Collaborative Contract (Project leader : G. Vo-Thanh, ECM, ICMMO) with Roquette & Freres (2017-2018), amount of funding: 70 k€, confidential.

Cifre fellowships

Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*

Start-ups

Click4Tag SAS – Cofounder Boris Vauzeilles – Dec. 4th, 2014 – Concours Scientifique 2015-2016 – 2 subsidiaries created in 2016 (C4Hydro) and 2017 (C4Diagnostics) – Staff : Click4Tag (4), C4Hydro (3), C4Diagnostics (5).

Clinical trials *(Biology only)*

8- Expertise

Consulting

Scientific Advisor (Concours Scientifique) – Click4Tag – 2015-2016 (B. Vauzeilles).

Participation in expert committees (ANSES etc.)

Legal expertise

9- Expert and standardization reports

10- Public outreach

Radio broadcasts, TV shows, magazines

Journal articles, interviews, book edition, videos, etc.

Une idée lumineuse pour traquer les légionelles, B. Vauzeilles, La Recherche, février **2016**, 508, 64-67.

Other popularization outputs

Debates on science and society

- Village de la Chimie - Chercheur, pourquoi pas moi : Grands témoins – Vincennes 2018 – B. Vauzeilles

- *Interroger le Vivant avec le Langage de la Chimie,* Forums Régionaux du Savoir - Hôtel de Région, October 13, **2016**, Rouen – B. Vauzeilles

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

7- Educational outputs

Books

8- For humanities only, published PhD theses

9- Quality of PhD student supervision

During the 2013-2018 period, 6 PhD were supported. Among them, 2 were financed by MESRI, 2 by the ANR, 1 by Charm3at and 1 by Vietnam. Duration of the theses was 38.8 months and rate of withdrawals was 0. Thesis supervisors, supervisors, sources of funding, date of PhD defense are given in the following table.

Name	Thesis director(s) supervisor	Financial support	Duration (months)	Thesis defense
Tien-Xuan LE	G. Doisneau	Vietnam	43	06/05/2014
Justine PEZZOTTA	G. Doisneau	ANR	41	27/05/2014
Dany FREM	D. Urban	MESRI	36	29/10/ 2014
Sophie BEDEL	Ph. Roger B. Lepoittevin	ANR	38	08/12/2014
Alexandra GOUASMAT	J.-M. Beau Y. Bourdreux	MESRI	36	19/10/2015
Nacim ZIDELMAL	Ph. Roger et A.C. Gouget	LabEx Charmmmat	38	14/03/2018

10- Students' follow up in association with doctoral schools

The policy followed by the team in this area is that of the Doctoral School. We support our PhD students to direct them towards postdoctoral contracts and also put them in touch with all our private sector contacts for those who wish. The current position (if known) is indicated in the following table.

Name	Current position
Tien-Xuan LE	Assistant-professor, Vietnam.
Justine PEZZOTTA	Regulatory affairs scientist at UCB Pharma, Bruxelles, Belgium
Dany FREM	Unknown
Sophie BEDEL	Post-doc position, China
Alexandra GOUASMAT	Associate director of Chemistry - Molecular NeuroImaging, USA
Nacim ZIDELMAL	Searching for a post-doc position

11- Participation to international training programs (e. g. Erasmus Mondus)

12- PhD student participation to scientific animation and unit/team life

PhD students participate to team meetings which are held regularly during which interns, PhDs and post-doctoral fellows are especially invited to rehearse their oral presentations before scientific meetings or presentations at the end of the internship. They promote exchanges between the various actors and ensure good overall cohesion. They also participate to group meetings which are held regularly during which 1 person (permanent or non-permanent researcher) present ongoing work or a bibliographical study on a topic of interest to the thematic in order to federate the group on new projects.

13- Participation of team members in setting up Master courses

Most of the team members have a current teaching activity as part of the Masters of Paris Saclay and others and have set up the corresponding courses, tutorials and practical works (see table below).

Member name	Title of the teaching unit	Level	University/UFR/discipline
AUBRY-BARROCA	Bases de la chimie moléculaire moderne Stratégies et outils en synthèse organique avancée	M1 M1	UPSay/Sciences/Chimie

AYMES-CHODUR	Sciences du médicament - Qualité en développement et production des médicaments Sciences du médicament - Parcours - Contrôle de la qualité des médicaments Sciences du médicament - Parcours - Dispositifs médicaux : évaluation, enregistrement, vigilance	M1 M2 M2	UPSay/Pharmacy UPSay/Pharmacy UPSay/Pharmacy
BOURDREUX	TP de chimie analytique Stratégies et outils en synthèse organique avancée	M1 M1	UPSay/Sciences/Chimie UPSay/Pharmacy
DOISNEAU	Chimie Expérimentale Surfaces et fonctionnalisations organiques	M1 M1	UPSay/Sciences/Chimie UPSay/Pharmacy
GUIANVARC'H	Synthèse de biomolécules bioactives	M2	UPSay/Sciences/Chimie
LEPOITTEVIN	Chimie et physicochimie des polymères	M1	UPSay/Sciences/Chimie
ROGER	Chimie et physicochimie des polymères Chimie des polymères – Parcours GPB Chimie des polymères avancée Les matériaux polymères – Parcours Science de la vision	M1 M1 M2 M2	UPSay/Sciences/Chimie UPSay/Sciences/Chimie UPSay/Sciences/Chimie UPSay/Sciences/Biologie
SALMI-MANI	Chimie des polymères – Parcours GPB	M1	UPSay/Sciences/Chimie
VAUZEILLES	Glycochimie-Glycobiologie Chemical Biology Chimie Combinatoire Dynamique Activation et Etiquetage de Protéines et Biomolécules Bioorthogonal Chemistry	M2 M2 M2 M2 M2	Ecole Polytechnique Ecole Polytechnique UPSay/Pharmacy UPSay/Sciences/Chimie PSL

14- Student publications (for Biology only)

Appendix 4

Team 6 - RMN

EVALUATION CAMPAIGN 2018-2019

GROUP E

INFORMATION

Team name:	**RMN en Milieu Orienté**
Acronym:	**RMN**
Director's name (current contract):	**Denis MERLET**
Director's name (future contract):	**Denis MERLET**

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

25- Articles

Scientific articles

1) *"On-the-fly" kinetics of Enzymatic Racemization using Deuterium NMR in DNA-based Chiral Oriented Media.* M. Chan-Huot, P. Lesot, P. Pelupessy, L. Duma, G. Bodenhausen, P. Duchambon, M. D. Toney, U. V. Reddy, N. Suryaprakash, *Analytical Chemistry*, **2013**, *85*, 4694-4697

2) *Combining J-Edited and Correlation Spectroscopies within a Multi-dimensional Spatial Frequency Encoding: Toward Fully Resolved 1H NMR Spectra.* N. Giraud, D. Pitoux, J.-M. Ouvrard, D. Merlet, *Chemistry - A European Journal*, **2013**, *19*, 12221-12224

3) *The Conformational Behaviour of Naproxen and Flurbiprofen in Solution by NMR Spectroscopy.* M. E. Di Pietro, C. Aroulanda, G. Celebre, D. Merlet, G. De Luca, *New Journal of Chemistry*, **2015**, *39*, 9086-9097

4) *Pushing the Limits of Signal Resolution to Make Coupling Measurement Easier.* J. E. H. Pucheta, D. Pitoux, C. M. Grison, S. Robin, D. Merlet, D. J. Aitken, N. Giraud, J. Farjon, *Chem Commun*, **2015**, *51*, 7939-7942

5) *Probing the Limits of NMR and VCD Spectroscopy in the Stereochemical Assignment of Chiral $^{2}H_{6}$-Neopentane.* A. Masarwa, D. Gerbig, L. Oskar, A. Loewenstein, H. P. Reisenauer, P. Lesot, P. R. Schreiner, I. Marek, *Angew. Chem. Int. Ed.*, **2015**, *54*, 13106-13109

6) *Contribution of NAD 2D-NMR in Liquid Crystals to the Determination of Hydrogen isotope Profile of Methyl Groups in Miliacin.* P. Berdagué, P. Lesot, J. Jacob, V. Terwilliger, C. Le Milbeau, *Geochim. Cosmochim. Acta*, **2016**, *173*, 337-351

7) *Detection of Quadrupolar Nuclei by Ultrafast 2D NMR: Exploring the Case of Deuterated Analytes Aligned in Chiral Oriented Solvents.* P. Lesot, P. Berdague, P. Giraudeau, *Chemical Communications (Cambridge, United Kingdom)*, **2016**, *52*, 2122-2125

8) *Assessing the Stable Conformations of Ibuprofen in Solution by Means of Residual Dipolar Couplings.* M. E. Di Pietro, G. Celebre, C. Aroulanda, D. Merlet, G. De Luca, *European Journal of Pharmaceutical Sciences*, **2017**, *106*, 113-121

9) *Integrated Computational Protocol for the Analysis of Quadrupolar Splittings from Natural-Abundance Deuterium NMR Spectra in (Chiral) Oriented Media.* A. Navarro-Vazquez, P. Berdagué, P. Lesot, *ChemPhysChem*, **2017**, *18*, 1252-1266

10) Highly Accurate Quantitative Analysis of Enantiomeric Mixtures from Spatially Frequency Encoded ^{1}H NMR Spectra. B. Plainchont, D. Pitoux, M. Cyrille, N. Giraud, *Analytical Chemistry*, **2018**, *90*, 1595-1600

Review articles

Correlation 2D-NMR Experiments Involving both ^{13}C and ^{2}H Isotopes in Oriented Media: Methodological and Analytical Applications, P. Lesot, O. Lafon, P. Berdagué, *Magn. Reson. Chem.*, **2014**, *52*, 595-613

Enantiotopic Discrimination in the NMR Spectrum of Prochiral Solutes in Chiral Liquid Crystals. P. Lesot, C. Aroulanda, H. Zimmermann, Z. Luz, *Chem. Soc. Rev.*, **2015**, *44*, 230-275

Other articles (professional journals, etc.)

RMN 2D DAN dans les CLC: de Nouveaux Outils pour l'Etude du Fractionnement Isotopique Naturel (^{2}H/^{1}H) d'Acides Gras et de Triglycérides, P. Lesot, *Spectra Analyse*, **2014**, *299*, 62-72

Rapport de Conjoncture du CoNRS 2014 (INC / S-12), **2014**, Chap. 12, 255-274, CoNRS-CNRS, CNRS Editions, Paris

RMN de Paillasse à TF. Le renouveau de la RMN à Bas Champs, E. Auguste, E. Lucas, L. Poignez, D. Ramaurthyg, H. Vaneeckhoutte, P. Lesot, *Spectra Analyse*, **2017**, *315*, 32-62

La « 39th FGMR Annual Discussion Meeting 2017 »: La Spectroscopie Magnétique Franco-Allemande dans ses « Etats » !, P. Lesot, *Spectra Analyse*, **2017**, *318*, 12-15

26- Books

Scientific book edition

Book chapters

1) *Encyclopedia of Spectroscopy and Spectrometry (ESS),* " Natural Abundance ^{2}H NMR Spectroscopy" P. Lesot, O. Lafon, 3rd Edition, Vol. 3, 1-14, Eds. Lindon, Tranter and Kopenaal, Elsevier, (**2017**)

2) *Encyclopedia of Analycal Science (EAS),* "Nuclear Magnetic Resonance Spectroscopy-Applicable Elements | Hydrogen Isotopes: ^{2}H NMR", P. Lesot, (sous presse), 3rd Edition, 1-16, Eds. J. Lindon, Elsevier, (**2018**)

27- Meetings

Meeting abstracts

28- Meeting and congress organisation

Local organisation of "GBP NMR meeting" at Orsay (2014); Co-organisation of Tropea meeting, NMR in Oriented Phases (2013); GERM president with one conference/year to organize, Member of the Alpine NMR conference

29- Electronic tools and products

Softwares

Databases

Tools for decision-making

30- Instruments and methodology

Prototypes

Platforms and observatories

31- Other products

Artistic creations

Movie or theatre play creation

Movies

32- Editorial activities

Participation to journal editorial boards (books, collections)

One member of the team is in the editorial board of "spectra analyse"
http://www.spectraanalyse.fr/comite-scientifique/

33- Peer reviewing activities

Reviewing of journal articles

Reviewers for *Science*, *Nature Comm.*, *J. Am. Chem. Soc.*, *Ang. Chem, Int. Ed.*, *Chem. Commun.*, *Anal. Chem.*, *J. Magn. Reson.*, *ChemPhysChem, Concepts in MR(A), Magn. Reson. Chem., Chem. Eur. J., Chem. Phys. Lett. J. Chem. Phys., J. Chem. Phys. Lett., J. Phys Chem., New J. Chem., J. Mol. Liq., J. Agr. Food Chem., J. Nat. Products. Anal. Bioanal. Chem.*, *Analyst, RSC Advance, Geochim. Cosmo. Acta, Lett. Org. Chem., J. Org. Chem., CRChimie, Tetrahedron.*

Grant evaluation (public or charities)L

Expertise for ANR (**Défi 3, AAPG**); Agence régionale pour la région pays de la Loire; « European Science Fundation (www.esf.org) » ; « DFG » Allemagne, « Emmy Noether Programme », DIM « Ile-de France »

Participation to lab site visit committees (Hceres etc.)

Two expertise committees for HCERES : i) LCH (2014, Université de Lyon), ii) COBRA (2015, Université de Rouen)

Participation to institutional committees and juries (CNRS, INSERM, etc.)

Participation of the CoNRS committee (Section 12, 2012-2016) and CNU (Section 32, 2012-2016)

34- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

National public grants (ANR, PHRC, FUI, INCA, etc.)

- JCJC ANR grant (2014-2017)
- *Défi ISOTOP CNRS AAP-2018 (Mission pour interdisciplinarité)*, "*Détermination du Fractionnement Enantio-sélectif Position-Spécifique du Carbone-13 par Spectrométrie RMN*"
- Projet « ESPoIR » (*partenaire référent*), CEISAM (Univ. Nantes) / ICMMO (Univ. de Paris-Sud)

Local grants ("collectivités territoriales")

PIA (Labex, Equipex etc.) grants

- M2 internship grant (6 months) from the Labex CHARMMMAT
- Post doctoral grant (2 years) from the Labex CHARMMMAT

Grants from foundations and charities (ARC, FMR, FRM, etc.)

35- Visiting senior scientists and post-doc

Post-docs

2 post-docs :

- Dr. B. Plainchont, financial support : ANR
- Dr. J. E. Herbert-Pucheta, financial support : Labex CHARMMMAT

- *Multi-nuclear NMR of Axially Chiral Biaryls in Polypeptide Orienting Solvents: Spectral Discriminations and Enantiorecognition Mechanisms.* P. Berdagué, J.-E. Herbert-Pucheta, V. Jha, A. Panossian, F. R. Leroux, P. Lesot, *New Journal of Chemistry*, **2015**, *39*, 9504-9517

- *Pushing the limits of signal resolution to make coupling measurement easier.* J. E. Herbert-Pucheta, D. Pitoux, C. M. Grison, S. Robin, D. Merlet, D. J. Aitken, N. Giraud, J. Farjon, *Chem Commun*, **2015**, *51*, 7939-7942
- *Fully Resolved NMR Correlation Spectroscopy.* D. Pitoux, B. Plainchont, D. Merlet, Z. Hu, D. Bonnaffe, J. Farjon, N. Giraud, *Chemistry - A European Journal*, **2015**, *21*, 9044-9047
- *Magnetic field dependence of spatial frequency encoding NMR as probed on an oligosaccharide.* D. Pitoux, Z. Hu, B. Plainchont, D. Merlet, J. Farjon, D. Bonnaffe, N. Giraud, *Magn. Reson. Chem.*, **2015**, *53*, 836-844
- *Achieving High-Resolution and Optimizing Sensitivity in Spatially Frequency Encoding NMR Spectroscopy: From Theory to Practice.* B. Plainchont, D. Pitoux, G. Hamdoun, J.-M. Ouvrard, D. Merlet, J. Farjon, N. Giraud, *Physical Chemistry Chemical Physics*, **2016**, *18*, 22827-22839
- *Combining Pure Shift and J-Edited Spectroscopies: A Strategy for Extracting Chemical Shifts and Scalar Couplings from Highly Crowded Proton Spectra of Oligomeric Saccharides.* D. Pitoux, Z. Hu, B. Plainchont, D. Merlet, J. Farjon, D. Bonnaffe, N. Giraud, *Magnetic Resonance in Chemistry*, **2018**, *56*
- *Highly Accurate Quantitative Analysis of Enantiomeric Mixtures From Spatially Frequency Encoded ^{1}H NMR Spectra.* B. Plainchont, D. Pitoux, M. Cyrille, N. Giraud, *Analytical Chemistry*, **2018**, *90*, 1595-1600

Visiting senior scientists

2 visiting full professors

- Prof. G. De Luca, UNICAL (Italy), 1 week, Erasmus exchange
- Prof. R. Gil, Carnegie Mellon University (USA), 1 week, July 2017

36- Scientific recognition

Prizes

Distinctions

IUF members

Chair of learned and scientific societies

Invitations to meetings and symposia (out of France)

Recent Achievements of NMR in Chiral Anisotropic Media: NMR Methodology and Applications.
P. Lesot, SMASH 2013, Santiago de Compostella, Spain, September 2013.

New Challenges in Chiral Anisotropic NMR: Methodology and Applications 4th Tropea Meeting on NMR in Liquid Crystals, Tropea,
P. Lesot, Italie, Octobre (2013).

NMR using Chiral Anisotropic Solvents: Recent Methodological Advances and new Analytical Applications.
P. Lesot, "19th National Conference of NMR Society", Tezpur, India, February 2014.

Revisiting Correlation Spectra in NMR Spectroscopy: Recent Developments in the Field of Spatial Frequency Encoding.
N. Giraud, Small Molecule NMR Conference, Atlanta, GA, USA, September 2014.

Spectroscopie RMN, Anisotropie et Chiralité: une Aventure Méthodologique et Analytique dans les Cristaux Liquides Chiraux.
P. Lesot, Journées Pratiques Francophones des Sciences Analytiques 2017, Marrakesh, Maroc. April 2017.

Members' long-term visits abroad

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

11-Socio-economic interactions / Patents

Invention disclosures
Filed patents
Accepted patents
Licenced patents

12-Socio-economic interactions

Industrial and R&D contracts
Cifre fellowships
Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*
Member of GDR CHIRAFUN
Member of FR "RMN Ile de France"
Member of SCF
Member of the Indian NMR Society

Start-ups
Clinical trials *(Biology only)*

13-Expertise

14-

Consulting
Participation in expert committees (ANSES etc.)
Legal expertise

15-Expert and standardization reports

Expert member (ITRF) nominated by MESR

16-Public outreach

Radio broadcasts, TV shows, magazines

Journal articles, interviews, book edition, videos, etc.

- *C&E News of ACS, 2013*
  http://cen.acs.org/articles/91/web/2013/04/Watching-Enzymes-Change-MoleculesChirality.html
- *Site de RMN : « theresonance.com », 2016*
  http://www.theresonance.com/exploring-the-analytical-potential-of-anisotropic-natural-abundance-deuterium-nmr-spectroscopy/. Part I and part II
- *Article présenté sous la forme d'un communiqué de presse CNRS-INC/INSU et Paris-Sud, 2015-2016*
  http://www.cnrs.fr/inc/communication/direct labos/lesot2.htm
  http://www.actu.u-psud.fr/fr/recherche/actualites-2016/dans-l-intimite-isotopique-des-molecules-fossiles.html

Other popularization outputs
Debates on science and society

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

15- Educational outputs

Books

E-learning, MOOCs, multimedia lessons, etc.

- Among team permanent staff, one is member of the network “Chimactiv” dedicated to educational purposes in analytical chemistry. Local impact on Master students in the frame of Université Paris-Saclay.
- Among team permanent staff, one is co-organiser of “Challenge de Chimie”, one day each year, a dedicated event to Bachelor students involving industrial partners and academic staff to help them to better define their professional project in the different domains of the chemistry in the frame of Region Ile-de-France
- Among team permanent staff, one has been involved in “Fête de la Science”, a national event dedicated to the vulgarisation of Sciences and Chemistry within the unit ICMMO.

16- For humanities only, published PhD theses

17- Quality of PhD student supervision

- M.-E. Di-Pietro, PhD defense on December 2013, « NMR development in thermotropic and lyotropic liquid crystal solvent for the structural determination », financial support from Calabria Region, Italy, joint PhD, 3 years.
- D. Pitoux, PhD defense on March 2015, « Développement de nouvelles expériences de corrélation en RMN haute-résolution mettant en œuvre un encodage spatial de l'échantillon », ANR, 3 years.
- G. Alaoui, PhD defense foreseen on October 2018, Tunisian financial support, 3 years.
- T. Texier-Bonniot, PhD defense foreseen on October 2019, MENSR financial support, 3 years.

18- Students' follow up in association with doctoral schools

When supervising PhD student, it is a noteworthy part of our work to explain them the scientific frame and environment in France, academic and non-academic positions, as well as at international level, especially to find a post doc position. The team tries to keep in touch with the PhD students and follows their career. One is currently in 1-year postdoc position in Milano (Italy), after 2-years postdoc position in Karlsruhe (Germany) financially supported by a Von Humboldt grant and 6-months post-doc position in UNICAL (Italy) granted by the program “L'Oréal : Women in Science”. The second one is currently working as a permanent staff in a private company.

19- Participation to international training programs (e. g. Erasmus Mondus)

The NMR team provides the NMR lectures and NMR practical works in the Erasmus Mundus SERP-CHEM master.

20- PhD student participation to scientific animation and unit/team life

Among PhD students, one has been involved in “Fête de la Science”, a national event dedicated to the vulgarisation of Sciences and Chemistry within the unit ICMMO.

21- Participation of team members in setting up Master courses

All permanent staff of the ERMN team (full, associated professors and researchers) is involved in the Master of Chemistry of Université Paris-Saclay. Among us, one is the head of the first year of this Master and consequently performs an unavoidable significant work to set up and manage Master courses, especially in the frame of Université Paris-Saclay.

22- Student publications (for Biology only)

Appendix 4

Team 7 - ECI

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Chimie Inorganique**
Acronym:	**ECI**
Director's name (current contract):	**Talal MALLAH**
Director's name (future contract):	**Ally AUKAULOO**

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

37- Articles

Scientific articles

1. *Snapshots of Light Induced Accumulation of Two Charges on Methylviologen using a Sequential Nanosecond Pump–Pump Photoexcitation*. Tran, T.-T.; Ha-Thi, M.-H.; Pino, T.; Quaranta, A.; Lefumeux, C.; Leibl, W.; Aukauloo, A. *J. Phys. Chem. Lett.* **2018,** *9*, 1086-1091. FI 8.539
2. *Visible Light-Driven Reduction of CO2 to CO and Its Subsequent Valorization in Carbonylation Chemistry and 13C Isotope Labelling*. Gotico, P.; Del Vecchio, A.; Audisio, D.; Quaranta, A.; Halime, Z.; Leibl, W.; Aukauloo, A. *ChemPhotoChem* **2018,** 10.1002/cptc.201800012. FI inconnu
3. *Water Molecules Gating a Photoinduced One Electron Two Protons Transfer in a Tyr/His model of Photosystem II*. Chararalambidis, G.; Das, S.; Trapali, A.; Quaranta, A.; Orio, M.; Halime, Z.; Fertey, P.; Guillot, R.; Coutsolelos, A.; Leibl, W.; Aukauloo, A.; Sircoglou, M. *Angew. Chem. Int. Ed.* **2018,** *10.1002/anie.201804498*. FI 11.709
4. *Comparison of structural dynamics and coherence of d-d and MLCT light-induced spin state trapping*. Zerdane, S.; Wilbraham, L.; Cammarata, M.; Iasco, O.; Rivière, E.; Boillot, M. L.; Ciofini, I.; Collet, E. *Chem. Sci.* **2017,** *8*, 4978-4986. FI 9.144
5. *Mimicking the Regulation Step of Fe-Monooxygenases: Allosteric Modulation of FeIV-Oxo Formation by Guest Binding in a Dinuclear ZnII–FeII Calix[6]arene-Based Funnel Complex*. Ségaud, N.; De Thomasson, C.; Daverat, C.; Sénéchal-David, K.; Dos Santos, A.; Steinmetz, V.; Maître, P.; Rebilly, J. N.; Banse, F.; Reinaud, O. *Chem. Eur. J.* **2017,** *23*, 2894-2906. FI 5.771
6. *Macroscopic Magnetic Anisotropy Induced by the Combined Control of Size, Shape and Organization of NiFe Prussian Blue Analog Nanoparticles in an Ordered Mesoporous Silica Monolith*. Moulin, R.; Fornasieri, G.; Impéror-Clerc, M.; Rivière, E.; Beaunier, P.; Bleuzen, A. *ChemNanoMat* **2017,** *3*, 833-840. FI 2.937
7. *Elucidating the light-induced charge accumulation in an artificial analogue of methane monooxygenase enzymes using time-resolved x-ray absorption spectroscopy*. Moonshiram, D.; Picon, A.; Vazquez-Mayagoitia, A.; Zhang, X.; Tu, M.-F.; Garrido-Barros, P.; Mahy, J.-P.; Avenier, F.; Aukauloo, A. *Chem. Commun.* **2017,** *53*, 2725-2728. FI 6.567
8. *Time-Resolved Interception of Multiple-Charge Accumulation in a Sensitizer–Acceptor Dyad*. Mendes Marinho, S.; Ha-Thi, M. H.; Pham, V. T.; Quaranta, A.; Pino, T.; Lefumeux, C.; Chamaillé, T.; Leibl, W.; Aukauloo, A. *Angew. Chem. Int. Ed.* **2017,** *56*, 15936-15940. FI 11.709
9. *Light-Controlled Release and Uptake of Zinc Ions in Solution by a Photochromic Terthiazole-Based Ligand*. Guérin, J.; Leaustic, A.; Berthet, J.; Métivier, R.; Guillot, R.; Delbaere, S.; Nakatani, K.; Yu, P. *Chem. Asian J.* **2017,** *12*, 853-859. FI 4.592
10. *New method for the growth of single-walled carbon nanotubes from bimetallic nanoalloy catalysts based on Prussian blue analog precursors*. Castan, A.; Forel, S.; Catala, L.; Florea, I.; Fossard, F.; Bouanis, F.; Andrieux-Ledier, A.; Mazerat, S.; Mallah, T.; Huc, V.; Loiseau, A.; Cojocaru, C. S. *Carbon* **2017,** *123*, 583-592. https://doi.org/10.1016/j.carbon.2017.07.058 FI 6.198
11. *Unraveling σ and π Effects on Magnetic Anisotropy in cis-NiA4B2 Complexes: Magnetization, HF-HFEPR Studies, First-Principles Calculations, and Orbital Modeling*. Charron, G.; Malkin, E.; Rogez, G.; Batchelor, L. J.; Mazerat, S.; Guillot, R.; Guihery, N.; Barra, A. L.; Mallah, T.; Bolvin, H. *Chem. Eur. J.* **2016,** *22*, 16848-16860. FI 5.771
12. *Engineering the magnetic coupling and anisotropy at the molecule–magnetic surface interface in molecular spintronic devices*. Campbell, V. E.; …; …; …; …; Rivière, E.; …; …; …; …; …; …; …; …; …; …; …; …; …; …; …; Mallah, T. *Nat. Comm.* **2016,** *7*, 13646. FI 11.329
13. *Elastically driven cooperative response of a molecular material impacted by a laser pulse*. Bertoni, R.; Lorenc, M.; Cailleau, H.; Tissot, A.; Laisney, J.; Boillot, M.-L.; Stoleriu, L.; Stancu, A.; Enachescu, C.; Collet, E.. *Nat. Mater.* **2016,** *15*, 606. FI 38.891
14. *Molecular-scale dynamics of light-induced spin cross-over in a two-dimensional layer*. Bairagi, K.; Iasco, O.; Bellec, A.; Kartsev, A.; Li, D.; Lagoute, J.; Chacon, C.; Girard, Y.; Rousset, S.; Miserque, F.; Dappe, Y. J.; Smogunov, A.; Barreteau, C.; Boillot, M.-L.; Mallah, T.; Repain, V. *Nat. Comm.* **2016,** *7*, 12212. FI 11.329
15. *A New, Simple and Versatile Strategy for the Synthesis of Short Segments of Zigzag-Type Carbon Nanotubes*. André, E.; Boutonnet, B.; Charles, P.; Martini, C.; Aguiar-Hualde, J. M.; Latil, S.; Guérineau, V.; Hammad, K.; Ray, P.; Guillot, R.; Huc, V. *Chem. Eur. J.* **2016,** *22*, 3105-3114. FI 5.771
16. *Electrochemical study of a nonheme Fe(ii) complex in the presence of dioxygen. Insights into the reductive activation of O2 at Fe(ii) centers*. Segaud, N.; Anxolabéhère-Mallart, E.; Sénéchal-David, K.; Acosta-Rueda, L.; Robert, M.; Banse, F. *Chem. Sci.* **2015,** *6*, 639-647. FI 9.144

17. *Successive light-induced two electron transfers in a Ru-Fe supramolecular assembly: from Ru-Fe(ii)-OH2 to Ru-Fe(iv)-oxo*. Herrero, C.; Quaranta, A.; Sircoglou, M.; Senechal-David, K.; Baron, A.; Marin, I. M.; Buron, C.; Baltaze, J.-P.; Leibl, W.; Aukauloo, A.; Banse, F. *Chem. Sci.* **2015,** *6*, 2323-2327. FI 9.144
18. *Assessing the exchange coupling in binuclear lanthanide(iii) complexes and the slow relaxation of the magnetization in the antiferromagnetically coupled Dy2 derivative*. Chow, C. Y.; Bolvin, H.; Campbell, V. E.; Guillot, R.; Kampf, J. W.; Wernsdorfer, W.; Gendron, F.; Autschbach, J.; Pecoraro, V. L.; Mallah, T. *Chem. Sci.* **2015,** *6*, 4148-4159. FI 9.144
19. *Ising-type magnetic anisotropy and single molecule magnet behaviour in mononuclear trigonal bipyramidal Co(ii) complexes*. Ruamps, R.; Batchelor, L. J.; Guillot, R.; Zakhia, G.; Barra, A. L.; Wernsdorfer, W.; Guihery, N.; Mallah, T. *Chem. Sci.* **2014,** *5*, 3418-3424. FI 9.144
20. *Magnetization Reversal in CsNiIICrIII(CN)6 Coordination Nanoparticles: Unravelling Surface Anisotropy and Dipolar Interaction Effects*. Prado, Y.; Mazerat, S.; Rivière, E.; Rogez, G.; Gloter, A.; Stephan, O.; Catala, L.; Mallah, T. *Adv. Funct. Mater.* **2014,** *24*, 5402-5411. FI 11.382
21. *MnII-containing coordination nanoparticles as highly efficient T1 contrast agents for magnetic resonance imaging*. Paul, G.; Prado, Y.; Dia, N.; Riviere, E.; Laurent, S.; Roch, M.; Vander Elst, L.; Muller, R. N.; Sancey, L.; Perriat, P.; Tillement, O.; Mallah, T.; Catala, L. *Chem. Commun.* **2014,** *50*, 6740-6743. FI 6.567
22. *Photochromic-fluorescent-plasmonic nanomaterials: towards integrated three-component photoactive hybrid nanosystems*. Ouhenia-Ouadahi, K.; Yasukuni, R.; Yu, P.; Laurent, G.; Pavageau, C.; Grand, J.; Guerin, J.; Leaustic, A.; Felidj, N.; Aubard, J.; Nakatani, K.; Metivier, R. *Chem. Commun.* **2014,** *50*, 7299-7302. FI 6.567
23. *Solid-State Magnetic Switching Triggered by Proton-Coupled Electron-Transfer Assisted by Long-Distance Proton-Alkali Cation Transport*. Higel, P.; Villain, F.; Verdaguer, M.; Rivière, E.; Bleuzen, A. *J. Am. Chem. Soc.* **2014,** *136*, 6231-6234. FI 13.038
24. *Understanding Spin Structure in Metallacrown Single-Molecule Magnets using Magnetic Compton Scattering*. Deb, A.; Boron, T. T.; Itou, M.; Sakurai, Y.; Mallah, T.; Pecoraro, V. L.; Penner-Hahn, J. E. *J. Am. Chem. Soc.* **2014,** *136*, 4889-4892. FI 13.038
25. *Giant Ising-Type Magnetic Anisotropy in Trigonal Bipyramidal Ni(II) Complexes: Experiment and Theory*. Ruamps, R.; Maurice, R.; Batchelor, L.; Boggio-Pasqua, M.; Guillot, R.; Barra, A. L.; Liu, J. J.; Bendeif, E.; Pillet, S.; Hill, S.; Mallah, T.; Guihery, N. *J. Am. Chem. Soc.* **2013,** *135*, 3017-3026. FI 13.038
26. *Photoinduced Relaxation Dynamics in Iron(II) Spin-Crossover Nanoparticles: The Significance of Crystallinity*. Chakraborty, P.; Boillot, M. L.; Tissot, A.; Hauser, A. *Angew. Chem. Int. Ed.* **2013,** *52*, 7139-7142. FI 11.709
27. *XMCD at the Transition Metal K-Edges as a Probe of Small Pressure-Induced Structural Distortions in Prussian Blue Analogues*. Cafun, J.-D.; Lejeune, J.; Itié, J.-P.; Baudelet, F.; Bleuzen, A. *J. Phys. Chem. C* **2013,** *117*, 19645-19655. FI 4.509

Review articles

28. *Magnetism and Photomagnetism of Prussian Blue Analogue Nanoparticles Embedded in Porous Metal Oxide Ordered Nanostructures*. Fornasieri, G.; Bordage, A.; Bleuzen, A. *Eur. J. Inorg. Chem.* **2018**, 259-271. FI 2.686
29. *Nanoparticles of Prussian blue analogs and related coordination polymers: From information storage to biomedical applications*. Catala, L.; Mallah, T. *Coord. Chem. Rev.* **2017,** *346*, 32-61. FI 12.994
30. *Femtosecond photoswitching dynamics and microsecond thermal conversion driven by laser heating in FeIII spin-crossover solids*. Bertoni, R.; Lorenc, M.; Tissot, A.; Boillot, M. L.; Collet, E. *Coord. Chem. Rev.* **2015,** *282-283*, 66-76. FI 12.994

Other articles (professional journals, etc.)

38- Books

Scientific book edition

Editor of a special issue on Artificial Photosynthesis for Compte Rendus de l'Académie des Sciences on the occasion of 2015 Year of Light. Molecular chemistry offers immense possibilities in the optimisation of molecules that are capable to capture visible light energy and to drive redox catalysis at low overpotentials. However, research in this field is still at the stage of basic research. It is to be expected that the mobilised effort from chemists on an international level will contribute to step from exciting laboratory findings to potential technological deployment. This will only be possible by sharing our results and personal view. It is with this target that this issue of Comptes-Rendus de Chimie was planned and realised.

Book chapters

1. Photochromic Materials: Preparation, Properties and Applications, K. Nakatani, J. Piard, P. Yu, R. Métivier, 1, 1 to 45, He Tian & Junji Zhang, Wiley-VCH, Introduction: Organic Photochromic Molecules, 2016.
2. Artificial Photosynthesis, A. Aukauloo, W. Leibl, 79, 3, 63-98, B. Robert, Academic Press, Bioinspired Photocatalysis, 2016, Advances in Botanical Research
3. Porphyrins and Metalloporphyrins as Components in Artificial Photosynthesis Research, Chapter 179, Handbook of Porphyrin Science. 2014.

39- Meetings

Meeting abstracts

40- Meeting and congress organisation

1. Journées de Catalyse de Paris-Saclay (2nd edition, 28-29 april 2014, Campus de Gif-sur-Yvette, and 3rd edition, 5-6 april 2018, Campus de Gif-sur-Yvette https://jcps2018.sciencesconf.org/), F. Banse
2. GECOM-CONCOORD 2017, 15 - 18 may 2017, Domaine de Forges, Forges-les-Eaux (https://gecom2017.sciencesconf.org/), F. Banse
3. 8th European School on Molecular Nanoscience, October 25th – 29th, 2015 Paris France (http://www.icmol.es/esmolna2015/), T. Mallah

41- Electronic tools and products

Softwares

Databases

Tools for decision-making

Solver competition tools *(Science and technology only)*

42- Instruments and methodology

Prototypes

Platforms and observatories

43- Other products

Artistic creations

Movie or theatre play creation

Movies

44- Editorial activities

Participation to journal editorial boards (books, collections)

45- Peer reviewing activities

Reviewing of journal articles

The members of the group contribute to reviewing in the most selective journals such as Nature Materials, Nature Chemistry, Nature Communication, JACS, Angew. Chem., Chem. Soc. Rev, Coord. Chem. Rev., Chem. Sci. etc… The number of articles reviewed is around 150 per year among them around 15% in the journals mentioned above.

Grant evaluation (public or charities)

The members of the groups contribute to public grant evaluation at the national, European (ERC, COST actions, Marie Curie,.) and international level (NSF). The number of projects reviewed is around 15 per year.

Participation to lab site visit committees (Hceres etc.)

INAC, CEA-Grenoble 19-22 January 2015

Participation to institutional committees and juries (CNRS, INSERM, etc.)

1. Member of the ANR Energy committee 2013-2016 (A. Aukauloo)
2. Member of the Evaluation Committee of Institut Universitaire de France Junior (2016-2018), (A. Aukauloo)
3. Chairman of the Evaluation Committee of Institut Universitaire de France Senior (2018-), (A. Aukauloo)

46- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

1. IRSES, Universite Paris-Sud, CNRS, Uniwersytet Wroclawski, Universita Degli Studi di Parma, Taras Shevchenko National University of Kyiv, University of Michigan, CNRS, Metallacrowns, 2013-2017.
2. PHC Brancusi, M.-L. Boillot, T. Mallah, L. Catala, C. Enachescu, Faculty of Physics, Univ. Iasi, Roumanie, 2015-2017

National public grants (ANR, PHRC, FUI, INCA, etc.)

1. ANR, J.-P. Mahy, F. Banse, K. Sénéchal-David, B. Schöllorn; D. Mandon, ICMMO LCBB-ECI, Univ. Paris-Sud, LEM, Univ. Paris Diderot; LCBMT, Univ. Strasbourg, CATHYMETHOXY, 2012-2016
2. ANR, P. Rabu, A. Bleuzen, G. Fornasieri, IPCMS, CNRS Strasbourg ; C-BLUE, 2012-2014
3. ANR, V. Repain, T. Mallah, M.-L. Boillot, C. Barreteau, MPQ, Univ. Paris-Diderot; IRAMIS, CEA-Saclay, SPIROU, 2013-2018
4. ANR, C. Bicharra, V. Huc, Université de Paris-Sud, CiNam, ONERA, Ecole Polytechnique, SYNAPSE, 2013-2017
5. ANR, W. Wernsdorfer, T. Mallah, M. Ruben, Institut Néel-Grenoble, ICMMO, Institut de Physique et de Chimie des Matériaux de Strasbourg, MolQuSpin, 2013-2017
6. ANR, E. Collet, T. Mallah, M.-L. Boillot, L. Catala, G. Chastanet, A. Rousse, IPR, Univ. Rennes; ICMCB, Univ. Bordeaux; LOA, INSTA, Palaiseau, FEMTOMAT, 2014-2018
7. ANR, P. Viel, V. Huc, CEA/Université de Paris-Sud, CYTER, 2014-2017
8. ANR, P. Roger, GASP, 2016-2020
9. ANR, T. Tron, A. Aukauloo, W. Leibl, F. Banse, M. Sircoglou, K. Sénéchal-David, Multiplet, 2016-2019
10. ANR, E. Shilova, CEA/Université de Paris-Sud, NanoExtract, 2016-2018
11. ANR, V. Huc, Université de Paris-Sud/IPNOrsay Physics, HIBISCUS, 2017-2020
12. ANR, R. Métivier, P. Yu, A. Léaustic, PPSM ENS Cachan Université Paris-Saclay et ITODYS Université Paris-Diderot, SWIST, 2018-2021
13. ANR, R. Mattana, T. Mallah, P. Yu, A. Léaustic, Unité Mixte de Physique-UPSUD, Institut d'électronique de microélectronique et de nanotechnologie-Univ Lille1, Laboratory for Chemistry of Novel Materials-UMONS-Belgique, SpinFun, 2018-2021
14. ANR, A. Bordage, A. Bleuzen, G. Fornasieri, E. Rivière, MagDiDi, 2018-2021

Local grants ("collectivités territoriales")

1. PRES Universud, V. Huc, CAN, 2013-2014
2. Domaine d'Intérêt Majeur, OxyMore, Financement de stage Post-doctoral, M. Imperor, A. Bleuzen, LPS-ICMMO, 2014-2015
3. International Chair Pascal-Pr. Eugenio Coronado, T. Mallah, Institut Parisien de chimie-UPMC, Institut Lavoisier-UVSQ, Unité Mixte de Physique-UPSUD, MolSpin, 2014-2016
4. SATT Paris-Saclay, concours maturation, C. Martini, V. Huc, NOVECAL, 2015-2017
5. SATT Maturation, V. Huc, P. Viel, E. Shilova, CEA/Université de Paris-Sud, CYTER, 2015-2017
6. Domaine d'Intérêt Majeur RESPORE, T. Mallah, M.-L. Boillot, C. Serre, Institut des Matériaux Poreux de Paris, 2DFun, 2017-2019
7. Domaine d'Intérêt Majeur RESPORE, R. Lescouezec, M.-L. Boillot, E. Rivière, L. Catala, IPCM, Univ. Pierre et Marie Curie; Institut des Matériaux Poreux, ENS Paris, 2018-2019

PIA (Labex, Equipex etc.) grants

1. EQUIPEX, V. Huc, ANDROMEDE, 2011-2021

2. Labex NanoSaclay, T. Mallah, Project Molecular Spintronics, 2012-2015.
3. LabEx NanoSaclay/PALM, V. Huc, CEA, CYTER, 2013-2014
4. LabEx NanoSaclay, V. Huc, SYNACA, 2013-2014
5. Labex Charmmmat, F. Banse, C. Herrero, W. Leibl (CEA Saclay), Photoactivation des intermédiaires peroxydiques, 2013-2014
6. LABEX CHARMMMAT, A. Aukauloo, P. Dauban, 2014-2017
7. LABEX NanoSaclay, C. Martini, H. Vincent, 2014-2015
8. Labex NanoSaclay-Professeur invité, T. Mallah, J. Long, 2014-2014
9. Labex Charmmmat, F. Banse, K. Cheaib, Winfried Leibl (CEA Saclay), Photoanode Ruthénium-Fer pour l'activation de l'eau : vers une cellule photoélectrochimique, 2015-2016
10. Labex CHARMMMAT, P. Yu, V. Trannoy, A. Léaustic, Institut Lavoisier UVSQ Université Paris-Saclay et PPSM ENS Cachan Université Paris-Saclay, 2016-2017
11. Labex Charmmmat. Post-doc 12 mois (Dr H. Dridi), J.-N. Rebilly, Université Versailles Saint Quentin (Dr O. Oms), Hybrides polyoxométallates-complexes de FeII pour la catalyse d'oxydation par le dioxygène., 2016-2017
12. Labex CHARMMMAT, P. Yu, V. Trannoy, A. Léaustic, Institut Lavoisier UVSQ Université Paris-Saclay, PPSM ENS Cachan Université Paris-Saclay et LPCIM Ecole Polytechnique, 2017-2018
13. Labex CHARMMMAT, A. Aukauloo, Professeur Invité Lionel Cheruzel, 2017-2017
14. Labex NanoSaclay, T. Mallah, D. Mailly, Centre de Nanosciences et de Nanotechnologies-C2N, TransNanoSheet, 2017-2019
15. LabEx PALM/NanoSaclay, V. Huc, ICMMO/IPN, LEIS, 2018-2018
16. LabEx CHARMMMAT, Z. Halime, L. Benedikt, Synchrotron SOLEIL, 2018-2019
17. IDEX Prématuration, V. Huc, P. Viel, CYTER, 2014-2015
18. IDEX Prématuration, C. Martini, V. Huc, ANNEMOL, 2014-2015
19. Initiatives de Recherche Stratégiques (IRS) IDEX Paris-Saclay, S. Lacombe, L. Catala, NANOTHERAD, 2018-2018
20. Initiatives de Recherche Stratégiques (IRS) IDEX Paris-Saclay, A. Aukauloo, H. Remita, MOMENTUM, consortium of 26 Research teams, 2017-2020

Grants from foundations and charities (ARC, FMR, FRM, etc.)

47- Visiting senior scientists and post-doc

Post-docs

1. Shilova Ekaterina, 1/9/2012-31/8/2013, Labex LabEx NanoSaclay/PALM; AAP « Valo »
2. Viciano Marta, 1/1/2013-30/4/2014, Labex Nanosaclay
3. Iasco Olga, 1/1/2013-31/3/2013, ANR ULTIMATE, 1/4/2013-31/7/2015, ANR SPIROU, 1/8/2014-31/10/2016, ANR FEMTOMAT, 1/9/2017-1/7/2018 industrial project with VERNET
4. Martini Cyril, 1/9/2013-31/8/2014 : contrat LabEx NanoSaclay AAP émergence, 1/9/2014-31/8/2015, contrat IdEx Prématuration and 1/9/2015-31/8/2018 contrat SATT maturation
5. Lopez-Jorda Mauri, 1/9/2013-31/8/2014, Labex CHARMMAT and 1/9/2014-31/8/2015, ANR MolQuspin
6. Herrero Christian, 01/09/2013-31/08/2014, Labex CHARMMMAT, 01/09/2014-31/08/2015, ANR Cathymetoxy
7. Jheng□Guang Li, 1/9/2014-31/8/2015, DIUM Oxymore
8. Gros Guillaume, 1/9/2014-31/8/2015, IdEx « prématuration » Paris-Saclay, 1/9/2015-31/8/2017, contrat maturation SATT Paris-Saclay
9. Poirel Arnaud, 1/9/2014-31/8/2015, AAP « NEEDS » déchets, 1/9/2015-31/8/2017 contrat maturation SATT Paris-Saclay
10. Cheaib Khaled, 01/04/2016-31/03/2017, Labex CHARMMMAT and 1/4/2018-31/03/2018, Labex CHARMMMAT
11. Trannoy Virgile, 01/11/2016-01/10/2018, Labex CHARMMMAT
12. Farran Rajaa, 1/9/2016-31/8/2017, ANR MULTIPLET
13. Abdellah Ibrahim, 1/9/2016-31/8/2017 contrat SATT maturation, 1/9/2017-31/8/2018 contrat LabEx CHARMMMAT, AAP « valorisation »
14. Dridi Hachem, 01/11/2016-31/10/2017, Labex CHARMMMAT
15. Das Shyamal, 1/1/2017-31/12/2018, CEA grant
16. Buendia Julien, 1/1/2017-31/12/2018, Labex CHARMMMAT
17. Lai Thanh Loan, 1/9/2017-31/8/2018, ANR PRCE HISBICUS

18. Parchamoni Sri, 1/4/2018-31/3/2019, DIM Respore

Post-doc publications

1. *A Bis-Binuclear Ni-II Complex with Easy and Hard Axes of Magnetization: Complementary Experimental and Theoretical Insights*. El-Khatib, F.; Cahier, B.; Lopez-Jorda, M.; Guillot, R.; Rivière, E.; Hafez, H.; Saad, Z.; Guihéry, N.; Mallah, T. *Eur. J. Inorg. Chem.* **2018**, 469-476.
2. *Water Molecules Gating a Photoinduced One Electron Two Protons Transfer in a Tyr/His model of Photosystem II*. Chararalambidis, G.; Das, S.; Trapali, A.; Quaranta, A.; Orio, M.; Halime, Z.; Fertey, P.; Guillot, R.; Coutsolelos, A.; Leibl, W.; Aukauloo, A.; Sircoglou, M. *Angew. Chem. Int. Ed.* **2018,** *10.1002/anie.201804498*.
3. *Temperature-, Light-, and Soft X-ray-Induced Spin Crossover in a Single Layer of Fe-II-Pyrazolylborate Molecules in Direct Contact with Gold*. Bairagi, K.; Bellec, A.; Fourmental, C.; Iasco, O.; Lagoute, J.; Chacon, C.; Girard, Y.; Rousset, S.; Choueikani, F.; Otero, E.; Ohresser, P.; Sainctavit, P.; Boillot, M. L.; Mallah, T.; Repain, V. *J. Phys. Chem. C* **2018,** *122*, 727-731.
4. *Comparison of structural dynamics and coherence of d-d and MLCT light-induced spin state trapping*. Zerdane, S.; Wilbraham, L.; Cammarata, M.; Iasco, O.; Rivière, E.; Boillot, M. L.; Ciofini, I.; Collet, E. *Chem. Sci.* **2017,** *8*, 4978-4986.
5. *Hysteresis in a bimetallic holmium complex: A synergy between electronic and nuclear magnetic interactions*. Viciano-Chumillas, M.; Koprowiak, F.; Mutikainen, I.; Wernsdorfer, W.; Mallah, T.; Bolvin, H. *Phys. Rev. B* **2017,** *96*, 214427.
6. *Light-driven electron transfer in a modular assembly of a ruthenium(II) polypyridine sensitiser and a manganese(II) terpyridine unit separated by a redox active linkage. DFT analysis*. Tebo, A. G.; Das, S.; Farran, R.; Herrero, C.; Quaranta, A.; Fallahpour, R.; Protti, S.; Charlot, M. F.; Aukauloo, A.; Leibl, W. *C. R. Chim.* **2017,** *20*, 323-332.
7. *The disentangling of hysteretic spin transition, polymorphism and metastability in bistable thin films formed by sublimation of bis(scorpionate) Fe(II) molecules*. Iasco, O.; Boillot, M. L.; Bellec, A.; Guillot, R.; Riviere, E.; Mazerat, S.; Nowak, S.; Morineau, D.; Brosseau, A.; Miserque, F.; Repain, V.; Mallah, T. *J. Mater. Chem. C* **2017,** *5*, 11067-11075.
8. *Light-Induced Activation of the Du Bois [Rh-2(II)(Esp)(2)] Catalyst for Nitrogen Atom Transfer Reactions*. Farran, R.; Ducloiset, C.; Buendia, J.; Vo, N. T.; Guillot, R.; Halime, Z.; Dauban, P.; Leibl, W.; Sircoglou, M.; Aukauloo, A. *ChemPhotoChem* **2017,** *1*, 562-567.
9. *Design and Magnetic Properties of a Mononuclear Co(II) Single Molecule Magnet and Its Antiferromagnetically Coupled Binuclear Derivative*. El-Khatib, F.; Cahier, B.; Shao, F.; Lopez-Jorda, M.; Guillot, R.; Rivière, E.; Hafez, H.; Saad, Z.; Girerd, J. J.; Guihery, N.; Mallah, T. *Inorg. Chem.* **2017,** *56*, 4601-4608.
10. *Design of a Binuclear Ni(II) Complex with Large Ising-type Anisotropy and Weak Anti-Ferromagnetic Coupling*. El-Khatib, F.; Cahier, B.; Lopez-Jorda, M.; Guillot, R.; Rivière, E.; Hafez, H.; Saad, Z.; Girerd, J. J.; Guihery, N.; Mallah, T. *Inorg. Chem.* **2017,** *56*, 10655-10663.
11. *Imidazolidine Ring Cleavage upon Complexation with First-Row Transition Metals*. Cheaib, K.; Herrero, C.; Guillot, R.; Banse, F.; Mahy, J. P.; Avenier, F. *Eur. J. Inorg. Chem.* **2017**, 3884-3891.
12. *Alignment under Magnetic Field of Mixed Fe2O3/SiO2 Colloidal Mesoporous Particles Induced by Shape Anisotropy*. Li, J. G.; Fornasieri, G.; Bleuzen, A.; Gich, M.; Gloter, A.; Bouquet, F.; Imperor-Clerc, M. *Small* **2016,** *12*, 5981-5988.
13. *Oxidation catalysis via visible-light water activation of a [Ru(bpy)(3)](2+) chromophore BSA-metallocorrole couple*. Herrero, C.; Quaranta, A.; Ricoux, R.; Trehoux, A.; Mahammed, A.; Gross, Z.; Banse, F.; Mahy, J. P. *Dalton Trans.* **2016,** *45*, 706-710.
14. *Photoassisted Oxidation of Sulfides Catalyzed by Artificial Metalloenzymes Using Water as an Oxygen Source*. Herrero, C.; Nhung, N. T.; Hammerer, F.; Banse, F.; Gagne, D.; Doucet, N.; Mahy, J. P.; Ricoux, R. *Catalysts* **2016,** *6*.
15. *Unraveling sigma and pi Effects on Magnetic Anisotropy in cis-NiA(4)B(2) Complexes: Magnetization, HF-HFEPR Studies, First-Principles Calculations, and Orbital Modeling*. Charron, G.; Malkin, E.; Rogez, G.; Batchelor, L. J.; Mazerat, S.; Guillot, R.; Guihery, N.; Barra, A. L.; Mallah, T.; Bolvin, H. *Chem. Eur. J.* **2016,** *22*, 16848-16860.
16. *Molecular-scale dynamics of light-induced spin cross-over in a two-dimensional layer*. Bairagi, K.; Iasco, O.; Bellec, A.; Kartsev, A.; Li, D.; Lagoute, J.; Chacon, C.; Girard, Y.; Rousset, S.; Miserque, F.; Dappe, Y. J.; Smogunov, A.; Barreteau, C.; Boillot, M.-L.; Mallah, T.; Repain, V. *Nat. Comm.* **2016,** *7*, 12212.
17. *Successive light-induced two electron transfers in a Ru-Fe supramolecular assembly: from Ru-Fe(ii)-OH2 to Ru-Fe(iv)-oxo*. Herrero, C.; Quaranta, A.; Sircoglou, M.; Sénéchal-David, K.; Baron, A.; Marin, I. M.; Buron, C.; Baltaze, J.-P.; Leibl, W.; Aukauloo, A.; Banse, F. *Chem. Sci.* **2015,** *6*, 2323-2327.

18. *Tailoring the Structure of Two-Dimensional Self-Assembled Nanoarchitectures Based on Ni-II-Salen Building Blocks*. Viciano-Chumillas, M.; Li, D. Z.; Smogunov, A.; Latil, S.; Dappe, Y. J.; Barreteau, C.; Mallah, T.; Silly, F. *Chem. Eur. J.* **2014,** *20*, 13566-+.
19. *Using Prussian blue analogue nanoparticles confined into ordered mesoporous silica monoliths as precursors of oxides*. Trannoy, V.; Delahaye, É.; Fornasieri, G.; Beaunier, P.; Bleuzen, A. *C. R. Chim.* **2014,** *17*, 512-520.
20. *Ising-type magnetic anisotropy and single molecule magnet behaviour in mononuclear trigonal bipyramidal Co(II) complexes*. Ruamps, R.; Batchelor, L. J.; Guillot, R.; Zakhia, G.; Barra, A. L.; Wernsdorfer, W.; Guihery, N.; Mallah, T. *Chem. Sci.* **2014,** *5*, 3418-3424.
21. *Chemical tuning of the magnetic relaxation in dysprosium(III) mononuclear complexes*. Batchelor, L. J.; Cimatti, I.; Guillot, R.; Tuna, F.; Wernsdorfer, W.; Ungur, L.; Chibotaru, L. F.; Campbell, V. E.; Mallah, T. *Dalton Trans.* **2014,** *43*, 12146-12149.
22. *Giant Ising-Type Magnetic Anisotropy in Trigonal Bipyramidal Ni(II) Complexes: Experiment and Theory*. Ruamps, R.; Maurice, R.; Batchelor, L.; Boggio-Pasqua, M.; Guillot, R.; Barra, A. L.; Liu, J. J.; Bendeif, E.; Pillet, S.; Hill, S.; Mallah, T.; Guihery, N. *J. Am. Chem. Soc.* **2013,** *135*, 3017-3026.
23. *Origin of the Magnetic Anisotropy in Heptacoordinate Ni-II and Co-II Complexes*. Ruamps, R.; Batchelor, L. J.; Maurice, R.; Gogoi, N.; Jimenez-Lozano, P.; Guihery, N.; de Graaf, C.; Barra, A. L.; Sutter, J. P.; Mallah, T. *Chem. Eur. J.* **2013,** *19*, 950-956.
24. *Click Chemistry as a Convenient Tool for the Incorporation of a Ruthenium Chromophore and a Nickel-Salen Monomer into a Visible-Light-Active Assembly*. Herrero, C.; Batchelor, L.; Baron, A.; El Ghachtouli, S.; Sheth, S.; Guillot, R.; Vauzeilles, B.; Sircoglou, M.; Mallah, T.; Leibl, W.; Aukauloo, A. *Eur. J. Inorg. Chem.* **2013**, 494-499.
25. *Synergy in Photomagnetic/Ferromagnetic Sub-50 nm Core-Multishell Nanoparticies*. Dia, N.; Lisnard, L.; Prado, Y.; Gloter, A.; Stephan, O.; Brisset, F.; Hafez, H.; Saad, Z.; Mathonière, C.; Catala, L.; Mallah, T. *Inorg. Chem.* **2013,** *52*, 10264-10274.

Visiting senior scientists

1. Jeffrey Long, Univ. of Berkeley, USA,1, month, 29 April-28 May 2013 (Labex Nanosaclay)
2. Herre van der Zant, TU Delft, Netherlands, 1 week, 7-11 April 2014 (TU Delft)
3. Dr Feng-Lei Yang, China, 12 months 2014-2015 (Normal University of Jiangsu)
4. Marco Affronte, Italian CNR, Italy, 1 month, 26 January-25 February 2015 (Univ. Paris Sud 11)
5. Eugenio Coronado, Univ. of Valencia, Spain, 12 months in 2015 and 2016 in the framework of Blaise Pascal International Chair (Fondation de l'Ecole Normale, Ile de France)

48- Scientific recognition

Prizes

1. V. Huc, 23 July 2014, Concours Mondial de l'Innovation
2. T. Mallah, 22 April 2015, Prix Paul Pascal de l'Académie des Sciences
3. C. Martini, 15 juin 2017, lauréat du 19e édition du concours national d'aide à la création d'entreprises de technologies innovantes (concours I-LAB 2017)

Distinctions

IUF members

1. T. Mallah, 1 october 2012, Chair IUF Senior
2. L. Catala, 1 october 2013, Chair IUF Junior

Chair of learned and scientific societies

Invitations to meetings and symposia (out of France)

Selection of the invitations out of France (13/26)

1. Water a powerful ally! A. Aukauloo, 16th International Congress on Photosynthesis Research, 11-16 August, 2013, Saint Louis, USA

2. Coordination Nanoparticles, a Fascinating Playground for (nano)Chemists. T. Mallah, Indo-French Symposium on Functional Metal-Organics: Applications in Materials and Catalysis, 22-26 February, 2014, Bhubaneswar, India
3. Reversal of the magnetization in cor-shell molecule-based nanomagnets. T. Mallah, 41st International Conference on Coordination Chemistry, 21-25 July 2014, Singapore, Singapore
4. Reductive activation of O_2 by a nonheme FeII complex. A mechanistic study by cyclic voltammetry. F. Banse, COST CM1003, final meeting, 16-17 April, 2015, Oeiras, Portugal
5. The Molecular Approach for Artificial Photosynthesis. A. Aukauloo, Electro Chemical Society Meeting, 22-29 May 2015, Chicago, USA
6. Magnetic Anisotropy and Single Molecule Magnet behavior in trigonal bi pyramidal mononuclear Co(II) complexes. T. Mallah, 5th European Conference on Molecular Magnetism, 6-10 September 2015, Zaragoza, Spain
7. Engineering the exchange coupling at the molecule/electrode interface in molecular spintronic devices. T. Mallah, The International Chemical Congress of Pacific Basin Societies (PACIFICHEM 2015), 15-20 December 2015, Honolulu, USA
8. Magnetic cyanide-based coordination nanoparticles and heterostructures. L. Catala, Spring 2015 ACS National Meeting, 22-26 March 2015, Denver, USA
9. Magnetic anisotropy and SMM behavior in trigonal bipyramidal mononuclear Co(II) complexes. T. Mallah, American Chemical Society Meeting, 12-16 March 2016, San Diego, USA
10. Magnetic Anisotropy and Single Molecule Magnet behavior in trigonal bi pyramidal mononuclear Co(II) complexes. T. Mallah, Modern Trends in Molecular Magnets (MTMM), 19-21 Mai 2016, Mumbai, India
11. Dipyrrin containing ligands and their metal complexes. A. Aukauloo, 1st International Nanjing-Dijon Symposium on Functional Macrocycles and their metal complexes, 9-10 July 2016, Nanjing, China
12. Engineering the exchange coupling at the molecule/electrode interface in molecular spintronic devices. T. Mallah, V. Campbell, The 15th International Conference on Molecule-Based Magnets, 4-8 September 2016, Sendai, Japan
13. A supramolecular mimic of the regulation step of Fe-monooxygenases: Allosteric modulation of Fe(IV)-Oxo formation by guest binding in a heterodinuclear Zn(II)-Fe(II) calix[6]arene-based funnel complex. F. Banse, SABIC 2017, 5th Symposium on Advanced Biological Inorganic Chemistry, 7-11 Januray 2017, Kolkata, India

Members' long-term visits abroad

1. T. Mallah, University of Tohoku, Sendai, Japan, 1/3/2015-31/5/2015

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

17- Socio-economic interactions / Patents

Invention disclosures

4

Filed patents

1. Catalyseurs supportés cycliques 27 octobre 2016. V. Huc, C. Martini, I. Abdellah, CNRS, Université Paris-Sud, 27 octobre 2016, FR1660471
2. Cryptands à base de calix[4]arènes associés à un macrocycle azoté et leur utilisation pour l'extraction sélective de métaux stratégiques. G. Gros, V. Huc, CNRS, Université Paris-Sud, 11 octobre 2017, FR1759523

Accepted patents

1. Solid-liquid process for extraction of radionucleides from aqueous waste solutions. V. Huc, E. Shilova, P. Viel, CEA, 24 février 2012, F0263O00487/EP/OEB, 22 février 2013, PCT/IB2013/051460
2. High yield synthesis of *p*-(benzyloxy)calix[6,7,8]arenes. V. Huc, C. Martini, Université Paris-Sud, June 2013, FR2983853
3. Method of preparing a high yield p (r) calixarenes Giants. C. Martini, V. Huc, March 2014 FR2994971
4. Method for the high-yield production of *p*-(R-oxy)calix[9-20] arenes. V. Huc, C. Martini, Université Paris-Sud, March 2014, FR2994970

5. Novel complexes for the separation of metal cations in liquid medium" V. Huc, P. Viel, E. Shilova. Université Paris-Sud, CEA, 4 avril 2014, 22 mai 2015, PCT Int. Appl. (2015), WO 2015150588 A1 20151008
6. Procédé de préparation à hauts rendements de *p*-(R)calix[9-20]arènes. V. Huc, C. Martini, avril 2016, FR3018074

Licenced patents

2 in negociation

18- Socio-economic interactions

Industrial and R&D contracts

Two contracts with VERNET (35 k€, 2017) and PROTEX (19 k€, 2018)

Cifre fellowships

Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*

1. COST action, CA15128, Molecular Spintronics (MOLSPIN), 2016-2020, http://www.icmol.es/molspin/index.php
2. COST action, CM1305, ECOSTBio: Explicit Control Over Spin States in Technology and Biochemistry
3. 2014-2018, http://www.ecostbio.eu/
4. Groupement d'Intérêt Scientifique, Groupe Français de Chimie Bio-Inorganique, 2013-2018
5. Groupement de Recherche, Rencontres de Spectroscopie Théorique (REST), 2015-2018, http://gdr-rest.polytechnique.fr/
6. Groupement de Recherche, Magnétisme et Commutation Moléculaires, 2016-2020, http://www.gdr-mcm2.cnrs.fr/
7. Groupement de Recherche, Photo Electro Stimulation, 2018-2022, https://iscr.univ-rennes1.fr/umr/actualites/article/le-gdr-photo-electro-stimulation-vient-d-etre-cree-par-l-inc-les-equipes-omc-1315

Start-ups

One start-up AJELIS was created by V. Huc and E. Shilova on September the 23rd 2014 and another one NOVECAL created by C. Martini and V. Huc on March the12th 2018

19- Expertise

Consulting

Participation in expert committees (ANSES etc.)

Legal expertise

20- Expert and standardization reports

21- Public outreach

Radio broadcasts, TV shows, magazines

1. "Terres rares: le nouvel or noir" émission France culture "la méthode scientifique" 24 Avril 2018, https://www.franceculture.fr/emissions/la-methode-scientifique/la-methode-scientifique-du-mardi-24-avril-2018, V. Huc

Journal articles, interviews, book edition, videos, etc.

2. Une approche bioinspirée pour produire de l'hydrogène : Connaissances de énergies, 2013, https://www.youtube.com/watch?v=qjXwwOlyGyQ, A. Aukauloo
3. « Le big bang des possibles », conférence grand public au Zénith d'Angers, 17 Mlars 2015, (https://www.youtube.com/watch?v=psv3JWXLj8U), V. Huc
4. Photosynthèse artificielle, la quête d'une énergie bio-inspirée, Biofutur 2015 N° 364, 34-36, (https://biofutur.revuesonline.com/article.jsp?articleId=20225), A. Aukauloo

5. Interview de la Société Chimique de France, 2017 https://www.youtube.com/watch?v=cTMz0C_kXYo, A. Aukauloo
6. « La guerre des métaux rares » Interview réalisée pour le magazine « Socialter » n°Avril-Mai 2018, (https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=10&ved=0ahUKEwi8s4ubgrPbAhVQmbQKHc_4B60QFghRMAk&url=http%3A%2F%2Falternatives-projetsminiers.org%2Fwp-content%2Fuploads%2Fdocs%2Fdossier-socialter_la-guerre-des-metaux-rares.pdf&usg=AOvVaw17jc1YOeFj3wF1vQsrwvQ1) V. Huc
7. « La cage aux ions » interview réalisée pour le magazine « Industrie et technologie » n° Avril 2018, https://www.industrie-techno.com/terres-rares-une-start-up-invente-une-cage-aux-ions.52720, V. Huc
8. Interview pour la Société Chimique de France « Témoignage de chimiste : comment naît une start-up », https://www.youtube.com/watch?v=lhuTMxZEglo, V. Huc

Other popularization outputs

9. Actualités scientifiques de l'INC et de l'INP du CNRS 'Contrôler des Molécules Magnétiques Bistables Auto-Organisées avec de la Lumière' (2016); http://www.cnrs.fr/inp/spip.php?article4747, M.-L. Boillot, T. Mallah
10. Actualités scientifiques de l'INP du CNRS 'Une Vague Elastique pour Amplifier la Commutation Ultra-rapide de Matériaux ' (2016) (http://www.cnrs.fr/inp/spip.php?article4521), M.-L. Boillot
11. En direct des laboratoires de l'INC du CNRS 'Photosynthèse artificielle : le deuxième électron enfin accessible' (2017) (http://www.cnrs.fr/inc/communication/direct_labos/aukauloo6.htm), A. Aukauloo.

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

Please, highlight the most selective.

23- Educational outputs

Books

E-learning, MOOCs, multimedia lessons, etc.

24- For humanities only, published PhD theses

25- Quality of PhD student supervision

The financial support of the PhD students of the Inorganic Chemistry team comes mainly from the French ministry of education (11/21) and from foreign countries (5/21). The remaining five PhD were financed by Idex Paris-Saclay, ANR and Région Ile de France. The average duration of the PhDs is 38 months and there were no withdrawals during the last 6 years. The number of published papers with PhD students is 64, which leads to an average of 3.05 publications per student.
11 PhD students are preparing their PhD at ECI and 21 had their defence during the period 2013-2018 (see list below).

List of PhD defended during the period 2013-2018

1. Y. Raza, 22 mars 2013, « Spin Crossover Nanoparticles of Fe(pyrazine)[Pt(CN)4]: Role of the Environment on Thermal Bistability » T. Mallah, L. Catala, Gouvernement Pakistanais
2. N. Dia, 8 janvier 2013, « Nanoparticules photomagnétiques et agents de contraste à base de réseaux de coordination » T. Mallah, L. Catala, Gouvernement Libanais
3. J. Lejeune, 26 juin 2013, « Propriétés de Commutation des Analogues CoFe du Bleu de Prusse : Vers un Contrôle de la position en Energie des Etats Stable et Métastable » A. Bleuzen, Allocation Spécifique Normalien
4. S. Cherdo, 6 décembre 2013, « Des complexes cage aux nanoparticules, nouveaux catalyseurs pour la production d'hydrogène » A. Aukauloo, MESRI
5. N. Ségaud, 13 décembre 2013, « Etude de l'activation réductrice du dioxygène par un complexe de FeII et nouveaux complexes hétérodinucléaires : contributions pour le développement de catalyseurs d'oxydation bioinspirés » F. Banse, K. Sénéchal-David, MESRI

6. J. Guérin, 15 octobre 2013, « Synthèse et étude de ligands diaryléthènes photochromes de type Salen: Compréhension de l'interaction métal-ligand pour la commutation optique » P. Yu, A. Léaustic, ASN
7. S. R. Sheth, 11 décembre 2013, « Synthesis and Characterization of catalysts for photo-oxidation of water » W. Leibl, A. Aukauloo, IRTELIS CEA
8. L. L. Nguyen, 8 octobre 2014, « Nanoparticules de photocommutateurs moléculaires basés sur des complexes de FeII à conversion de spin et à ligand isomérisables » M.-L. Boillot, Vietnam (Consortium USTH-MEN)
9. B. Boutonnet, 12 décembre 2014, « Vers la synthèse totale de nanotubes de carbone zig-zag de diamètres controlés : utilisation de calixarènes » Vincent Huc, MESRI
10. V. Trannoy, 10 décembre 2015, « Vers l'élaboration de pistes magnétiques enregistrables : De la Molécule au Matériau » A. Bleuzen, Cnano IdF
11. G. Paul, 1 octobre 2015, « Nanoparticules de réseaux de coordination pour l'imagerie médicale » L. Catala, MESRI
12. J. Laisney, 23 janvier 2015, « Influence de l'environnement sur la commutation et la bistabilité thermique de micro-, nanoparticules à transition de spin. » M.-L. Boillot, MESRI
13. C. Buron, 17 juillet 2015, « Développement de nouveaux catalyseurs d'oxydation bioinspirés : greffage de complexes de fer(II) non hémiques sur électrodes d'or ou dans la β-lactoglobuline » F. Banse, K. Sénéchal-David, MESRI
14. G. Zakhia, 18 mai 2015, « Synthèse, caractérisation et propriétés magnétiques de nano-aimants moléculaires » T. Mallah, D. Naoufal, CNRS Liban
15. R. Moulin, 2 novembre 2016, « Matrices de silice mésoporeuses pour le développement de nanomatériaux multifonctionnels » A. Bleuzen, G. Fornasieri, MESRI
16. C. Ducloiset, 21 septembre 2017, « Etude de complexes pour les réactions par transfert d'atome d'oxygène ou d'azote : de la synthèse à la photoactivation » A. Aukauloo, M. Sircoglou, MESRI
17. S. Mendes Marinho, 6 octobre 2017, « Combustible solaire : caractérisation du mécanise de transfert de charge dans des molécules photocatalytiques, vers la production d'énergie par la photosynthèse artificielle » A. Aukauloo, IDEX
18. F. El Khatib, 24 janvier 2017, « Synthèse, caractérisation et étude magnétique des complexes de Co (II) et de Ni (II) avec des ligands de type cryptands » T. Mallah, Z. Saad, Bourse Liban
19. F. Shao, 30 juin 2017, « Study of the magnetic anisotropy in mononuclear Co(II) Single Molecule Magnets » T. Mallah, Bourse CSC
20. A. Castan, 25 janvier 2018, « Croissance et caractérisations de nanotubes de carbone monoparois à partir de précurseurs de catalyseurs synthétisés par voie chimique » V. Huc, A. Loiseau, ANR
21. B. Cahier, 27 mars 2018, « Etude théorique de l'anisotropie magnétique dans des complexes de métaux de transition: application à des complexes mono- et binuculéaires de Ni(II) et Co(II) » T. Mallah, N. Guihéry, MESRI

26- Students' follow up in association with doctoral schools

The policy followed by the team in this area is the same as that of the Doctoral School. We support our PhD students to direct them towards postdoctoral contracts and also put them in touch with all our private sector contacts for those who wish.

27- Participation to international training programs (e. g. Erasmus Mondus)

1. A. Aukauloo: one week stay in the lab of Pr. Athanassis Coutsolelos University of Heraklion August 2016. Electron Transfer courses to PhD and master students on internship.
2. T. Mallah, 15 hours/year lecture Master 2 Inorganic Chemistry at Lebanese University, Beirut, Lebanon, 2013-2018
3. T. Mallah, 15 hours/year lecture Master 2 NanoChemistry at USTH, Hanoi, Vietnam, 2013-2018

The interaction with the foreign universities allowed receiving PhD students with local grants, 3 from Lebanon and 1 from Vietnam

28- PhD student participation to scientific animation and unit/team life

PhD students fully participate to the scientific life of the team. This is done at two levels: 1) they attend the seminars given by invited external personalities (1/month) and 2) they present their work in a quasi-formal form during the team meetings that take place twice a month. In average, each PhD student has the opportunity to give three presentations. In addition, a final formal presentation is given a week before the defence.

29- Participation of team members in setting up Master courses

1. A. Aukauloo in charge of the Bioinorganic unit of a Master 2 at the interface Chemistry-Biology 2016-
2. T. Mallah in charge of the Master 2 "Chimie Inorganique: molecules, surfaces et nano-objets". He is in charge of leading the discussions for setting up the courses for each of the 5 units (40 hours per unit) of the Master.

30- Student publications (for Biology only)

Département d'évaluation
de la recherche

Appendix 4

Team 8 – SP2M

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Synthèse, Propriétés & Modélisation des Matériaux**
Acronym:	**SP2M**
Director's name (current contract):	**Nita DRAGOE / Jerome CREUZE**
Director's name (future contract):	**Nita DRAGOE / Jerome CREUZE**

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

1. Articles

Scientific articles

1. *Bulk, surface and point defect properties in UO2 from a tight-binding variable-charge model*. G. Sattonnay, R. Tétot, Journal of Physics-Condensed Matter, 2013, 25 FI 2.209
2. *Stabilization of the tetragonal phase in large columnar zirconia crystals without incorporating dopants*. Z. Chen, G. Ji, N. Prud'Homme, A. Addad, V. Ji, J. Chevalier, G. Bernard-Grangere, Scripta Materialia, 2013, 68, 559 FI 3.305
3. *Microstructure characterization and deposition mechanism studies of ZrO2 thin films deposited by LI-MOCVD*. Z. Chen, N. Prud'Homme, B. Wang, P. Ribot, V. Ji, Surface & Coatings Technology, 2013, 218, 7 FI 2.139
4. *Influence of humidity on high temperature oxidation of Inconel 600 alloy: Oxide layers and residual stress study*. J. Xiao, N. Prud'Homme, N. Li, V. Ji, Applied Surface Science, 2013, 284, 446– 452
5. *Internal stresses in polycrystalline zirconia: microstructure effects*. C. Berdin, Z. Yao, S. Pascal, Computational Materials Science, 2013, 70, 140 FI 2.086
6. *Residual stress study of nanostructured Zirconia films obtained by MOCVD and by Sol-gel routes*. M. Jouili, M. Andrieux, P. Ribot, A. Bleuzen, G. Fornasieri, V. Ji, Applied Surface Science, 2013, 276, 138 FI 3.150
7. *Asymmetric Orientational Writing in glass with femtosecond laser irradiation*. B. Poumellec, M. Lancry, R. Desmarchelier, E. Hervé, F. Brisset, J.C. Poulin, Optical Materials Express, 2013, 3, 1586 FI 2.657
8. *Broadband anisotropy of femtosecond laser induced nanogratings in fused silica*. M. Beresna, M. Gecevičius, M. Lancry, B. Poumellec, P. G. Kazansky, Applied Physics Letters, 2013, 103, 131903 FI 3.142
9. *Ultrafast nanoporous silica formation driven by femtosecond laser irradiation*. M. Lancry, B. Poumellec, J. Canning, K.Cook, J. C. Poulin, F. Brisset, Laser Photonics Review, 2013, 7, 953 FI 7.486
10. *Anisotropic propagating excitations and quadrupolar effects in Tb$_2$Ti$_2$O$_7$*. S. Guitteny, J. Robert, P. Bonville, J. Ollivier, C. Decorse, P. Steffens, M. Boehm, H. Mutka, I. Mirebeau, S. Petit, Physical Review Letters, 2013, 111, 087201 FI 7.645
11. *High thermoelectric properties of n-type AgBiSe$_2$*. L. Pan, D. Bérardan, N. Dragoe, Journal of the American Chemical Society, 2013, 135, 4914 FI 13.038
12. *Texturation boosts the thermoelectric performance of BiCuSeO oxyselenides*. J. Sui, J. Li, J. He, Y-L. Pei, D. Bérardan, H. Wu, N. Dragoe, W. Cai, L-D. Zhao, Energy and Environmental Science, 2013, 6, 2916 FI 25.427
13. *An examination of microstructural evolution in a Cu-Ni-Si alloy processed by HPT and ECAP*. A. Y. Khereddine, F. H. Larbi, M. Kawasaki, T. Baudin, D. Bradai, T. G. Langdon, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2013, 576, 149 FI 2.647
14. *Effect of recrystallization and degree of order on the magnetic and mechanical properties of soft magnetic FeCo-2V alloy*. B. Nabi, A.-L. Helbert, F. Brisset, G. Andre, T. Waeckerle, T. Baudin, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2013, 578, 215 FI 2.647
15. *Microstructure and texture evolution during the ultra grain refinement of the Armco iron deformed by accumulative roll bonding (ARB)*. E. Bonnot, A.-L. Helbert, F. Brisset, T. Baudin, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2013, 561, 60 FI 2.647
16. *Layered oxychalcogenide in the Bi-Cu-O-Se system as good thermoelectric materials*. C. Barreteau, L. Pan, E. Amzallag, L. Zhao, D. Bérardan, N. Dragoe, Semiconductor Science & Technology, 2014, 29, 064001 FI 2.098
17. Residual stresses in oxide scale formed on Fe–17Cr stainless steel. N. Li, J. Xiao, N. Prud'Homme, Z. Chen, V. Ji, Applied Surface Science, 2014, 316, 108 FI 3.150
18. *Residual stress and micro-structure of GCr15 steel after multistep shot peening*. P. Fu, C. Jiang, Z. Zhang, V. Ji, Surface Engineering, 2014, 30, 847 FI 1.081
19. *Direct evidence of polar nature of ferroelastic twin boundaries in CaTiO3 obtained by second harmonic generation microscope*. H. Yokota, H. Usami, R. Haumont, P. Hicher, J. Kaneshiro,E. K. H. Salje, Y. Uesu, Physical Review B, 2014, 89, 144109 FI 3.718

20. *Low-field magnetoresistance up to 400 K in double perovskite Sr_2FeMoO_6 synthesized by a citrate route*. L. Harnagea, B. Jurca, P. Berthet, Journal of Solid State Chemistry, 2014, 211, 219 FI 2.265
21. *One-step photoinscription of asymmetrically oriented fresnoite-type crystals in glass by ultrafast laser*. X. He, B. Poumellec, Q. Liu, F. Brisset, M. Lancry, Optics Letters, 2014, 39, 5423 FI 3.040
22. *Effect of long range order on mechanical properties of partially recrystallized Fe49Co-2V alloy*. B. Nabi, A.-L. Helbert, F. Brisset, R. Batonnet, G. Andre, T. Waeckerle, T. Baudin, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2014, 592, 70 FI 2.647
23. *Influence of stored energy on twin formation during primary recrystallization*. W. Wang, F. Brisset, A. L. Helbert, D. Solas, I. Drouelle, M. H. Mathon, T. Baudin, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2014, 589, 112 FI 2.647
24. *Measurement of stored energy in Fe-48%Ni alloys strongly cold-rolled using three approaches: Neutron diffraction, Dillamore and KAM approaches*. Y. A. Betanda, A.-L. Helbert, F. Brisset, M.-H. Mathon, T. Waeckerle, T. Baudin, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2014, 614, 193 FI 2.647
25. *Monte Carlo simulation of primary recrystallization and annealing twinning*. W. Wang, A. L. Helbert, F. Brisset, M. H. Mathon, T. Baudin, Acta Materiala, 2014, 81, 457 FI 5.058
26. *Ageing of out-of-equilibrium nanoalloys by a kinetic mean-field approach*. F. Berthier, A. Tadjine, B. Legrand, Physical Chemistry Chemical Physics, 2015, 17, 28193 FI 4.449
27. *Metal organic precursor effect on the properties of SnO2 thin films deposited by MOCVD technique for electrochemical applications*. R. Drevet, C. Legros, D. Bérardan, P. Ribot, D. Dragoe, C. Cannizzo, M. G. Barthes-Labrousse, A. Chausse, M. Andrieux, Surface & Coatings Technology, 2015, 271, 234 FI 2.139
28. *Finite element analysis of laser shock peening of 2050-T8 aluminum alloy*. N. Hfaiedh, P. Peyre, H. Song, I. Popa, V. Ji, V. Vignal, International Journal of Fatigue, 2015, 70, 480 FI 2.162
29. *Quantitative study of particle size distribution in an in-situ grown Al–TiB2 composite by synchrotron X-ray diffraction and electron microscopy*. Y. Tan, Z. Chen, A. Borbély, G. Ji, S.-Y. Zhong, D. Schryvers, V. Ji, H.-W. Wang, Materials Characterization, 2015, 102, 131 FI 2.383
30. *Spin dynamics in the presence of competing ferromagnetic and antiferromagnetic correlations in $Yb_2Ti_2O_7$*. J. Robert, E. Lhotel, G. Remenyi, S. Sahling, I. Mirebeau, C. Decorse, B. Canals, S. Petit, Physical Review B, 2015, 92, 064425 FI 3.718
31. *Experimental evidence that a high electric field acts as an efficient external parameter during crystalline growth of bulk oxide*. P. Hicher, R. Haumont, R. Saint-Martin, X. Mininger, P. Berthet, A. Revcolevschi, Journal Crystal Growth, 2015, 409, 23 FI 1.462
32. *Experimental realization of long-distance entanglement between spins in antiferromagnetic quantum spin chains*. S. Sahling, G. Remenyi, C. Paulsen, P. Monceau, V. Saligrama, C. Marin, A. Revcolevschi, L. P. Regnault, S. Raymond, J. E. Lorenzo, Nature Physics, 2015, 11, 255 FI 18.791
33. *Microstructure, mechanical properties and texture of an AA6061/AA5754 composite fabricated by cross accumulative roll bonding*. K. Verstraete, A. L. Helbert, F. Brisset, A. Benoit, P. Poniard, T. Baudin, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2015, 640, 235 FI 2.647
34. *3D numerical modeling of dynamic recrystallization under hot working: Application to Inconel 718*. J. De Jaeger, D. Solas, O. Fandeur, J.-H. Schmitt, C. Rey, Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing, 2015, 646, 33 FI 2.647
35. *CO adsorption-induced surface segregation and formation of Pd chains on AuPd(100) alloy: DFT-based Ising model and Monte Carlo simulations*. B. Zhu, J. Creuze, C. Mottet, B. Legrand, H. Guesmi, The Journal of Physical Chemistry C, 2016, 120, 350 FI 4.509
36. *Finite element modelling of the oxidation kinetics of Zy-4 with a controlled metal-oxide interface and the influence of growth stress*. G. Zumpicchiat, S. Pascal, M. Tupin, C. Berdin, Corrosion Science, 2016, 100, 209 FI 5.154
37. *Key role of the short-range order on the response of the titanate pyrochlore $Y_2Ti_2O_7$ to irradiation*. G. Sattonnay, S. Cammelli, D. Menut, N. Sellami, C. Grygiel, I. Monnet, J. Béchade, J.-P. Crocombette, A. Chartier, A. Soulié, R. Tétot, C. Legros, P. Simon, S. Miro, L. Thomé, Physical Review B, 2016, 94, 224109 FI 3.718
38. *XPS-nanocharacterization of organic layers electrochemically grafted on the surface of SnO2 thin films to produce a new hybrid material coating*. R. Drevet, D. Dragoe, M. G. Barthes-Labrousse, A. Chausse, M. Andrieux, Applied Surface Science, 2016, 384, 442 FI 3.150

39. *Microstructure and residual stresses in Ti-6Al-4V alloy pulsed and unpulsed TIG welds*. B. Mehdi, R. Badji, V. Ji, B. Allili, D. Bradai, F.-D. Beaume, F. Soulié, Journal of Materials Processing Technology, 2016, 231, 441 FI 2.359
40. *Parity violation in chiral structure creation under femtosecond laser irradiation in silica glass?*. B. Poumellec, M. Lancry, R. Desmarchelier, E. Hervé, B. Bourguignon, Light: Science & Applications, 2016, 5, 16178 FI 13.600
41. *Form birefringence induced in multicomponent glass by femtosecond laser direct writing*. J. Cao, L. Mazerolles, M. Lancry, D. Solas, F. Brisset, B. Poumellec, Optics Letters, 2016, 41, 2739 FI 3.040
42. *Nematicity in stripe-ordered cuprates probed via resonant x-ray scattering*. A. J. Achkar, M. Zwiebler, C. Mcmahon, F. He, R. Sutarto, I. Djianto, Z. Hao, M. J. P. Gingras, M. Hücker, G. D. Gu, A. Revcolevschi, H. Zhang, Y. J. Kim, J. Geck, D.-G. Hawthorn, Science, 2016, 351, 576 FI 34.661
43. *Room temperature lithium superionic conductivity in high entropy oxides*. D. Bérardan, S. Franger, A.K. Meena, N. Dragoe, Journal of Materials Chemistry A, 2016, 4, 9536 FI 8.262
44. *Colossal dielectric constant in high entropy oxides.* D. Bérardan, S. Franger, D. Dragoe, A.K. Meena, N. Dragoe, Physica Status Solidi RRL, 2016, 10, 328 FI 2.580
45. *Effective site-energy model: A thermodynamic approach applied to size-mismatched alloys* F. Berthier, J. Creuze, B. Legrand, Physical Review B, 2017, 95, 224102. FI 3.718
46. *Room-temperature soft mode and ferroelectric like polarization in $SrTiO_3$ ultrathin films: Infrared and ab initio study*. W.-W. Peng, R. Tétot, N. Gang, E. Amzallag, B. Vilquin, J.-B. Brubach, P. Roy, Scientific Report, 2017, 7, 2160 FI 4.857
47. *Microstructure study of cold rolling nanosized in-situ TiB_2 particle reinforced Al composites*. C.-Y. Dan, Z. Chen, G. Ji, S.-H. Zhong, Y. Wu, F. Brisset, H.-W. Wang, V. Ji, Materials & Design, 2017, 130, 357-365
48. *Effects of TiO_2 doping on the defect chemistry and thermo-physical properties of Yb2O3 stabilized ZrO_2*. L. Guo, C. Zhang, L. Xu, M. Li, Q. Wang, F. Ye, C. Dan, V. Ji, Journal of the European Ceramic Society, 2017, 37, 4163 FI 2.933
49. *Surface mechanical property and residual stress of peened nickel-aluminum bronze determined by in-situ X-ray diffraction*. C. Wang, C. Jiang, Y. Zhao, M. Chen, V. Ji, Applied Surface Science, 2017, 420, 28 FI 3.150
50. *Chiroptical properties photo-induced by femtosecond laser irradiation in silica glass*. R. Desmarchelier, M. Lancry, J. Tian, B. Poumellec, Applied Physics Letters, 2017, 110, 021112 FI 3.142
51. *Study of femtosecond laser-induced circular optical properties in silica by Mueller matrix spectropolarimetry*. J. Tian, M. Lancry, S. H. Yoo, E. Garcia-Caurel, R. Ossikovski, B. Poumellec, Optics Letters, 2017, 42, 4103 FI 3,040
52. *Disorder and Quantum Spin Ice*. N. Martin, P. Bonville, E. Lhotel, S. Guitteny, A. Wildes, C. Decorse, M. Ciomaga Hatnean, G. Balakrishnan, I. Mirebeau, S. Petit, Physical Review X, 2017, 7, 041028 FI 12.789
53. *Finite size effect on the magnetic excitations spectra and magnetic heat conduction of the quasi- one dimensional spin chains system $SrCuO_2$*. D. Bounoua, R. Saint-Martin, S. Petit, F. Bourdarot, L. Pinsard-Gaudart, Physica B, 2017, 536, 323 FI 1.352
54. *Impurity-induced spin pseudogap in $SrCuO_2$ doped with Mg, Zn, or La*. D. Bounoua, R. Saint-Martin, S. Petit, P. Berthet, F. Damay, Y. Sidis, F. Bourdarot, L. Pinsard-Gaudart, Physical Review B, 2017, 95, 224429 FI 3.718
55. *Relaxation path of nanoparticles in an oxygen-enriched ferritic oxide-dispersion-strengthened alloy*. M.A.Thual, J. Ribis, T. Baudin, V. Klosek, Y. de Carlan and M.H. Mathon, Scripta Materialia, 2017, 136, 37 FI 3.305
56. *Direct measurement of the surface energy of bimetallic nanoparticles: Evidence of Vegard's rule-like dependence*. A. Chmielewski, J. Nelayah, H. Amara, J. Creuze, D. Alloyeau, G. Wang, C. Ricolleau, Physical Review Letters, 2018, 120, 025901 FI 7.645
57. *Cold rolling texture evolution of TiB_2 particle reinforced Al-based composites by Neutron Diffraction and EBSD analysis*. C.-Y. Dan, Z. Chen, M.-H. Mathon, G. Ji, L.-W. Li, Y. Wu, F. Brisset, L. Guo, H.-W. Wang, V. Ji, Materials Characterization, 2018, 136, 293 FI 2.383
58. *Investigation on surface layer characteristics of shot peened graphene reinforced Al composite by X-ray diffraction method*. K. Zhan, Y. Wu, J. Li, B. Zhao, Y. Yan, L. Xie, L. Wang, V. Ji, Applied Surface Science, 2018, 435,1257 FI 3.150

Review articles

1. *UV laser processing and multiphoton absorption processes in optical telecommunication fiber materials.* M. Lancry, B. Poumellec, Physics Reports 522, 2013, 239 FI 16.240
2. *BiCuSeO oxyselenides: new promising thermoelectric materials.* L-D. Zhao, J. He, D. Bérardan, Y. Lin, J-F. Li, C-W. Nan, N. Dragoe, Energy and Environmental Science, 2014, 7, 2900 FI 25.427 (WOS Higly cited paper)

Other articles (professional journals, etc.)

2. Books

Scientific book edition

Book chapters

1. EBSD: Analyse par diffraction des électrons rétrodiffusés - Applications et techniques couplées, D. Solas, chap. 3, caractérisation de la texture cristallographique, comparaison des techniques expérimentales de diffraction : Rayons X, Neutrons et EBSD, EDP Sciences (2015).

3. Meetings

Meeting abstracts

1. Experimental approach and atomistic simulations to investigate the radiation tolerance of complex oxides: Application to the amorphization of pyrochlores. G. Sattonnay, L. Thomé, N. Sellami, I. Monnet, C. Grygiel, C. Legros, R. Tétot, 17th International Conference on Radiation Effects in Insulators (REI), 30 juin-5 juillet 2013, Helsinki, Finland, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2013, 326, 228
2. Porous nanogratings existence and related form birefringence in binary and ternary silica-based glasses. M. Lancry, B. Poumellec, F. Brisset. LAMP2013, LPM 2013 14th International Symposium on Laser Precision Microfabrication, HPL2013 6th International Symposium on High Power Laser Processing, Niigata, Japan (2013),), https://www.jlps.gr.jp/Booklet80F/LAMP2013_80_F_ Booklet.pdf
3. Impact of fictive temperature on glass density and structure of Ge-doped silica glasses. M. Heili, M. Lancry, B. Poumellec, E. Burov, D. R. Neuville, C. Le Losq. 12th International Conference on the Structure of Non-Crystalline Materials (NCM12), in Riva del Garda (Trento) Italy (7-12 Juillet 2013), http://events.unitn.it/en/ncm12/proceedings.
4. Porous nanogratings and related form birefringence in silicate and germanate glasses. F. Zimmerman, N. Guth, F. Brisset, S. Nolte, B. Poumellec, M. Lancry, R. Desmarchelier. Bragg Gratings, Photosensitivity and Poling in Glass Waveguides (BGPP), 25-28 July 2014, Barcelona, Spain, paper N°1997125 in Advanced Photonics, (Optical Society of America, 2014), paper BW2D.2.
5. Space selective oriented crystallization of optically non-linear crystals in glass by femtosecond laser irradiation. B. Poumellec, M. Lancry, X. He, F. Brisset, Q. Liu. 15th International Workshop on Nanoscience and Nanotechnology, NANO 2013, 21-23 November 2013, Sofia, Bulgarie, Nanoscience & Nanotechnology, http://ecad.tu-sofia.bg/e-conf/?r=12
6. High strength soft magnetic FeCo alloys, delivered in a "fully process" state for machining. T. Waeckerlé, T. Wéry, F. Petit, A.-L. Helbert, T. Baudin, B. Nabi, WMM'14, Magnetism and Metallurgy Conference, 17-19 juin 2014, Cardiff, United Kingdom
7. Effect of microalloying elements on the Cube texture formation of Fe48%Ni alloys tapes. Y. Ateba Betanda, A.-L. Helbert, F. Brisset, M. Wehbi, M.-H. Mathon, T. Waeckerlé, T. Baudin, Effect of microalloying elements on the Cube texture formation of Fe48%Ni alloys tapes, ICOTOM 17, 24-29 août 2014, 012036, Dresden, Germany
8. Influence of Al/Ge ratio on radiation-induced attenuation in nanostructured erbium-doped fibers preforms. M. Leon-Pichel, M. Lancry, N. Ollier, L. Bigot, H. Elhamzaoui, I. Savelli, A. Pastouret, E. Burov, B. Poumellec, M. Bouazaoui. Conference on Lasers and Electro-Optics (CLEO) 2015 in San Jose, CA. 10-15 May 2015. Symposium - Science and Technology of Laser Three Dimensional Printing, paper SM3L8

9. Influence of beta-forging on texture development in Ti 6246 alloy. S. Le Corre, R. Forestier, F. Brisset, M.-H. Mathon, D. Solas, TI 2015 - 13th World Conference on Titanium, 16-20 août 2015, 757-764, San Diego, USA
10. Fictive temperature reduction as an efficient approach for improving radiation resistance of silica glass. M. Lancry, B. H. Babu, N. Ollier, B. Poumellec. 24th International Congress on Glass, Shanghai from April. 7 to 11, 2016
11. Anisotropic circular optical properties photo-induced by femtosecond laser irradiation in silica glass. R. Desmarchelier, M. Lancry, J. Tian, B. Poumellec. Photonics and Fiber Technology 4-8/9/2016 (ACOFT, BGPP, NP), OSA Technical Digest (online) (Optical Society of America, 2016), Sydney, Australia, paper BT3B.3
12. Study Of Femtosecond Laser Induced Circular Optical Properties By Mueller Matrix Spectropolarimetry. J. Tian, M. Lancry, E. Garcia-Caurel, R. Ossikovski, B. Poumellec. CLEO PACIFIC RIM Singapore 31 July to 4 Aug 2017 in Singapore, paper s1279

4. Meeting and congress organisation

International conferences :

General chair of IVC-19/ICSS-15/ICN+T 2013, 19th Int. Conference on Vacuum/15th International Conference on Surface Science/International Conference on Nanoscience and Technology, Paris, 9-13 September 2013, 2300 participants

Committee member, "SiO2 and advanced dielectrics", June 2014, Cagliari, Italy
President of scientific committee, "Bragg Gratings Photosensitivy and Poling" (BGPP) 2016, Sydney
Committee member, RomPhysChem16, 21-23 September 2016, Galati, Romania
Committee member, "SiO2 and advanced dielectrics", June 2016, Nice, France
Committee member, "SiO2 and advanced dielectrics", June 2018, Bari, Italy
Committee member "ESG-PNCS 14th European Society of Glass Conference 2018", St Malo, France
Co-president of scientific committee of "Bragg Gratings Photosensitivy and Poling (BGPP)", 2018, Zurich, Suisse.
Committee member, ICTMC21, September 2018, Denver, USA

Workshops and national meetings :

Committee member, « Modélisation des oxydes » in GDR « ModMat » et « Co-DFT », 2013
Committee member, Winter School INSTN « Computational mechanics of materials damage », Saclay, 2013
Organizer, "Single crystals : Growth and physico-chemical properties", 18 déc 2014, Orsay
Committee member, « Cinétique et diffusion » GdR « Nanoalliages », 2015
Committee member, "National network CNRS CRISTECH", 2016
Committee member, "Diagrammes de phases" GdR « ModMat » 2017
Committee member, "Which teaching, research and business synergies to promote innovation?" 19 jan 2017, Saclay, France
Committee member, "National network CNRS CRISTECH", 2018
Organizer, « Anisotropy and Texture » (joint national associations of metallurgy from France, Germany, Belgium, Holland), april 2018, Orsay, France

5. Electronic tools and products

Softwares

Implementation of the variable charge model in tight binding formalism (SMTB-Q) in the LAMMPS code, a free molecular simulation software (lammps.sandia.gov).

Databases

Tools for decision-making

Solver competition tools *(Science and technology only)*

6. Instruments and methodology

Prototypes

Prototype image furnace with electric field: Development of an adaptable module within a growth furnace for applying several KV/cm. (J. Cryst. Growth 409, 23 (2015))
Development of a magnetic field electric transport measuring device (Hall effect, magnetoresistance) as a function of temperature with an original system of generating an alternative magnetic field by a Halbach magnet attached to a rotating platform. (Meas. Sci. Technol. 28, 105905 (2017))

Platforms and observatories

UV (nanosecond) or IR (femtosecond) laser irradiation platform of refractory and transparent insulating materials for their modification. Optical and microscopic characterizations. Platform published on www.pluginlabs-universiteparissaclay.fr

7. Other products

Artistic creations
Movie or theatre play creation
Movies

8. Editorial activities

Participation to journal editorial boards (books, collections)

9. Peer reviewing activities

Reviewing of journal articles

Advanced Materials, Physical Review Letters, Physical Review B, Laser & Photonics Reviews, J. of Applied Physics, Applied Physics Letters, Journal of Non-Crystalline Solids, Solid State Communications, Optics Express, Optics Letters, Applied Optics, Energy & Environ. Sci., J. Mater. Chem., Journal of Nanoparticle Research, Nanoscale, Surface Science, Computational Materials Science, Chemical Physics Letters, Materials Letters

Grant evaluation (public or charities)

French National Agency (PNANO, Young Researchers, Open Call, Matetpro)
National Science Center (Pologne)
DFG (Allemagne)
CIFRE projects

Participation to lab site visit committees (Hceres etc.)
Participation to institutional committees and juries (CNRS, INSERM, etc.)

10. Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

Coordinator of a European project e-FLAG (Exchanges around Femtosecond Laser Applications in Glasses, 247635), FP7-PEOPLE-IRSES, 11/2010 - 11/2014

Marie-Curie Individual Fellowship (HyTeChan), 10/2016 - 10/2018

FeCoProGen : Fe-Co based magnetic alloy with high strength and minimized iron losses for new high speed aerospace generator, Thales, APERAM, ENS Cachan, 2013-2015

PHC Tassili, "Texture and microstructure of FeNi and Cu alloys after severe plastic deformation", USTHB, Algeria, 2012-2015.

PHC Maghreb, "Hyperdeformation for hypertexturation {100}", Faculty of Physics, Alger ; LMCN, Marrakech, Maroc ; Laboratoire for Inorganic Chemistry, Sfax, 2016-2018.

National public grants (ANR, PHRC, FUI, INCA, etc.)

ANR MatetPro : Nanofiber
ANR JCJC : Recipe
BPI France, D. Solas, AL Helbert, T. Baudin. SOFIA «Solutions for industrial metal additive manufacturing », 2016-2022
CNRS Energy Programme, 2017

Local grants ("collectivités territoriales")

PIA (Labex, Equipex etc.) grants

SATT Paris-Saclay, T. Baudin, A.-L. Helbert, ENS Cachan, CNAM, ONDALU : Study and production of heat exchanger tubes for the automobile by a colamination method, 2016-2018
SATT Paris-Saclay, B. Poumellec, M. Lancry : Development of birefringent Optical components (with Horiba Jobin-Yvon), 2014
SATT Paris-Saclay, B. Poumellec, M. Lancry : Optofluidics (with LighFab), 2016

Grants from foundations and charities (ARC, FMR, FRM, etc.)

11. Visiting senior scientists and post-doc

Post-docs

Zhiyong YANG (01/2014-02/2015), CSC scholarship (1 paper)
Xuanguo WANG (03/2014-02/2015), CSC scholarship
Changyong ZHAN (03/2014-02/2015), CSC scholarship (7 papers)
Richard DREVET (10/2014-10/2015), IdF scholarship (4 papers, 1 international conference)
Lei GUO (Septembre 2016- Août 2017), CSC scholarship (7 papers)
Rudy DESMARCHELIER (11/2014-02/2016), IDEX Paris Saclay scholarship (2 papers)
Monica Leon PICHEL (1/2014-12/2014), ANR Mat&Pro. (1 paper)
Babu Hari BABU, (2/2015-6/2016), ANR Mat&Pro (7 papers).
Murat GUNES (10/2016-10/2018), CEE Marie-Curie Individual Fellowship (1 paper)
Antoine PARIS (11/2015-11/2017), Airbus and Aubert&Duval, Industrial development
M. REKIK (11/2013-07/2014), CEE project FeCoProGen (1 international conference)
M. TEBIB (10/2016-03/2018), SATT Paris-Saclay (2 national conferences)

Visiting senior scientists

Huan XUE, R&D Center of Wuhan Iron & Steel Group Corp, 6 months 2013
Torataro KURITA Kyoto University, Japon, 2014
Kevin COOK, Université de Sydney, Australia, 2014
Niculae SPATARU, Institute of Physical Chemistry, Bucarest, Romania, 2014
Qiu LIU, Photonics Laboratory, Wuhan University, China, 2016
Lei LI, North-Western Institute for non-ferrous metals, Chine, 3 months, 2014
Qiang HONG, North-Western Institute for non-ferrous metals, Chine, 3 months, 2014
Anchao REN, R&D Center of Wuhan Iron & Steel Group Corp, China, 6 months, 2015
Xiaonan MAO, North-Western Institute for non-ferrous metals, China, 6 months, 2015
Liao KAI, Central South University of Forestry and Technology, China, 1 year, 2016

12. Scientific recognition

Prizes

Thesis Prize of French Neutron Society, D. Bounoua, 2017
Thesis Prize, Department of Physics, Waves and Matter, University Paris Saclay, Jing CAO, 2017.

Distinctions

Awarded OSA (Optical Society of America) Senior Member: Bertrand Poumellec, 2015
Awarded OSA (Optical Society of America) Senior Member: Matthieu Lancry, 2017

IUF members

Chair of learned and scientific societies

Member of the Board of Directors USTV (Union for science and technology of glass) 2014-2017
Treasurer and Member of the Board of Directors USTV (Union for science and technology of glass) 2017-2020

Invitations to meetings and symposia (out of France)

During the reference period, team members gave a total of 53 invited conferences abroad, some of them in major conferences in their field and listed below:

V. Ji, M. Andrieux, N. Prud'Homme, ICMCTF 2013, "Residual Stress and Crystallographic Texture in Zirconia Thin Films Obtained by MOCVD", 29 April-3 May 2013, San Diego, USA

V. Ji, W. Seiler, 17th National Conference on Residual Stresses, "XRD peak width and its engineering applications" 29-31 October 2013, Shanghai, China
G. Sattonnay, N. Sellami, I. Monnet, C. Grygiel, C. Legros, R. Tétot, L. Thomé, D. Menut, J.-L. Béchade, Spring Meeting MRS 2014, symposium ZZ "Advanced Characterization Techniques for Ion-Beam-Induced Effects in Materials", 22-24 April 2014, San Francisco, USA

D. Berardan, L. Zhao, C. Barreteau, L. Pan, J. Li, N. Dragoe, 5th International Congress on Ceramics ICC5, "BiCuSeO-layered oxychalcogenides with high ZT values, from basic science to applications", 17-21 August 2014, Beijing, China

B. Poumellec, M. Lancry, Advances on functional doped glasses: technologies, properties and applications, "Optical functionalization of glasses by femtosecond laser irradiation", 15-19 September 2014, Warsaw, Poland

B. Poumellec and M. Lancry, 24th International Congress on Glass, "Femtosecond laser direct writing of optical functions in glasses for photonics", 7-11 April 2016, Shanghai, China

R. Haumont, RCBJSF-IWRF, "Crystalline growth under high electric field, a new tool for new materials design", 19 June 2016, Matsue, Japan

V. Ji, N. Li, N. Prud'Homme, The 10th International conference on Residual Stresses (ICRS 10), "Internal stress analysis for oxide-metallic substrate system due to high temperature oxidation", 3-7 July 2016, Sydney, Australia

N. Dragoe, D. Berardan, S. Franger, D. Dragoe, A. K. Meena, 20th International Conference on Ternary and Multinary Compounds, "High entropy oxides: a new class of functional materials". 5-9 September 2016, Halle, Germany

N. Dragoe, D. Bérardan, S. Franger, D. Dragoe, A. K. Meena, Novel quantum and functional materials, "Structure and properties of high entropy oxides", 7-9 August 2017, Stuttgart, Germany

C. Ricolleau, A. Chmielewski, J. Nelayah, J. Creuze, H. Amara, H. Prunier, D. Alloyeau, XXVI International Materials Research Congress, "Reactivity and thermodynamical properties of nanoalloys studied by in situ TEM experiments", 20-25 August 2017, Cancun, Mexico

F. Berthier, J. Creuze, B. Legrand. 4th International Conference on Physical and Theoretical Chemistry, "What is hidden behind a phase diagram ?", 18-19 September 2017, Dublin, Ireland

D. Berardan, N. Dragoe, 15th European Conference on Thermoelectrics, "The potential of oxychalcogenides for thermoelectric applications", 25-27 September 2017, Padova, Italy

M. Lancry, B. Poumellec, The 7th Annual World Congress of Nano Science and Technology-2017, "Creation and orientation of nano-crystals by femtosecond laser for controlling second harmonic generation in silica-based glasses", 24-26 October 2017, Fukuoka, Japan

D. Berardan, A. K. Meena, N. Dragoe, S. Franger, Advanced Materials World Congress, "High entropy oxides as promising materials for safe and efficient green solid state batteries", 4-8 February 2018, Singapore, Singapore

V. Ji, The 5th China National Conference and International Seminar on Shot-Peening Technologies, "Shot-peening effect on fatigue life of samples with foreign object defects", 11-14 June 2018, Shanghai, China

M. Lancry, B. Poumellec, Progress in Ultrafast Laser Modifications of Materials, "Femtosecond laser induced crystallization from Glasses", 13-16 June 2018, Telluride, USA

Members' long-term visits abroad

Waseda university, Tokyo, several stays totaling one month since 2013
The University of Sydney, Australia, 15 days in 2014
East China University of Science and Technology, Shanghai, Chine, 10 days in 2014
The University of Sydney, Australia, 15 days in 2015
The University of Sydney, Australia, 15 days in 2016
Beihang University, Beijing, 10 days in november 2017,
Beihang University, Beijing, 10 days in april 2018
University Caddi Ayyad, Marrakech, two visits of one week each, PHC Mahgreb
University of Science and Technology « Houari Boumediene », Alger, two visits of one week each, PHC Tassili

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

1. Socio-economic interactions / Patents

Invention disclosures

Filed patents

T. Waeckerlé, T. Baudin, A.L. Helbert and O. Hubert, "FeCo alloy, FeSi alloy or Fe sheet or strip and production method thereof, magnetic transformer core produced from said sheet or strip, and transformer comprising same", Patent WO2017017256 (A1) 29 juillet 2016.

Accepted patents

Licenced patents

2. Socio-economic interactions

Industrial and R&D contracts

PRES UniverSud, LAMBE – Evry : "Electrochemical grafting for thermoelectric Applications and sensors" 2013-2013
CHPOLANSKY, "Optimization of welding by laser cladding. Microstructure and strain study", 2015-2015
VALLOUREC, "Residual stress analysis on Inconel 690", 2015-2016
VALLOUREC-VALINOX, "Residual stress analysis by XRD on Ni based alloy tubes", 2015-2016
CHPOLANSKY, "Cladding Laser Recharging of Molds for Glassware: Study of Metallurgical Behavior and Damage", 2015-2018
TE-OX, NANOX, 2016-2019
ANR/FCS, LAMBE - Evry, LABEX CHARMMMAT : 2016-2018
APERAM, "Cube hypertexture {100}<001> Fe-Ni and Fe-W sheats for epitaxial substrates", 2012-2015
APERAM, "Texture analysis of Fe49%Co after laminating", 2014-2014
APERAM, "Characterization of sample texture components (AFK1)", 2014-2014
APERAM, "Controlling Goss texture of Fe-27%Co F A.-L. Helbert, T. Baudin, Contrôle de la texture Goss d'échantillons de Fe-27%Co for a reduction of magnetostriction in embedded transformers", 2015-2018
APERAM, "Metallurgical study of textured Fe-48%Co", 2015-2015
APERAM, "Anomal growth in superalloys", 2016-2016
AUBERT & DUVAL, "Influence of thermo-mechanical treatment on microstructure and mechanical properties of Ti6246 alloy", 2013-2015
AUBERT & DUVAL – AIRBUS, "Study of the growth kinetics of beta grains in titanium alloys Ti6AlV", 2015-2017
CHPOLANSKI, "Optimization of cladding laser welds. Study of microstructure and constraints", 2015-2015
SAINT-GOBAIN, " Comparison of textures measured by X-ray diffraction and EBSD", 2015-2015
MICHELIN, "Characterization of pearlitic steel wire", 2018-2018

Cifre fellowships

S. Le Corre, "Influence of thermo-mechanical treatment on microstructure and mechanical properties of Ti6246 alloy". Thesis defence february 15, 2016 (Aubert&Duval).

F. Bourahima, "Cladding laser reloading of moulds for glassware: study of metallurgical behaviour and damage", 2015-2018, (Chpolansky).

Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*

GDR Meeticc, GDR Nanoalliages, GDR Nanoperando, GDR Recristallisation, GDR Thermoélectricité, GDR ModMat, GDR Oxyfun, IRN Nanoalloys, reseau CRISTECH

Start-ups

3. Expertise

Consulting
Participation in expert committees (ANSES etc.)
Legal expertise

4. Expert and standardization reports

V. Ji is a member of the AFNOR Standardization Commission for "non-Destructive testing" since 2014.

5. Public outreach

Radio broadcasts, TV shows, magazines

R. Haumont is involded in several TV shows: E=m6 (M6), Les carnets de Julie (France 3, weekly, since 2017), Le magazine de la santé (chronicle twice a month since 2018)

Journal articles, interviews, book edition, videos, etc.

Other popularization outputs

raphaelhaumont.wordpress.com

Un chimiste en cuisine
R. Haumont,
Dunod, octobre 2013

Le petit chimiste en cuisine
R. Haumont,
Dunod, octobre 2014

Innovation aux fourneaux
T. Marx, R. Haumont
Dunod, mai 2015

Les papilles du Chimiste
R. Haumont
Dunod, octobre 2017

Debates on science and society

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

1. Educational outputs

Books
E-learning, MOOCs, multimedia lessons, etc.

2. For humanities only, published PhD theses

3. Quality of PhD student supervision

2013

S. Costes, 4 juin 2013, « Extension de l'approche par la courbe maitresse de la prédiction des durées de vie de réseaux d'indice complexes inscrits par UV dans les fibres » B. Poumellec, M. Lancry, Industriel

X. He, 2 décembre 2013, « thèse suivante Oriented micro/nano-crystallization in silicate glasses under thermal or laser field for mastering optical non-linear optics in bulk » B. Poumellec, M. Lancry, co-tutelle CHine

M. Heili, 19 novembre 2013, « Influence de l'histoire thermique sur la diffusion optique dans les préformes et les fibres optiques GeO2-SiO2 : F » B. Poumellec, M. Lancry, CNRS-industriel

C. Barreteau, 26 septembre 2013, « Matériaux céramiques thermoélectriques pour la production d'électricité propre » N. Dragoe, D. Bérardan, Financement MESRI

J. De Jaeger, 17 janvier 2013, « Effet du procédé multi-passes sur la microstructure et le comportement mécanique de l'Inconel 718 forgé à chaud » J.-H. Schmitt, Industriel

2014

S. Denis, 20 novembre 2014, « Cristallogénèse et caractérisations physico-chimiques des solutions solides supraconductrices $La_{2-x}Sr_xCuO_4$ et $La_{1,6-x}Nd_{0,4}Sr_xCuO_4$ et » P. Berthet, C. Decorse, Financement MESRI

B. Nabi, 27 janvier 2014, « Etude d'alliages FeCo magnétiques à microstructure partiellement recristallisée ou fortement texturée » T. Baudin, A.-L. Helbert, Pole ASTech

J. Xiao, 12 décembre 2014, « Etude du comportement et de contraintes résiduelles de l'Inconel 600 oxydé sous air humide » V. Ji, N. Prud'Homme, Bourse CSC

W. Wang, 14 janvier 2014, « Etude des mécanismes de précipitation et de recristallisation en vue de l'optimisation des microstructures de nouveaux alliages base Ni à hautes propriétés mécaniques » T. Baudin, A.-L. Helbert, Financement MESRI

Y. Zhang, 26 septembre 2014, « Theoretical study of the transition-metal oxides Pb2FeMoO6 and ZrO2 » V. Ji, Bourse CSC

N. Salles, 11 septembre 2014, « Etude des différents polymorphes de l'alumine et des phases transitoires apparaissant lors des premiers stades d'oxydation de l'aluminium. Simulations à l'échelle atomique par un modèle à charges variables en liaisons fortes » R. Tétot, O. Politano, CNRS/Région Bourgogne

R. Desmarchelier, 4 juillet 2014, « Analyses des forces photo-induites par le laser femtoseconde dans les verres à base de silice » B. Poumellec, M. Lancry, ANR

E. Malheiros, 3 avril 2014, « Experimental study of the diffusion of oxygen, chromium and iron in oxide films formed by the oxidation of the AISI 439 ferritic stainless steel (thèse en co-tutelle) » A. Sabioni, V. Ji, bourse brésilienne

P. Ramos, 2 avril 2014, « Ionic diffusion in Cr2O3 films and its relation with the oxidation rate if AISI 304 austenitic stainless steel (thèse en co-tutelle) » A. Sabioni, V. Ji, bourse brésilenne

2015

Y. Ateba Betanda, 1 octobre 2015, « Hypertexture Cube {100}<001> de feuillards d'alliages Fer-Nickel et Nickel-Tungstène pour substrats d'épitaxie » A.-L. Helbert, T. Baudin, Financement MESRI

N. S. Beesetty, 10 juillet 2015, « Single crystal growth and magnetic heat transport study of the spin chain compound Sr2CuO3 » A. Revcolevschi, Européen

C. Byl, 2 avril 2015, « Synthèse et caractérisation de nanocomposites à base d'oxyde de zinc pour des applications thermoélectriques » N. Dragoe

T. T. X. Vo, 17 septembre 2015, « Nanomatériaux pour applications thermoélectriques » N. Dragoe

J. Li, 24 juillet 2015, « Structure and properties of BiCuSeO-type thermoelectric materials » N. Dragoe, C. Wei, allocation CSC

G. Zumpicchiat, 16 décembre 2015, « Modélisation numérique de la diffusion-corrosion des alliages de zirconium » C. Berdin, bourse CEA

2016

S. Le Corre, 15 février 2016, « Influence du traitement thermomécanique sur la microstructure et les propriétés mécaniques de l'alliage Ti6246 » A.-L. Helbert, D. Solas, Industriel

J. N. V. De Souza, 29 avril 2016, « Experimental Determination of diffusibility of Oxygen, Chromium and Iron in oxide films obtained during oxidation of Fe-15%Cr alloy (thèse en co-tutelle) » A. C. S. Sabioni, V. Ji, Université Fédéral de Oura Preto (Brésil)

N. Li, 4 avril 2016, « Etude du comportement à l'oxydation et des contraintes résiduelles lors de l'oxydation sous air humide de l'alliage AISI 430 » V. Ji, N. Prud'Homme, Bourse CSC

B. Mehdi, 4 décembre 2016, « contribution à l'étude de la texture, l'anisotropie et le comportement mécanique des soudures de l'alliage de Titane TA6V (thèse en co-tutelle) » B. Alili, V. Ji, bourse algérienne

S. Mitra, 15 décembre 2016, « Chalcogénures de type I-V-VI pour applications thermoélectriques » D. Berardan, financement MESRI

P. Hicher, 16 décembre 2016, « Croissance cristalline d'oxydes sous champ électrique » P. Berthet, R. Haumont, bourse ministère

2017

J. Cao, 3 mars 2017, « Création et orientation de nano-cristaux par irradiation laser femtoseconde pour le contrôle de l'orientation des propriétés optiques non-linéaires dans des verres à base de silice » B. Poumellec, M. Lancry, bourse CSC

K. Verstraete, 28 mars 2017, « Étude du multi-colaminage de matériaux différents » T. Baudin, A.-L. Helbert, Financement MESRI

B. Hary, 16 novembre 2017, « Compréhension et modélisation de l'influence du taux de renforts et de la texture de déformation sur la recristallisation des aciers ODS ferritiques » T. Baudin, R. Logé, Bourse CEA

M.-A. Thual, 20 décembre 2017, « Étude de la cinétique de coalescence de nano-oxydes et incidence sur la recristallisation dans des alliages ODS » M.-H. Mathon, T. Baudin, Bourse CEA

D. Bounoua, 12 décembre 2017, « Synthèse et étude de cuprates de basse dimensionnalité à propriétés thermiques fortement anisotropes » L. Pinsard-Gaudart, R. Saint-Martin, DIM oxyMORE - île de France

2018

J. Djuidje-Dzumgam, 30 janvier 2018, « synthèse et résistance mécanique de couches d'oxyde de zirconium » C. Berdin, M. Andrieux, Financement MESRI

4. Students' follow up in association with doctoral schools

The policy is the same as that of the Doctoral School. We support our PhD students to direct them towards postdoctoral contracts and also put them in touch with all our private sector contacts for those who wish.

5. Participation to international training programs (e. g. Erasmus Mondus)

6. PhD student participation to scientific animation and unit/team life

Each year, one day is devoted to presentations given by all the PhD students of the team to summarize their work and the organization of this day is done by the PhD students.

Each year, the PhD students organize a day for presentations given by the internship students (L3, M1 and M2) on the form "my internship in 300 seconds".

The proper functioning of the chemistry laboratory is in charge of one PhD student and one permanent staff and it turns each month.

7. Participation of team members in setting up Master courses

L. Pinsard-Gaudart (2015-2016) then J. Creuze (since 2016): In charge of M1 "Functional Materials" of the Master "Materials Science and Engineering" (University Paris Saclay)

A.-L. Helbert: In charge of M2 "Materials for Energy and Transports" of the Masters "Materials Science and Engineering" and "Energy", INSTN/CEA/University Paris-Saclay

8. Student publications (for Biology only)

Appendix 4

Team 9 - ERIEE

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Recherche et Innovation en Electrochimie pour l’Energie**
Acronym:	**ERIEE**
Director's name (current contract):	**Pierre MILLET**
Director's name (future contract):	**Pierre MILLET**

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

1- Articles

Scientific articles

1. *Multiscale morphological and electrical characterization of charge transport limitations to the power performance of positive electrode blends for lithium-ion batteries*. N. Besnard, A. Etiemble, T. Douillard, O. Dubrunfaut, P. Tran-Van, L. Gautier, S. Franger, J.-C. Badot, E. Maire, B. Lestriez, *Advanced Energy Materials*, 7 (**2017) 1602239.** Impact factor of the Journal : 15.230

2. *Influence of iridium oxide loadings on the performance of PEM water electrolysis cells: Part I – Pure IrO2-based anodes*. C. Rozain, E. Mayousse, N. Guillet, P. Millet, Appl. Catalysis B: Environmental, 182 (**2016**) 153 – 160. Impact factor of the Journal : 8.328
3. *Influence of iridium oxide loadings on the performance of PEM water electrolysis cells: Part II – Advanced anodic electrodes*. C. Rozain, E. Mayousse, N. Guillet, P. Millet, *Appl. Catalysis B: Environmental*, **2016**, *182*, 123 – 131. Impact factor of the Journal : 8.328
4. *The role of surface states during photocurrent switching: Intensity Modulated Photocurrent Spectroscopy analysis of BiVO4 photoelectrodes*. M. Antuch, P. Millet, A. Iwase, A. Kudo, Appl. Catalysis B: Environmental, x (**2018**) xxx. In Press. Impact factor of the Journal : 8.328

5. *Direct Evidence of Lithium Ion Migration in Resistive Switching of Lithium Cobalt Oxide Nanobatteries*. V. S. Nguyen, V. H. Mai, P. Auban Senzier, C. Pasquier, K. Wang, P. Lecoeur, P. Aubert, S. Franger, R. Salot, B. Dkhil, O. Schneegans, *Small*, **2018**, *5*, 1801038-1801045 FI 8.315
6. *Room temperature lithium superionic conductivity in high entropy oxides*. D. Berardan, S. Franger, A. K. Meena, N. Dragoe, *Journal of Materials Chemistry A*, **2016**, *6*, 9536 FI 8.262
7. *Comprehensive characterization of all-solid-state thin films commercial microbatteries by Electrochemical Impedance Spectroscopy*. S. Larfaillou, D. Guy-Bouyssou, F. Le Cras, S. Franger, *J. Power Sources*, **2016**, *319*, 139-146 FI 6.333
8. *Core-shell amorphous silicon-carbon nanoparticles as high performance anodes for Li-ion batteries*. J. Sourice, A. Bordes, A. Boulineau, S. Franger, A. Quinsac, A. Habert, Y. Leconte, E. De Vito, W. Porcher, C. Reynaud, N. Herlin-Boime, C. Haon, *J. Power Sources*, **2016**, *328*, 527-535 FI 6.333

Other articles (professional journals, etc.)

Main documents other than scientific publications of the team

1. Expert report for the French PS2E Institute for Energy Transition : Methodologies for the *qualification of MW-scale PEM water electrolysers for hydrogen production and mobility applications* (2015 - 2016).
2. Expert reports in contribution to the work of the International Energy Association (IEA) and the European Commission (Joint Research Center & Joint Undertaking Fuel Cell & Hydrogen) on the harmonization of test protocols and characterization techniques of water electrolysis cells. Publication of a corpus of reference documents to support the development of codes and standards in the field of water electrolysis.
3. Multiples expert reports for national and international research laboratories and agencies (ex . French Labexes, French ANR, H2020 and Marie Curie-Sklodowska of the European Commission, Belgian FRS).

2- Books

Scientific book edition

1. D. Bessarabov, P. Millet, PEM water electrolysis, 1st Edition, Volume 1, B.G. Pollet Series Editor, Elsevier, ISBN: 978-01-28-11145-1 (**2018**).
2. D. Bessarabov, P. Millet, PEM water electrolysis, 1st Edition, Volume 2, B.G. Pollet Series Editor, Elsevier, ISBN: 978-01-28-11145-2 (**2018**).

Book chapters

1. P. Millet, chapters 13 and 18 in *Handbook of Membrane Reactors*. Volume 2: Reactor types and industrial applications', A. Basile and S. Pereira Nunes Editors, WoodHead Publishing, ISBN: 978-0-85709-414-8 (**2013**).
2. P. Millet, Chapters 4 and 6 in *Water Electrolysis,* A. Godula-Jopek Ed., Wiley-VCH, ISBN 9783527333424 (**2015**).
3. P. Millet, Chapters 7 and 10 in *PEM water Electrolysis for hydrogen production: Principles and Applications*, D. Bessarabov, H. Wand, H. Li, N. Zhao, CRC Press, ISBN 9781482252293, (**2015**).
4. P. Millet, chapters 9 and 10 in *Compendium of Hydrogen Energy'* Vol.1 : Hydrogen Production and Purification; S. Subramani, A. Basile, T.N. Veziroglu Editors, WoodHead Publishing, ISBN: 978-1-78242-361-4 (**2016**)

3- Meetings

Meeting abstracts

1. R. Ngameni, P. Millet**,** *EIS analysis of hydrogen incorporation into Pd-based planar, spherical and cylindrical bi-layers,* 9th International Symposium on Electrochemical Impedance Spectroscopy, Okinawa, Japan, 16-21 June **2013.**
2. A. Fateeva, E. Demessence, T. Puzenat, T. Devic, P. Millet, *Functional Metal Organic Frameworks based on Porphyrinic Linkers: Optical and Electronic Properties and Applications,* 41st International Conference on Coordination Chemistry, Singapore, 21-25 July **2014**.
3. S.A. Grigoriev, V.N. Kuleshov, N.V. Kuleshov, P. Millet, *Development and characterization of a high-temperature PEM fuel cell with H3PO4-doped PBI as solid polymer electrolyte,* 20th World Hydrogen Energy Conference, Gwangju, South Korea, 15-20 June **2014.**
4. P. Millet, A. Ragupathy, A. Villagra, A. Ranjbari, *Implementation of Metallic Clathrochelates at the Surface of Carbonaceous Substrates for Hydrogen Evolution in Acidic Media,* 16th Topical Meeting of the International Society of Electrochemistry, Angra dos Reis, Brazil, Brasil, 22-26 March **2015**.
5. A. Villagra, A. Ranjbari, A. Kudo, P. Millet, *Surface Modification of Rhodium-doped Strontium Titanate by Adsorption of Cobalt Clathrochelates for Water Photo-Dissociation,* 3rd South African Solar Energy Conference (SASEC 2015), Skukuza, Kruger National Park, South Africa, 11-13 May **2015**.
6. P. Millet, *Electrocatalysis of the Hydrogen Evolution Reaction in Acidic Media using Transition Metal Clathrochelates*, 6th Baltic Electrochemistry Conference Electrochemistry of Functional Interfaces and Materials, Helsinki, Finland, June 15-17, **2016**.
7. B. Verdin, F. Fouda-Onana, P. Millet, *Current distribution in large-surface area PEM electrolysis cells*, 20th Topical Meeting of the International Electrochemical Society, Advances in Lithium and Hydrogen Electrochemical Systems for Energy Conversion and Storage, Buenos-Aires, Argentina, 19-22 March, **2017**.
8. A. Villagra, M. Antuch, A. Kudo, P. Millet, *Photochemical Water Dissociation using Rh-doped $SrTiO_3$ Surface-modified by Pt-nanoparticles or Cobalt-clathrochelate Co-catalysts,* 21st Topical Meeting of the International Society of Electrochemistry on '*Photoelectrochemistry of semiconductors at the nanoscale: from fundamental aspects to practical application*', Szeged, Hungary, 23-26 April **2017**.
9. P. Millet, *Performance comparison of main water electrolysis technologies*, 8th International Conference on Hydrogen Production 2017 (ICH2P-2017), Sydney, Australia, 29-31 July 2017.
10. B. Verdin, H. Bounoua, A. Moussabbir, P. Millet, *Distribution of current lines in catalytic layers of PEM water electrolyzers*, 68th Annual Meeting of the International Society of Electrochemistry, Providence, Rhode-Island, USA, Aug 27–Sept 1 **2017**.

4- Meeting and congress organisation

1. L. Assaud: **co-organization of a Workshop on 'Solar fuels', IRS Momentom (Paris-Saclay university),** UPSud-Cachan, 11 October 2017 (≈ 50 participants)
2. P. Millet: **co-organisation of two French academic colloquium on Basic Science for energy** *(organized by the French Alliance on energy Ancre)*:
   Colloquium n°1 : *Simulations multi-échelles de la molécule aux systèmes en fonctionnement*, CNRS, Paris, 16 octobre **2017** (≈ 30 participants).
   Colloquium n°2 : *Caractérisation couplée des matériaux et interfaces solides et fluides – instrumentation*, IFPEN, Rueil-Malmaison, 8 décembre **2017** (≈ 30 participants).

3. P. Millet: **organisation of the annual workshop of the International Energy Agency** (task 30 : global hydrogen systems analysis), UPSud-Orsay, 18-20 April **2018** (≈ 50 participants from Europe, USA and Japan).

5- Electronic tools and products

Softwares

1. Set of numerical tools developed for analyzing the efficiency of water electrolysis stacks (patent pending, 2018).

Tools for decision-making

1. Protocols and methodology for the quality control of PEM water electrolysis stacks (FlexiPEM2, patent pending, 2018).

6- Instruments and methodology

Prototypes

- Design of prototype PEM water electrolysis cell and stack; application in the water electrolysis industry.
- Development of prototype test benches for the characterization of hydrogen absorbing materials and hydrogen compression. Application to the development of thermal hydrogen compressors.

Platforms and observatories

1. **AMiCE** Platform: AFM-SECM characterization platform allowing operation in tapping and peakforce tapping modes; AFM, QNM, SECM, KPA; equipment (260 k€) was purchased using fundings from the industry (≈ 70%), Paris-Sud University and the Char3mat Labex (≈ 30%).
2. **GenHyTech** Platform: test platform (ATEX) of PEM water electrolysis cells and stacks for the production of pressurized hydrogen.

7- Other products

Video

- *Regards sur nos horizons énergétiques*, SCAVO, Faculté des sciences d'Orsay, Université Paris-Sud (2013).

8- Editorial activities

Participation to journal editorial boards (books, collections)

9- Peer reviewing activities

Reviewing of journal articles

1. Team members are involved in regular peer review of scientific papers for electrochemistry and material science Journals.
2. Same for book chapters.

Grant evaluation (public or charities)

1. Agence National de la Recherche
2. FNRS Belge
3. Proposal evaluation of Marie Sklodowska-Curie mobility program (chemistry panel).
4. H2020, European Commission.

Participation to lab site visit committees (Hceres etc.)

Participation to institutional committees and juries (CNRS, INSERM, etc.)

P. Millet. Nominated member of the Conseil National des Universités (CNU), section 33 (Chimie des Matériaux).

10- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants

1. H2020 research grant, P. Millet, CEOPS, 2013-2015.
2. CCUFB research Grant, L. Assaud (in coll. with Univ. of Erlangen Nuremberg, Germany) 2016.

National public grants (ANR, PHRC, FUI, INCA, etc.)

1. ANR research grant, S. Franger, Pépite, 2015-2019
2. ANR research grant, P. Millet, Chalco-cat, 2015-2018
3. ANR research grant, P. Millet, Moïse, 2017-2020
4. ADEME research grant, P. Millet, Mhyel, 2016-2019
5. ADEME research grant, P. Millet, Vitrhydrogène, 2017-2020
6. ADEME research grant, P. Millet, Méthycentre, 2018-2021

Local grants ("collectivités territoriales")

1. DIM Oxymore, S. Franger, 2013-2013
2. RTRA Triangle de la Physique, S. Franger, 2014-2014
3. Cnano (Région IdF), S. Franger, 2014-2014
4. ASTRE (Conseil Général 91), P. Millet, 2015-2018
5. Idex Paris Saclay, S. Franger, ECOPTER, 2015-2016
6. DIM Oxymore, S. Franger, 2016-2017
7. Initiative de Recherche Stratégique, L. Assaud, MOMENTOM, 2017-2018

PIA (Labex, Equipex etc.) grants

1. IEED/ITE Paris-Saclay Efficacité Energétique (PS2E), P. Millet, FlexiPEM1, 2015-2017.
2. IEED/ITE Paris-Saclay Efficacité Energétique (PS2E), P. Millet, FlexiPEM2, 2018-2020.
3. Charm3at Labex, post-doc grant, A. Ranjbary, 2015-2016.
4. Charm3at Labex, AMicE, L. Assaud, 2017-2018.

Grants from foundations and charities (ARC, FMR, FRM, etc.)

11- Visiting senior scientists and post-doc

Post-docs

1. R. Ngameni-Jiembou, ANR grant, HydroPEM project, France (02-2013/10-2013). 6 papers published.
2. K. Ramirez, ANR grant, HydroPEM project (04-2013/07-2013).
3. C. Thibault, grant from the industry (08-2013/12-2013).
4. P. Vorburger, H2020 European project, (01-2014/12-2014).
5. R. Ngo-Biboum Bimbong, grant from the Charm3at Labex (11-2014/12-2015).
6. P. Vorburger, grant from the industry (01-2015/12-2015).
7. G. Mouchaham, grant from the Charm3at Labex (03-2015/03-2016).
8. A. Villagra, ANR grant, ChalcoCat project (03-2017/09-2017).
9. A. Pradon, grant from IDEX Université Paris-Saclay, IRS MOMENTOM (04-2017/04-2018) 2 papers in preparation.
10. A. Villagra, ADEME grant, Mhyel project (09-2017/03-2018).
11. C. Bongu, CSIR/CECRI, Karaikudi, India (09-2017/06-2018); grant from the Idex program - IRS Momentum; 01 paper submitted; 01 paper in preparation.
12. W. El Rouby, Beni-Suef University, Beni-Suef city, Egypt (12-2017/12/2018); grant from the French-Egyptian scientific cooperation program STDF-IFE; several papers in preparation.
13. A. Pradon, ADEME grant, Mhyel project (05-2018/11-2018).
14. J. Sebile-Meilleroux, ADEME grant, Méthycentre project (06-2018/05-2019).
15. M. S. Reck, ADEME grant, Vitrhydrogène project (04-2018/03-2019).

Visiting senior scientists

1. S. Grigoriev, Kurchatov Institute, Moscow, Federation of Russia (2013 and 2015). Invitation from Paris-Sud University (16 papers published over the period, 3 papers in preparation).
2. A. Kudo, Tokyo University of Science, Tokyo, Japan (April-May 2015). Invitation from Paris-Sud University (3 papers published recently, 5 papers in preparation).

12- Scientific recognition

Prizes

Distinctions

IUF members

Chair of learned and scientific societies

Invitations to meetings and symposia (out of France)

5 invitations to give oral communications in international conferences by team members

1. P. Millet, F. Auprêtre, Keynote lecture *: Polymer Electrolyte Membrane Water Electrolysis : status, perspectives and technological developments,* European Hydrogen Energy Conference, Sevilla, Spain, 12-14 March **2014.**
2. L. Assaud, N. Gauthier, O. Dubrunfaut, J.C. Badot, B. Lestriez, S. Franger, *Multiscale charge transport characterization of carbon black/electrolyte interfaces in a γ-Al_2O_3/PVdF/CB composite electrode for lithium batteries*, ACSSI **2016**, Patna, India.
3. P. Millet, *Conventional and Innovatice Electrocatalysts for PEM Water Electrolysis*, Pacific Rim Meeting on Electrochemical and Solid State Science, Honolulu, Hawai, USA, 02-07 October **2016**.
4. P. Millet, *Characterization of MW-scale PEM water electrolyzers, 1st International Conference on Water Electrolysis*, Copenhague, Denmark, June 13-16, **2017**.
5. D. Berardan , A.K. Meena, N. Dragoe, S. Franger, *High entropy oxides as promising materials for safe and efficient green solid state batteries*, Advanced Materials World Congress, Singapore, 4-8 February **2018**.

Members' long-term visits abroad

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

1- Socio-economic interactions / Patents

Invention disclosures

- Several reports have been written for the industry.

Filed patents

1. Two patents under examination on water electrolysis (2017 & 2018).

Accepted patents

1. *Procédé de réalisation de couches minces structurées en 3D.* H. Porthault, F. Le Cras, S. Franger, CNRS, Université Paris-Sud, CEA, 25 février **2013**, FR 13/00426,

Licenced patents

1. E. Anxolabéhère, A. Aukauloo, P. Millet, O. Pantani*, Cellule pour électrolyse de l'eau avec électrolyte solide à base d'oximes métalliques,* Brevet Français UPSud-CNRS (30/11/2007), Brevet EP n°10172519, déposé le 28/11/2009, licence CETH2 2013-2016.

2- Socio-economic interactions

Industrial and R&D contracts

1. P. Millet, leave of absence in the industry at the French Institute on energy transition Paris-Saclay Efficacité Energétique (PS2E, 2015-2016).
2. P. Millet, coordination of the FlexiPEM1 R&D projects, Qualification of industrial PEM water electrolysis plants for grid services, Program d'investissement d'avenir.
3. Council of Essonne (ASTRE project) to develop an automated water electrolysis platform for pressurized H_2 production (R&D + training).
4. P. Millet, ArévaH2Gen, *R&D contract on PEM water electrolysis for pressurized hydrogen production*, 2013-2016.
5. P. Millet, Italcementi, PhD-support contract, *R&D contract on CO_2 electro-reduction*, 2012-2015.
6. S. Franger, Renault, Limitations électroniques/ioniques dans électrodes de batteries Li-ion, 2013-2016.

7. S. Franger, EDF, *Cyclage batteries Li-ion pour stockage stationnaire*, 2016.
8. S. Franger, EDF, *Modélisation du vieillissement de batteries Li-ion pour stockage stationnaire*, 2017.
9. S. Franger, ST Microelectronics, *Microbatteries Li-free*, 2017.
10. S. Franger, PSA, *Vieillissement électrothermique de batteries Li-ion pour usage automobile*, 2017.
11. L. Assaud, Greenfish, PhD-support contract, *Électrodes nanostructurées*, 2017.
12. L. Assaud, Greenfish, PhD-support contract, *Électrodes nanostructurées* pour la (photo)réduction du CO_2, 2018.
13. S. Franger, Greenfish, PhD-support contract, *Batteries tout solide au sodium*, 2018.

Fellowships for PhD studies

1. Caroline ROZAIN, *Développement de nouveaux matériaux d'électrode pour la production d'hydrogène par électrolyse*. Grant : CEA-industrie. Thesis defense : 27th of September **2013**.
2. Séverin Larfaillou, *Application de la spectroscopie d'impédance électrochimique à la caractérisation et au diagnostic de microbatteries tout solide*. Grant : Cifre, ST Microelectronics, Thesis defense : 03rd of March **2015**.
3. Anuradha Ragupathy, *Synthèse du méthanol par réduction électrochimique du CO_2* ; financement Italcementi. Grant : Cifre, Italcementi. Thesis defense : 14th of September **2015**.
4. Angel Villagra; *Photo-dissociation de l'eau et photo-réduction du CO_2 assistées par co-catalyse moléculaire*, grant : Idex Paris-Saclay, MESRI. Thesis defense : 28th of September **2016**.
5. Baptiste Verdin, *Etude des électrodes grandes surfaces d'électrolyseur PEM : homogénéité de fonctionnement et intégrations de catalyseurs innovants.* Grant : CEA-industrie. Thesis defense : 21st of March **2018**.
6. Manuel Antuch, *Photoelectrochemical kinetics of visible-light driven water splitting at Rh :$SrTiO_3$ based electrodes* , Grant : Paris-Saclay Idex. Thesis defense : 21st of March **2018**.
7. Franck Fereirra-Gomes, *Caractérisation électrochimique de micro-batteries Li-free*, financement ST Microelectronics. Grant : Cifre. Started in September 2015. Thesis defense : September **2018**.
8. Tiphaine Deletang, *Vieillissement d'une batterie Li-Ion : Couplage d'un modèle de fatigue et d'un modèle de circuit équivalent (MCE) paramétré par spectroscopie d'impédance*; financement EDF. Started in November 2016. Thesis defense : November **2019**.
9. Yi Peng, *Copper-Graphene quantum dots for water photo-reduction*, Grant : University of Santa Cruz in California + laureate of a Chateaubriand Fellowhip for one semester internship in France (February -> July 2018).Thesis defense : December **2019**.
10. Juan Ugalde, *Modélisation semi-empirique du comportement thermique des batteries Lithium-ion et de leur vieillissement*; Grant : Cifre, PSA. Started in May 2017. Thesis defense : May **2020**.
11. Arun Kumar Meena, *All-solid-state batteries for high energy and power density applications*; Grant : Cifre, Greenfish. Started in December 2017. Thesis defense : December **2020**.
12. Parviz Allazov, *Electrodes nano-structurées pour l'électro(photo)réduction du dioxyde de carbone,* Grant : Cifre, Greenfish-ANRT. Started in December 2017. Thesis defense : December **2020**.
13. Sheng-Mu You, *MOF deposition atop titanium dioxide nanotubes for water photo-reduction.* Grant : National Tsing Hua University + laureate of a mobility fellowship for two years long PhD studies in France. Thesis defense : December **2020**.

Creation of labs with private-public partnerships

Networks and mixed units *(Science and technology only)*
The Eriée team (or individual team members) is official member and contributor of :

- the HySPàC Groupe de Recherche (GdR) of the French CNRS.
- the Charm3at Labex.
- the IEA Annex 30 work group on electrolysis.
- the FCH-JU/JRC working group of the European Commission for the normalisation of water electrolysis test protocols.
- The international society of electrochemistry and the US electrochemical society.

Start-ups

1. P. Millet. Founding member of the French start-up CETH company, later purchased by Aréva and Ademe; close collaborator of the new ArévaH2Gen company (manufacturing of MW-scale PEM water electrolysers for hydrogen refueling stations); the company is located in Les Ulis, France (http://www.arevah2gen.com/fr/societe).

3- Expertise

Consulting

- P. Millet: consultant for private companies on water electrolysis technology.

Participation in expert committees (ANSES etc.)

- S. Franger, P. Millet: experts for the French Agence Nationale de la Recherche.
- S. Franger, P. Millet: H2020 experts of the European Commission.
- P. Millet: expert and vice-president of the chemistry panel for the Marie Sklodowska-Curie mobility action of the European Commission.

Legal expertise

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4- Expert and standardization reports

* P. Millet *et al.*, in : *EU Harmonised Terminology for Low Temperature Water Electrolysis for Energy Storage Applications*, G. Tsotridis and A. Pilenga Edts., JRC science for policy report, European Commission, Luxembourg, 2017, in press.
* P. Millet *et al.*, in : *EU Harmonised Polarisation Curve Test Method for Low Temperature Water Electrolysis*, G. Tsotridis and A. Pilenga Edts., JRC science for policy report, European Commission, Luxembourg, 2017, in press.
* P. Millet *et al.*, in : *EU Harmonised Cyclic Voltammetry Procedure for Low Temperature Water Electrolysis*, G. Tsotridis and A. Pilenga Edts., JRC science for policy report, European Commission, Luxembourg, 2018, in press.
* P. Millet *et al.*, in : *EU Harmonised Electrochemical Impendance Spectroscopy Procedure for Low Temperature Water Electrolysis*, G. Tsotridis and A. Pilenga Edts., JRC science for policy report, European Commission, Luxembourg, 2018, in press.

5- Public outreach

Radio broadcasts, TV shows, magazines

1- TV interview : *Comment produire des jets fuels à partir d'eau de mer*, P. Millet, FR3 Ile de France, 7 avril 2014.

Journal articles, interviews, book edition, videos, etc.

1. P. Millet, A. Aukauloo, *Des électrodes à bas prix pour une planète qui revit,* Plein-sud Recherche, n° 83, p. 35, Université Paris-sud, janvier **2013**.

Other popularization outputs

1. P. Millet, A. Villagra, forum CNRS, *L'hydrogène : l'énergie du futur ?*, démonstration mobilité hydrogène, Cité internationale universitaire, Paris, 25-26 novembre **2017**.

Debates on science and society

1. P. Millet, séminaire journée des Sciences, Mairie de Gif-sur-Yvette, 25 janvier **2018**.
2. P. Millet, séminaire ile de Science Tour, Université Paris-Saclay, 31 janvier **2018**.
3. L. Assaud, participation à l'atelier Energie Renouvelable de la Maison d'Initiation et Sensibilisation aux Sciences (MISS, Université Paris Saclay, **2018**).
4. P. Millet, débat public sur la programmation pluriannuelle de l'énergie (PPE), Atelier « recherche et innovation » sur le power-to-gas et l'hydrogène, CentraleSupélec Saclay, 25 juin **2018**.

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

1- Educational outputs

Books

All books and book chapters published by team members and listed above are for both research and educational purposes.

E-learning, MOOCs, multimedia lessons, etc.

1. P. Millet, French corresponding agent of the EUA/UNI-SET (http://www.eua.be/activities-services/projects/current-projects/research-and-innovation/uni-set.aspx) for UPSud training (MOOC development) and research on energy.
2. L. Assaud, participation au MOOC '*Hydrogène pour la transition énergétique*', IRS Momentom, 2018.

2- For humanities only, published PhD theses

3- Quality of PhD student supervision

- PhD students of the team get their funding from the Ministry of Higher Education (MESRI), from the CEA and from the industry (Cifre grant contracts)
- The mean duration of PhD thesis is close to 3 years.

4- Students' follow up in association with doctoral schools

- Specific PhD thesis actions taken to facilitate PhDs careers are managed directly by the doctoral school (Sciences Chimiques: Molécules, Matériaux, Instrumentation et Biosystèmes, 2MIB).
- However, team leaders are also strongly committed to help PhD students finding positions after leaving the teams; contacts are maintained long (in some cases decades after) after the student has left the team; the academic and industrial networks of team members are used to find either post-doctoral or permanent positions.

5- Participation to international training programs (e. g. Erasmus Mondus)

- L. Assaud, P. Millet: teaching in the Serp+ Chem Erasmus Mundus Master Course (http://www.master-serp.eu/); course title : *Chemistry for Renewable Energy: from advanced research to industrial applications*.

6- PhD student participation to scientific animation and unit/team life

PhD students and post-doc Fellow of the team are involved in **scientific animation and Eriée team life via:**

- Weekly scientific team meeting
- Monthly presentation of research results

7- Participation of team members in setting up Master courses

1. Setup and management of the Master of Energy, Paris-Saclay University (S. Franger)
2. Setup and management of the Master of Chemical Engineering, Paris-Saclay University (P. Millet)
3. Setup and management of the Master of Materials and Industrial Management, Paris-Saclay University (apprenticeship cursus) (J.M. Duffault)
4. Management of one of the first year (M1) of the Master of Energy (Energy Materials), Paris-Saclay University (L. Assaud).
5. Management of various teaching modules, Orsay Institute of technology, Chemistry Department (A. Ranjbari).

8- Student publications (for Biology only)

Appendix 4

Team 10 – SST (SC)

EVALUATION CAMPAIGN 2018-2019
GROUP E

INFORMATION

Team name:	**Soutien Scientifique & Technique (Services Communs)**
Acronym:	**SST (SC)**
Director's name (current contract):	**Anne BLENZEN**
Director's name (future contract):	**Anne BLENZEN**

This SST part of appendix 4 lists the research production exclusively for the SST service. The items listed here have not been taken into account by the research teams. They highlight the visibility of the PICMMO Instrument Platform and the recognition of qualifications of the SST team.

I - SCIENTIFIC OUTPUTS AND ACTIVITIES, ACADEMIC REPUTATION AND APPEAL

13- Articles

Scientific articles

1. *Revealing the Origins of Mechanically Induced Fluorescence Changes in Organic Molecular Crystals.* L. Wilbraham, M. Louis, D. Alberga, A. Brosseau, R. Guillot, F. Ito, F. Labat, R. Métivier, C. Allain, I. Ciofini, *Advanced Materials*, **2018**
2. *Nd 3+ doped transparent tellurite ceramics bulk lasers.* M. Dolhen, M. Tanaka, V. Couderc, S. Chenu, G. Delaizir, F. Brisset, P. Thomas, J.-R. Duclère, *Scientific Reports*, 2018, *8*, 4640-4649
3. *Ballistic edge states in Bismuth nanowires revealed by SQUID interferometry.* A. Murani, A. Kasumov, F. Brisset, S. Guéron, *Nature Comm.*, **2017**, *8*, 1-7
4. *In situ optical monitoring of new pathways in the metal induced crystallization of amorphous Ge.* D. Pelati, G. Patriarche, O. Mauguin, L. Largeau, F. Brisset, F. Glas, F. Oehler, *Crystal Growth & Design*, **2017**, *17*, 5783–5789
5. *A Metallo Pro-Drug to Target CuII in the Context of Alzheimer's Disease.* A. Conte-Daban, V. Ambike, R. Guillot, N. Delsuc, C. Policar, C. Hureau, *Chemistry – A European Journal*, **2018**, *24,* 5095-5099
6. *Anticancer Activity of Polyoxometalate-Bisphosphonate Complexes: Synthesis, Characterization, In Vitro and In Vivo Results.* A. Boulmier, X. Feng, O. Oms, P. Mialane, E. Rivière, C. J. Shin, J. Yao, T. Kubo, T. Furuta, E. Oldfield, A. Dolbecq, Inorg. Chem., **2017**, 56, 7558-7565
7. *Photocatalytic Hydrogen Evolution Using Ni−Pd/TiO2: Correlation of Light Absorption, Charge-Carrier Dynamics, and Quantum Efficiency.* A. L. Luna, D. Dragoe, K. Wang, P. Beaunier, E. Kowalska, B. Ohtani, D. Bahena Uribe, M. A. Valenzuela, H. Remita, C. Colbeau-Justin, *The J. Phys. Chem. C*, **2017**, *121*, 14302-14311
8. *Electronic Structures of Mono-Oxidized Copper and Nickel Phosphasalen Complexes.* C. Herrero, A. Auffrant, G. Nocton, C. Clavaguéra, M. Cordier, R. Singh Chauhan, T. Cheisson, I. Mustieles-Marín, *Chemistry – A European Journal*, **2017**, *23 (71)*, 17940-17953
9. *Copper(II)-Controlled Molecular Glue for Mismatched DNA.* N. Kotera, R. Guillot, M.-P. Teulade-Fichou, A. Granzhan, *ChemBioChem*, **2017**, *18, Issue 7*, 618–622
10. *N-terminal domain of PB1-F2 protein of influenza A virus can fold into amyloid-like oligomers and damage cholesterol and cardiolipid containing membranes* Ajjaji, D. ; Richard, C.-A. ; Mazerat, S. ; Chevalier, C. ; Vidic, J. Biochemical and Biophysical Research Communications, 12 August **2016**, Vol.477(1), pp.27-32
11. *Role of PF6- in the radiolytical and electrochemical degradation of propylene carbonate solutions.* D. Ortiz, I. Jimenez Gordon, S. Legand, V. Dauvois, J.-P. Baltaze, J.-L. Marignier, J.-F. Martin, J. Belloni, M. Mostafavi, S. Le Caër, *J. Power Sources*, **2016**, *326*, 285
12. *Hexanuclear, Heterometallic, Ni3Ln3 Complexes Possessing O-Capped Homo- and Heterometallic Structural Subunits: SMM Behavior of the Dysprosium Analogue.* J. Goura, R. Guillaume, E. Rivière, V. Chandrasekhar, Inorg. Chem., **2014**, 53, 7815-7823

Review articles

Other articles (professional journals, etc.)

14- Books

Scientific book edition

Book chapters

Three chapters in the book: *EBSD : Analyse par diffraction des électrons rétrodiffusés - Applications et techniques couplées*, éd. F. Brisset, publ. EDP Sciences, ISBN : 978-2-7598-1912-6, 300 pages, 2015.

1. EBSD – Historique, p. 31-46, F. Brisset
2. Analyse EBSD et échantillons isolants, p. 83-94, F. Brisset
3. Traction et recuit in-situ analysés par EBSD, p. 127-140, F. Brisset

Five chapters in the book: Microscopie Electronique à Balayage et Microanalyses.

1. Le spectromètre de rayons X à sélection d'énergie (EDS), p. 287-346, F. Brisset
2. L'analyse EDS, p. 347-356, F. Brisset
3. L'analyse EBSD, p. 563-596, F. Brisset
4. L'EBSD : historique, principe et applications, p. 597-604, F. Brisset
5. Diffraction de type Kikuchi en mode transmission (TKD), p. 873-906, F. Brisset

15- Meetings

Meeting abstracts

16- Meeting and congress organisation

1. Co-organization of the symposium 'Cartographie d'orientation et de déformation', 14th colloquium of the Sfmu (Société Française des Microscopies), 2015, F. Brisset.
2. F. Brisset, as a member of the scientific council of EMAS (European Microbeam Analysis Society), has co-organized the EMAS international meetings every years
   - EMAS Porto, Portugal, 2013
   - EMAS Loeben, Austria, 2014
   - EMAS Portoroz, Slovenia, 2015
   - EMAS Marcoule, France, 2016
   - EMAS Konstance, Germany, 2017
   - EMAS Bristol, UK, 2018
3. Organization by of a Mini-colloquium 'GN-MEBA : Caractérisation physico-chimique en MEB et microsonde ' during the 'Journées de la Matière Condensée', SFP, Grenoble, France, F. Brisset.

17- Electronic tools and products

Softwares
Databases
Tools for decision-making

18- Instruments and methodology

Prototypes

1. Participation to the development of an original method for distortion correction during an EBSD measurement (Method presented at the international congress ICOTOM18, St George, Utah, USA), F. Brisset.

Platforms and observatories

19- Other products

Artistic creations
Movie or theatre play creation
Movies

20- Editorial activities

Participation to journal editorial boards (books, collections)

1. *Book. EBSD : Analyse par diffraction des électrons rétrodiffusés - Applications et techniques couplées*, éd. F. Brisset, publ. EDP Sciences, ISBN : 978-2-7598-1912-6, 300 pages, 2015.
2. *Book. Microscopie Electronique à Balayage et Microanalyses*, éd. F. Brisset, publ. EDPsciences ISBN 978−2−7598−0082−7. 1050 pages, 2018, ré-édition complétée, in press.
3. Participation to the editorial process of congress proceedings on the occasion of four EMAS meetings, F. Brisset :
   - EMAS Porto, Portugal, 2013
   - EMAS Loeben, Austria, 2014
   - EMAS Portoroz, Slovenia, 2015
   - EMAS Marcoule, France, 2016

21- Peer reviewing activities

Reviewing of journal articles
Grant evaluation (public or charities)
Participation to lab site visit committees (Hceres etc.)

1. Member of the expert committee for the evaluation of the Laboratoire de Glycochimie des Antimicrobiens et des Agro-ressources – LG2A in Amiens, November 8-9, 2016, J.-P. Baltaze.

Participation to institutional committees and juries (CNRS, INSERM, etc.)

1. Concours interne CNRS pour l'accession au corps des Ingénieurs de Recherche de la BAP B, chairman of the jury, E. Rivière.
2. Concours externe CNRS, chairman of the jury for 1 IE position 'diffraction des RX', 2015, F. Brisset
3. Concours externe CNRS, chairman of the jury for 2 IE positions 'croissance de couches minces sous ultra-vide', 2016, F. Brisset
4. Concours externe CNRS, chairman of the jury for 1 IE position, 'Microscopie électronique', 2018, F. Brisset
5. Concours externe CNRS, member of the jury, for 2 AI positions, 'Techniques d'analyse chimique', 2016, J.-P. Baltaze

22- Academic research grants

European (ERC, H2020, etc.) and international (NSF, JSPS, NIH, World Bank, FAO, etc.) grants
National public grants (ANR, PHRC, FUI, INCA, etc.)

Local grants ("collectivités territoriales")

1. Sésame, Region île de France, ATOMA, participation to the funding of a MET LaB_6 200KV, F. Brisset, 2017

PIA (Labex, Equipex etc.) grants

1. Labex Charm3at, Participation to the funding of a single-crystal diffractometer, R. Guillot, 2014
2. Labex Charm3at, Projet ECH-RPE, (EPR-Electrochemistry coupling) C. Herrero, 2017
3. Labex Charm3at, ATOMA, Participation to the funding of a MET LaB_6 200KV, F. Brisset, 2017
4. Labex LaSIPS, ATOMA, Participation to the funding of a MET LaB_6 200KV, F. Brisset, 2017

Grants from foundations and charities (ARC, FMR, FRM, etc.)

23- Visiting senior scientists and post-doc

Post-docs

Visiting senior scientists

1. Dr. M. Bieda from Poland, two weeks, 2013, F. Brisset.
2. Dr. M. Miszczyk from Poland, two weeks, 2016, F. Brisset.
   Associated publication : *Microstructure and phase constitution in the bonding zone of explosively welded tantalum and stainless steel sheets*, H. Paul, M.M. Miszczyk, R.Chulist, M.Prażmowskib, J.Morgiel, A.Gałka, M.Faryna, F.Brisset, Materials and Design 153 (2018) 177–189, 10.1016/j.matdes.2018.05.014.
3. Pr. W. Bose from Brazil, two months, 2017, F. Brisset.
   Associated publication: *Advanced characterization of microstructural changes during recrystallization in aluminum alloy 6013*, IOP Conference Series Materials Science and Engineering 82(1), M Bieda, J Kawalko, F Brisset, K Sztwiertnia, 10.1088/1757-899X/82/1/012081.

24- Scientific recognition

Prizes
Distinctions
IUF members

Chair of learned and scientific societies

1. Member of the scientific council of EMAS (European Microbeam Analysis Society), F. Brisset
2. Chairman of the GN-MEBA (Groupement National de Microscopie Électronique à Balayage et de microAnalyses), F. Brisset.

Invitations to meetings and symposia (out of France)
Members' long-term visits abroad

II - INTERACTIONS WITH THE NON-ACADEMIC WORLD, IMPACTS ON ECONOMY, SOCIETY, CULTURE OR HEALTH

6- Socio-economic interactions / Patents

Invention disclosures
Filed patents
Accepted patents
Licenced patents

7- Socio-economic interactions

Industrial and R&D contracts
Cifre fellowships
Creation of labs with private-public partnerships
Networks and mixed units *(Science and technology only)*
Start-ups

8- Expertise

Consulting
Participation in expert committees (ANSES etc.)
Legal expertise

9- Expert and standardization reports

10- Public outreach

Radio broadcasts, TV shows, magazines
Journal articles, interviews, book edition, videos, etc.
Other popularization outputs
Debates on science and society

III - INVOLVEMENT IN TRAINING THROUGH RESEARCH

9- Educational outputs

Books
E-learning, MOOCs, multimedia lessons, etc.

10- For humanities only, published PhD theses

11- Quality of PhD student supervision

12- Students' follow up in association with doctoral schools

13- Participation to international training programs (e. g. Erasmus Mondus)

14- PhD student participation to scientific animation and unit/team life

15- Participation of team members in setting up Master courses