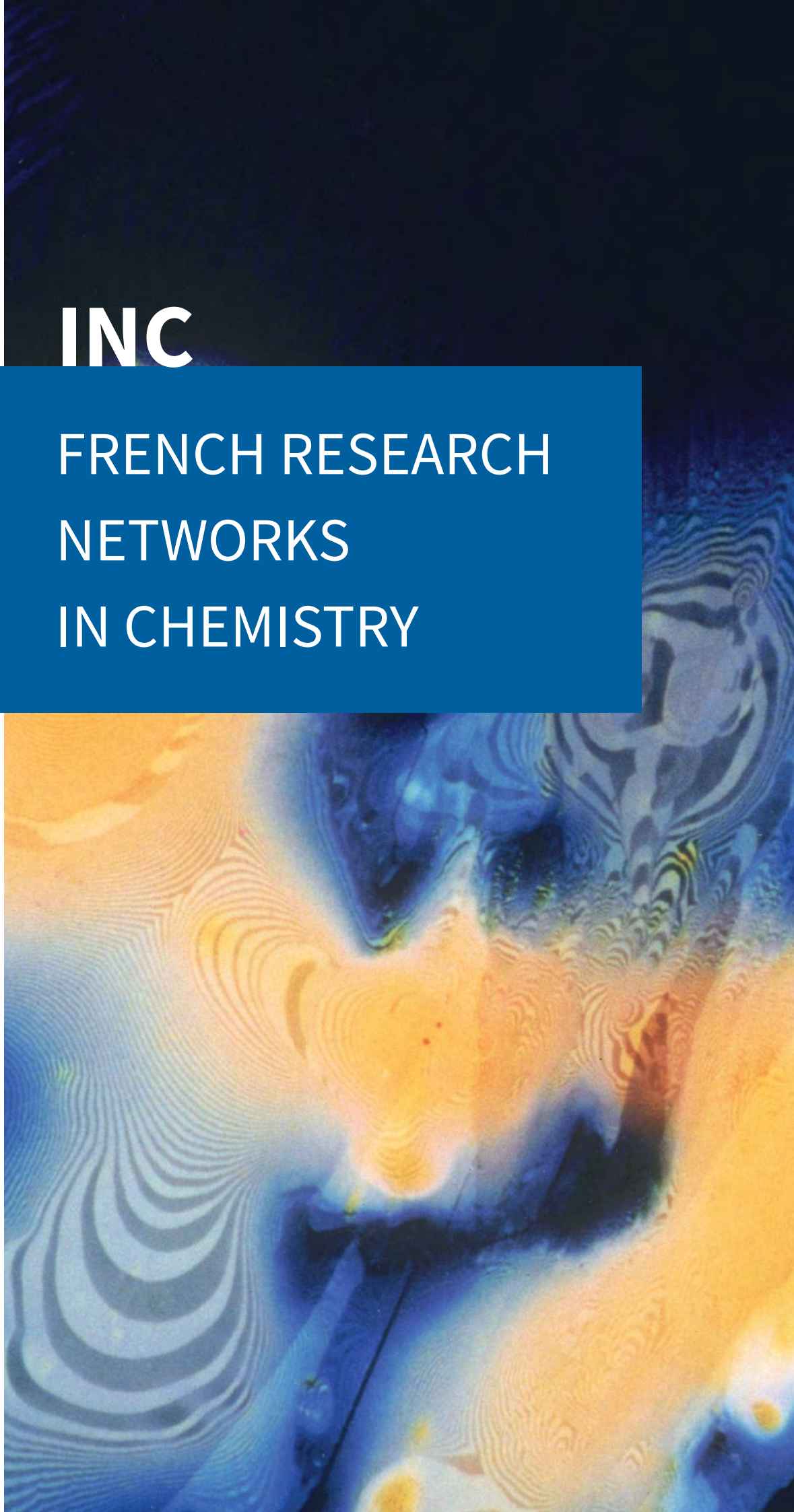
INC

FRENCH RESEARCH NETWORKS IN CHEMISTRY



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FRENCH RESEARCH NETWORKS IN CHEMISTRY
EDITION 2020

This booklet compiles the research groups led by the Institute of chemistry active in december 2020, the oldest of which were created in 2010.

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Editorial

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The CNRS French research networks in chemistry, called GDR for “groupement de recherche”, are unique structures in which different scientific communities share their own knowledge and join forces to make a well-defined field thrive. Interdisciplinarity and the resulting multi-scale approaches are the originality and strength of these networks. This specificity is important in a complex research environment with increasingly competitive national and / or European calls for projects. From this point of view, the GDR can become a powerful instrument for defining new scientific orientations, making new strategic choices and even, in the extreme, transforming new theoretical or practical knowledge into a scientific field in its own right.

Until now, the creation of GDRs has been proposed based on an upstream reflection initiated by a group of researchers and teacher-researchers who can be associated with other organizations, such as CEA, IFPEN, INSERM, INRIA ... The GDR framework then offers these research teams the opportunity to meet. Industry can also be a stakeholder if developments are likely to give rise to the enhancement and / or maturation of pre-industrial projects.

The analysis of motivations and objectives is carried out in consultation with the CNRS Institute of Chemistry, which entrusts the GDRs with three essential missions:

- Animation of a community that recognizes itself around a thematic area;
- Structuring and coordination of research activities;
- Scientific and foresight watch making it possible to monitor developments in the field in terms of results, new scientific challenges and societal issues.

The GDRs also fulfil a training mission. They are indeed a source of innovation, innovation that must spread to the communities concerned. They are also a place for sharing and transferring knowledge to the youngest researchers, doctoral students and postdoctoral fellows. The organization of thematic schools is therefore an essential point, which often falls within the framework of the continuing training policy implemented by the CNRS for all of its employees.

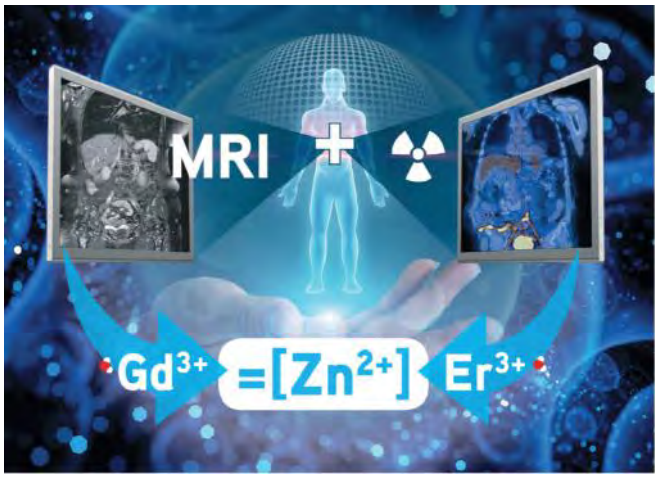
This booklet honors the 34 GDRs that the Institute of Chemistry is piloting. Each group presents its objectives and perspectives in a synthetic way. We hope that its dissemination will arouse the attention of many colleagues and encourage them to join a network related to their scientific activity, or even to propose new GDRs. In this case, they will ensure that their project is placed at the intersection of disciplinary fields and will have the ambition to develop a new activity there.

In short, the GDRs appear to us to be the place where tomorrow’s research axes are imagined, and the INC is happy to support those who invent and evaluate, for the French chemistry community, the fertility of the interfaces of tomorrow.

Jacques Maddaluno
Director of the CNRS Institute of Chemistry

GDR AIM
Molecular imaging agents

OBJECTIVES



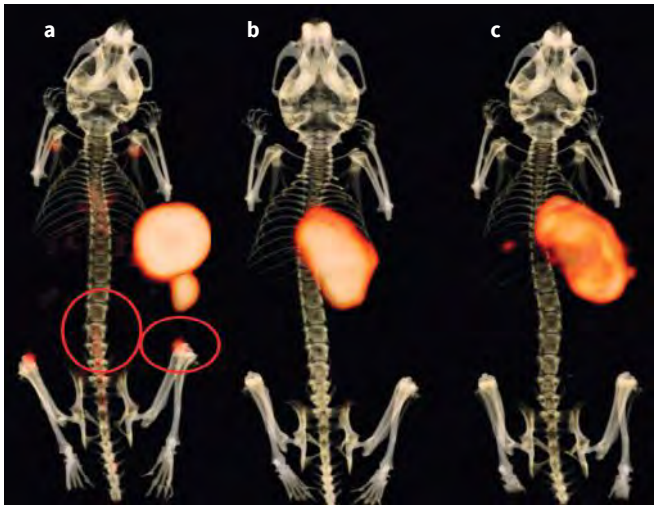
A cocktail of ^{165}Er(III) and Gd(III) complexes allows for quantifying zinc by combining SPECT and MRI.

The GDR gathers all French research groups working on the design and development of chemistry tools for imaging and their complementary expertise allows addressing current scientific challenges in the field.

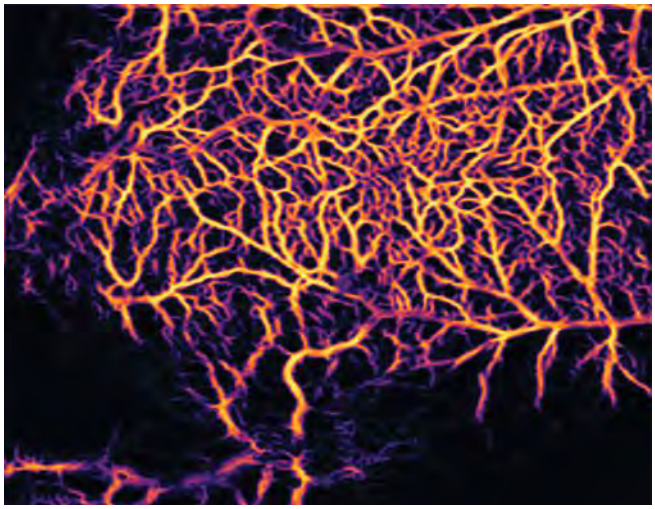
The objective is to develop innovative molecular probes for optical, nuclear or magnetic resonance imaging applications, as well as theranostic agents. These novel molecules will facilitate early diagnostics, help evaluate disease progression or treatment efficacy in clinical applications, and provide unprecedented investigation tools for biomedical research. The GDR promotes an interdisciplinary approach of imaging agent development between chemistry, biology and imaging sciences.

THEMATICS

- Optical agents
- MRI agents
- Nuclear imaging probes
- Targeting approaches
- Nanoparticle probes
- Multimodal and theranostic approaches



PET images of tumor-bearing mice injected with ^{89}Zr-DFO-trastuzumab (a), ^{89}Zr- DFOcyclo*-trastuzumab (b) and ^{89}Zr-DFO*-trastuzumab (c). New DFO* chelators prevent bone accumulation.



NIR image of a mouse (ventral side) following intravenous injection of indocyanine green, with a near-infrared detection window (1500-1700 nm); artificial intelligence is used for image treatment.

250 RESEARCHERS
INVOLVED IN
50 LABORATORIES

PROSPECTS

Molecular imaging aims the *in vivo* or *in vitro* detection of molecular events at the cellular level. Approaches that allow the visualization of molecular signatures of diseases represent a major progress for clinical diagnostics and provide a remarkable tool for biomedical research. Thanks to molecular imaging, the characterization and the non-invasive, repetitive visualization of gene expression, biological function or dysfunction, protein-protein interactions, signalling, etc. become possible in preclinical animal models of pathologies, as well as in patients. This new generation of imaging agents will enable detection of the molecular processes underlying the diseases, thus contributing to a better understanding of pathological phenomena.

As each molecular imaging procedure requires a specific probe, chemistry plays a central role in molecular imaging developments.

Multimodal imaging combines the advantages of various techniques, for example by associating functional information with morphological data. For some years now, theranostic approaches, combining molecular imaging and therapy, have led to a paradigm change and to the development of personalized medicine. Their objective is to image and to characterize *in vivo* the molecular profile of the disease, the delivery of drugs to the site of interest, or the efficacy of the treatment. Theranostics is often associated to nanomedicine, since nanoparticles can be relatively easily loaded with multiple imaging and therapeutic agents. In contrast, molecular theranostic probes can offer the advantage of easier characterization and controlled physicochemical properties. All these developments require an interdisciplinary vision where chemistry, physics, biology, medical sciences and imaging technology converge towards novel therapeutic solutions.

Although the GDR is centred on chemistry, we promote a fully pluridisciplinary approach which is the unique way to succeed in the optimization of radiotracers, MRI or optical probes and their translation to realistic applications. Via interactions between GDR research groups and including also industrial partners, the chemists of the GDR AIM network will develop innovative synthetic, bioconjugation and coordination chemistry methodologies and create novel imaging probes of higher efficacy and specificity to aid biomedical research and clinical medicine.

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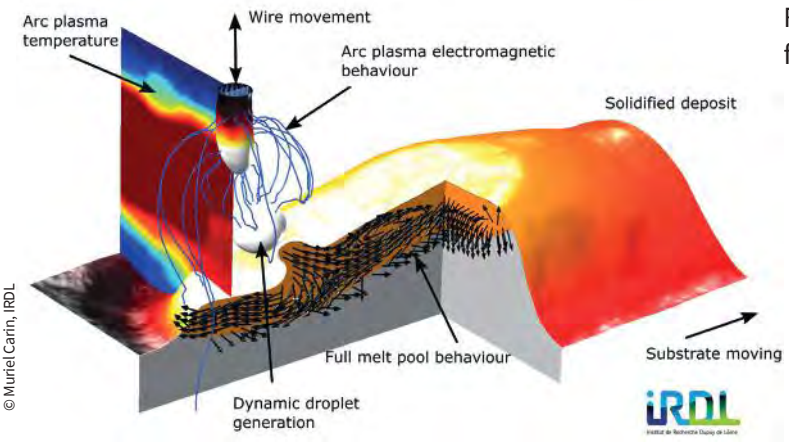
cnrs GDR Groupement de recherche
AIM Molecular imaging agents

GDR ALMA

Metallic alloys by/for additive manufacturing

OBJECTIVES



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3D multiphysics modeling of the WAAM process.

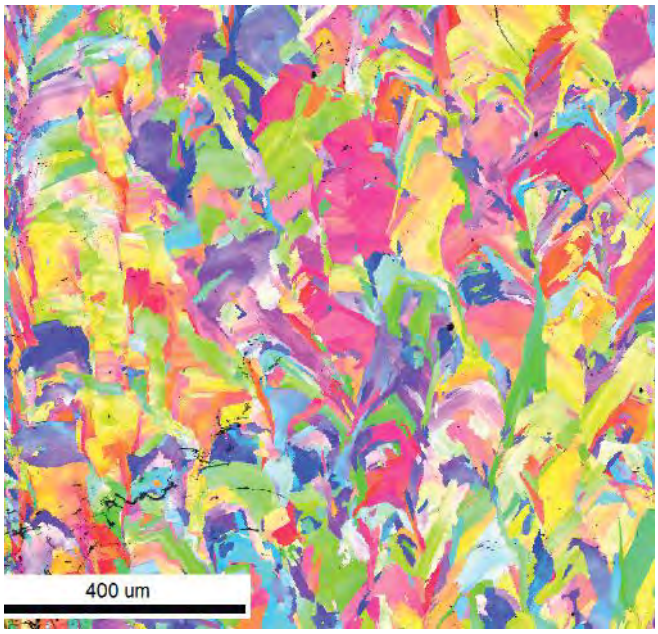
The ambition of the GDR ALMA is to bring together French scientists around fundamental issues arising from Additive manufacturing (AM). It concerns the interactions between materials science, mechanics and process engineering. The main missions of the GDR are as follows:

– bring out innovative and transversal projects at the frontiers of the conventional properties of metal alloys;

– identify and organize experimental platforms by promoting academic research;

– train young researchers in materials science, mechanics and process engineering and

– contribute to efforts to revitalize metallurgy and its professional opportunities.

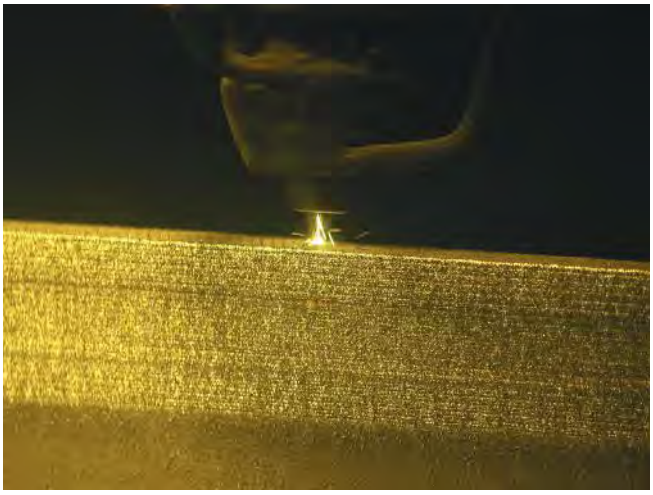


© François Brisset de l'ICMMO, Orsay

Microstructure of a SLM-built nickel-based superalloy.

THEMATICS

- Energy-matter interactions
- Materials for AM
- Materials obtained by AM
- Mechanical properties
- Physicochemical properties
- Characterization / modeling / training



© Thierry Malot, PIMM-AMValor, Paris

3D manufacturing of a Titanium alloy with the Laser Metal Deposition technique.

245 RESEARCHERS
INVOLVED IN
34 LABORATORIES

PROSPECTS

The mission of the GDR ALMA is to structure the scientific community interested with AM of metal alloys in France. The ambition is to bring together national scientists around academic research on subjects targeted around major scientific issues. This synergy, these exchanges and these collaborations initiated at the national level through the activities of the GDR should ultimately contribute to the visibility of research teams at the international level. The work of the GDR focuses on the properties of materials for additive manufacturing and on the properties of alloys obtained by AM. This manufacturing method should make it possible to imagine a new metallurgy, based on the behavior of non-equilibrium alloys and gradient alloys (composition, microstructure, properties).

The work of the GDR ALMA covers both elementary physical mechanisms, the materials used and the final properties of metallic parts.

PHYSICAL MECHANISMS

In the various processes involved, a high energy source (electric arc, laser, electron beam) is used to melt materials in the form of powder or wire, and structure a 3D part by accumulation of solidified layers. If the physics of these processes seems mastered, many scientific fields remain poorly understood.

MATERIALS

The GDR must allow the emergence of families of metallic alloys identified for their original structural or functional properties. In addition, the manufacture of metal powders with optimized properties (specific particle size with low dispersion, purity of alloys, oxidation of powders, flowability, spreadability) remains a challenge due to their large specific surface area and their affinity for oxygen.

PROPERTIES

AM parts require specificities in terms of mechanical strength, post-process heat treatments and surface properties. However, many properties remain little studied or poorly understood: plasticity mechanisms, role of metallurgical defects, properties of functional surfaces, electrical and magnetic properties, degradation and wear.

Finally, this GDR will also allow:
– the establishment of comparative studies and benchmarks;
– the organization of French platforms dedicated to metallic AM;
– academic training, for instance the establishment of summer schools;
– the emergence of collaborative projects in the frame of national or European calls for proposal and
– support for the development of new parametric machines assisted by design.

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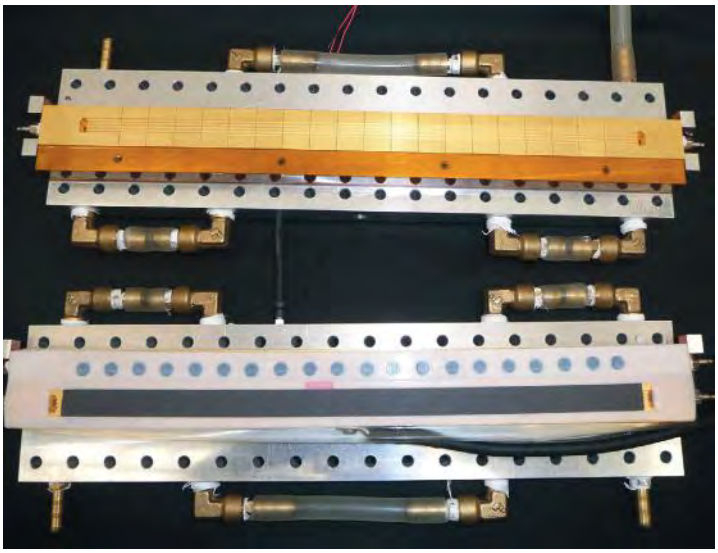
cnrs GDR Groupement de recherche
ALMA metallic alloys by/for additive manufacturing

GDR REDOXFLOW
Redox flow batteries

OBJECTIVES

The RedoxFlow research group aims at bringing together a large community of academic and industrial experts who can coordinate their research actions on redox-flow batteries, from fundamental research to problems related to their industrialization. Our objective is to create synergy and emulation effects to promote new competitive solutions for the storage of renewable energies.

The GDR organized in 2019 a first thematic school on redox-flow technology, and in 2020 a first European congress on redox-flow batteries, with the aim of perpetuating it and extending to the European scale this work of structuring and critical analysis of this field of research for the storage of renewable energies.



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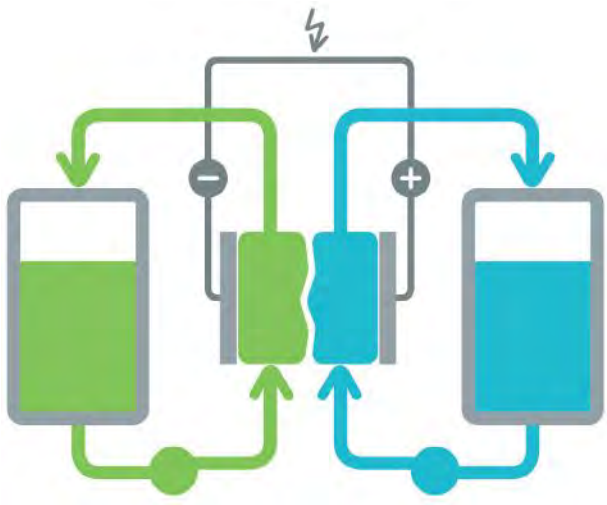
Segmented cell developed.



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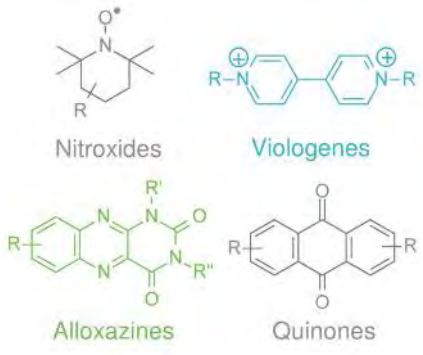
Schematic representation of a redox flow battery.

THEMATICS

- New soluble electrolytes
- Redox targeting and suspensions
- Materials
- System and modelization
- standardization et applications



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Families of organic molecules for electrolytes.

100 RESEARCHERS
INVOLVED IN 20 LABORATORIES
AND COMPANIES

PROSPECTS

Redox flow technologies have been studied for over fifty years. Today's most mature technology, the all-vanadium battery, still suffers from a lack of competitiveness to become a leader in renewable energy storage. A major challenge is the cost of the electrolyte, and of certain materials such as the ion exchange membrane. In addition, the energy and power densities of redox flow systems remain modest. Research must be oriented towards the discovery and optimization of new low-cost electrolytes, high-performance and competitive materials, and a better understanding and management of these systems in which material, electron and heat flows must be optimized to achieve the best performance and longest life.

Several actions are identified:

CONFRONTING THE CHALLENGES POSED BY THE DEVELOPMENT OF NEW ELECTROLYTES for redox flow batteries: synthesis of new molecules, optimization of synthesis processes to reduce the cost and environmental impact of the molecules, study of the electrochemical properties, stability and formulation of electrolytes. This includes theoretical studies and methodological developments to better understand the behaviour of molecules at high concentrations.

INCREASING ENERGY DENSITY through systems based on the use of suspensions or solid materials interacting with flowing electrolytes. Two technologies are treated: the approach with electrochemical mediators (redox-targeting/solid boosters) comprises a circulating liquid electrolyte together with insertion materials in tanks, the semi-solid approach for which an electroactive solid suspension is suspended under flow. Theoretical and technological aspects are also included here.

OPTIMIZING THE MATERIALS to exceed current battery limits in terms of efficiency, power density and cost. This includes polymeric membranes or porous separators, porous electrode materials, bipolar plates, gaskets or solid electrolyte materials. It also includes studies on corrosion and aging of materials during battery operation.

DIMENSION AND OPTIMIZE THE REDOX FLOW BATTERY as an electrochemical system through engineering and modeling approaches. This includes the optimization of electrolyte flows in volume and time, minimization of leakage currents, reduction of different resistance phenomena, heat exchanges and optimization of the BMS (battery monitoring system).
Finally, to evaluate innovations in the field of redox flow batteries by applying relevant standard tests that will achieve a consensus for the community. The envisaged applications must be defined in terms of service for the power grid with the aim of defining realistic cost objectives for the emergence of redox flow technologies in a competitive market.

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https://gdr-redoxflow.cnrs.fr

cnrs GDR Groupement de recherche
REDOXFLOW Redox flow batteries

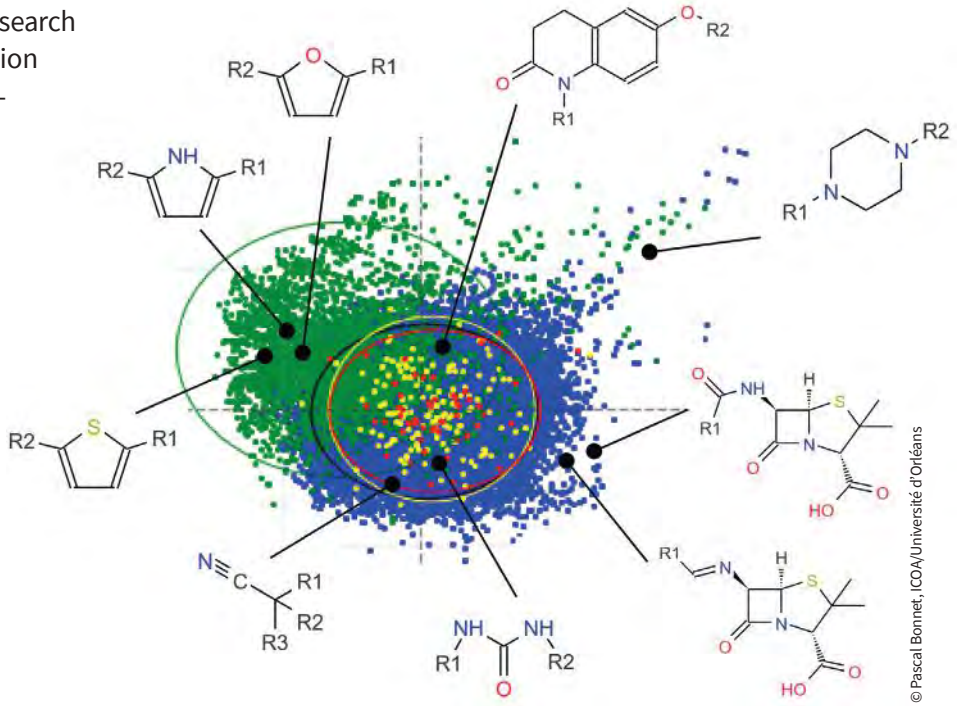
GDR BIGDATACHIM

Big data in chemistry

OBJECTIVES

The mission of the GDR BigDataChim is to promote and animate interdisciplinary research activities in cheminformatics. The main goals are research and structuration of chemical information to establish correlations between chemical structure and properties.

The GDR BigDataChim is composed of working groups representative of themes such as quantum chemistry, molecular simulations, chemical reactivity or rational molecule design. A significant component of this GDR is also devoted to studying the interactions between molecules and living organisms.



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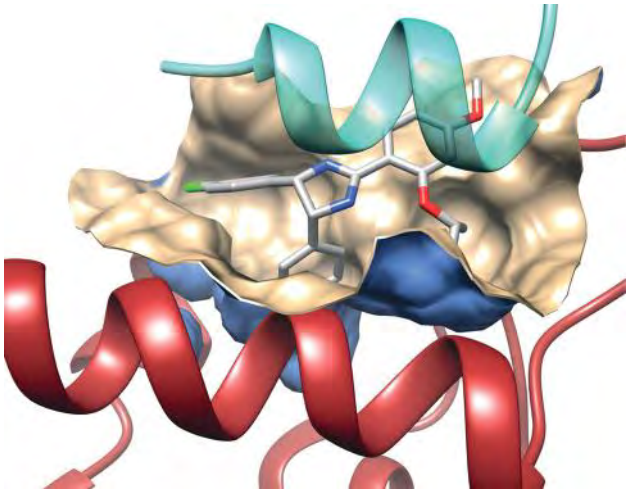
Explore the chemical space.



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Predict molecular interactions.

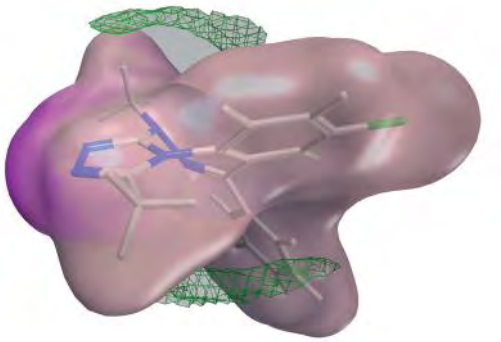
THEMATICS

- Databases
- Development of methods for data acquisition, processing and analysis in order to rationalize, simulate and predict the properties of molecules
- Modeling and prediction of biological activities

90 RESEARCHERS
INVOLVED IN
29 LABORATORIES

PROSPECTS

The GDR BigDataChim is intended to create a dynamic environment favorable to the use of massive data in chemical sciences. Cheminformatics is at the crossroads of multiple disciplines in chemistry, computer science, statistics, biology, physics, with the molecule as the object of study. As an example of the organization of data in chemical sciences, the “Chemical Abstracts”, appeared more than a century ago, while databases in biology appeared in the early 1980s. The advent of various “omics” techniques in biology (genomic, proteomic, metabolomic) accelerate the generation of megadata, massive data that are also called “Big Data”. The last is a recent term that covers different aspects related to mass data: collection, storage, sharing, mining, analysis, prediction and visualization. Big Data poses new challenges in all of these components.



Estimate properties.

Cheminformatics is interested in fundamental questions such as the development of molecular descriptors, force fields in molecular mechanics, machine learning methods or virtual reality tools, but it is also at the origin of many applications, as for example, the rational design of “green” solvents, complexing agents and chemicals to extract radionuclides, the development of new molecules that make up flavors and fragrances, and the predictions of the chemical reactivity including the development of high-performance algorithms dedicated to retrosynthesis and based on learning methods and on artificial intelligence. New predictive methods for bio-profiling chemical compounds are also expected to alert on potential side effects such as toxicity and ecotoxicity but also as an alternative to the use of animals in the laboratory to assess the chemical risks of molecules.

A feature of cheminformatics, whether for French or foreign research groups, is the small size of the majority of these teams, which are often a component of much larger research units. This GDR reinforces the research efforts of its participants through actions such as the organization of seminars in association with the French Society on Cheminformatics (SFCi, Société Française de Chémoinformatique), the setting up of high level training courses (Strasbourg summer school in cheminformatics), or the setting up of hackathons dedicated to the design and sharing of innovative methods and tools.

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gdr-bigdatachim.cn.cnrs.fr/web/accueil

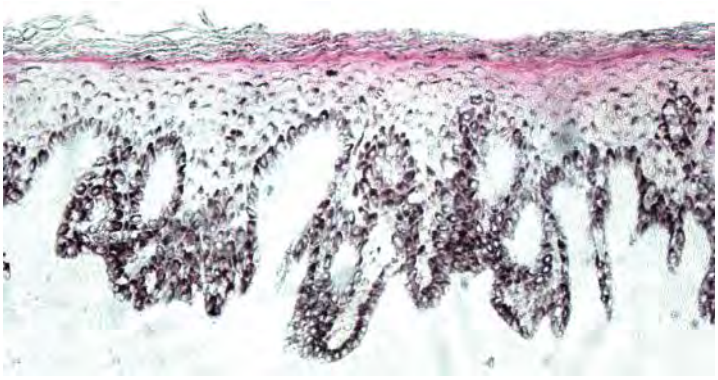
cnrs GDR Groupement de recherche
BigDataChim Big data in chemistry

GDR COSM'ACTIFS
Bioactive & cosmetics

OBJECTIVES

The main mission of the GDR COSM'ACTIFS is to promote the advancement of knowledge in "cosmetics" themes related to face and body skincare with various properties (moisturizing, firming, slimming, depigmenting, anti-stain, anti-wrinkle, anti-aging, sun protection, grassy skin…).

The scope of the GDR has been defined to respond more specifically to the following scientific challenges: innovation in active ingredients and ingredients on the basis of sustainable development of biodiversity; innovation in formulation and vectorization; innovation in new biological and technological tools at the service of a better knowledge of healthy skin.



An action on the skin.

THEMATICS

- Sourcing: bioactives / ingredients
- Formulation and vectorization
- Targets and biological models
- Safety and conservation

Bioproduction of actives.

250 RESEARCHERS
INVOLVED IN
48 LABORATORIES

PROSPECTS

After an initial period of 4 years, where the main mission was to unite the teams and give them visibility, we must now go further in the initiated dynamics. The following expectations emerged from events organized in recent years (round table during national days, industrial survey):

– academic needs: mutual knowledge, industrial support for experiments, identification of industrial needs and
– industrial needs: knowledge of teams, having contact points, technology watch, experiments.

Skin explants.

The presence of representatives of industrial partners will therefore be encouraged and expected during this renewal. The GDR will propose the creation of an Industrial Partners Club to carry out actions promoting exchanges between these two worlds and thus meet their expectations. By joining this club, industrial partners will be able to establish a privileged dialogue with research teams, monitor scientific issues and technology transfer, participate in setting up projects to respond to calls for tenders, acquire and share technical skills, establish a privileged relationship with graduates trained in research laboratories in modern and innovative technologies: specialized masters, young doctors and doctor-engineers or even post-docs who constitute more experienced researchers.

Particular effort will also be placed on the development of research themes transversal to the 4 axes of GDR and more particularly concerning the development of multifunctional cosmetic ingredients, sustainable processes and skin microbiota / cosmetics and environment interactions. This will allow us to respond competitively to national (ANR) or European calls for tender through an academic or mixed academic / industrial consortium.

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cnrs GDR Groupement de recherche
COSM'ACTIFS Bioactive & cosmetics

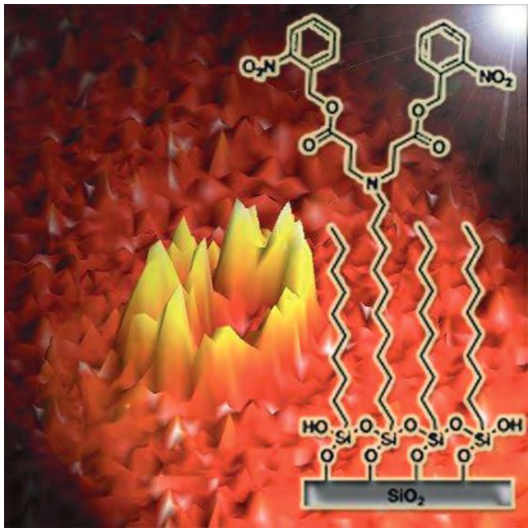
GDR B2i
Bioengineering of interfaces

OBJECTIVES

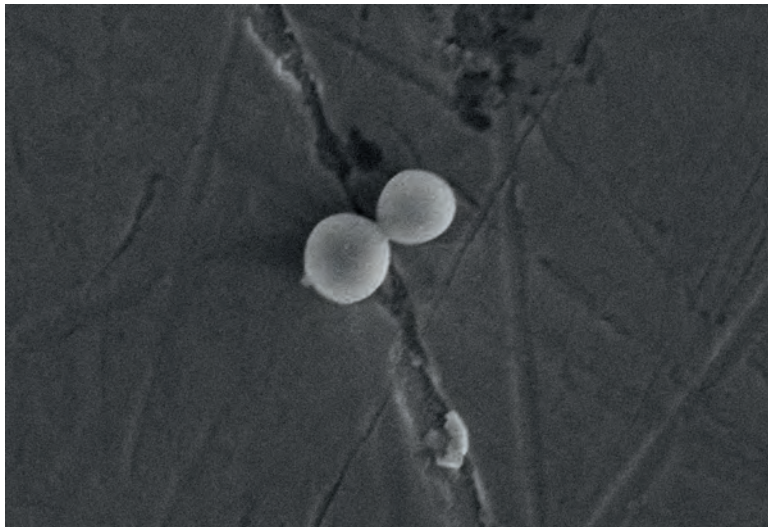
The mission of the GDR B2i is to federate the French and French-speaking European communities around a multidisciplinary theme whose research activities focus on biointerfaces.

The purpose of the GDR B2i is to encourage synergies between the different disciplines in order to allow the emergence of innovative and transversal projects. Faced with current public health challenges, medical devices (biomaterials, implantable devices), biochips, Lab-on-a-chips, biosensors and nanomaterials are used in a wide range of applications ranging from medical to environmental analysis through food control (dosage of GMOs, mycotoxins, pathogens, etc.).

The bioengineering of interfaces therefore aims to control the physical, chemical and biochemical properties at the interfaces of materials in order to control their stealth and specificity.



Engineering of mixed SAMs on SiO_2



***Staphylococcus aureus* (golden staphylococcus) @ titanium surface.**

THEMATICS

- Development of complex biointerfaces: functionalization, printing and nano-structuring
- Characterization of biointerfaces, opportunities and perspectives: towards *operando* characterizations and *in silico* calculations
- Biointerfaces at the heart of medical devices
- Transversal action: a major issue: microorganism / surface interactions

Titanium #Total hip prothesis.

200 RESEARCHERS
INVOLVED IN
50 LABORATORIES

PROSPECTS

The multidisciplinarity and transversality of biointerface research are clearly highlighted when considering the fields of research of GDR B2i teams.

From a scientific point of view, the actions of GDR B2i have highlighted new directions but also new needs both in the development and in characterization of biointerfaces. Thus, the scientific axes have seen their scope redrawn by the arrival of new teams, but also with the creation of a new transversal axis targeting the wanted or unwanted interactions between microorganisms and interfaces.
Thus, new ways of functionalization and development of complex interfaces are investigated with the contribution of nanostructured architectures in 3 or 4 dimensions but also with more selective and multiple functionalizations. *In situ* and / or *operando* characterizations, but also the coupling of spectroscopic and microscopic techniques, are highlighted while emphasizing *in silico* calculations aspects. New directions towards the field of biomedicine are undertaken, with applications in the field of on-board sensors and miniaturized devices; we also note the emergence of the application for diagnosis and therapy of the use of nanoparticles. Finally, a major issue, which is the interaction between various microorganisms and surfaces, is now addressed; these interactions can be harmful as in the case of biofilm formation or desired in the context of the detection of pathogens or the use of microorganisms in the field of energy.

Finally the GDR B2i wishes to:

IMPROVE ITS EUROPEAN INFLUENCE, in particular with the integration of French-speaking European laboratories providing new skills both in characterization (with for example the JRC laboratory in Ispra in Italy), and in development and application (with the CSEM in Neuchâtel in Switzerland).

IMPROVE INTERACTIONS WITH INDUSTRIAL PARTNERS AND END-USERS with the creation of an "industrial club" but also the integration of laboratories from other institutions, namely CEA, INSERM, UGA, working on biomaterials, bioengineering and life sciences.

IMPROVE ITS NETWORK AND THE TRAINING OF YOUNG RESEARCHERS creating a club of doctoral and post-doctoral students who would allow them to take a more active part in the life of GDR B2i, to be a driving force for new actions and for the future to create at the end of the 10 years life of the GDR B2i. This club would also make it possible to set up networking for the future of young graduates and their integration into the world of research, both academic and industrial.

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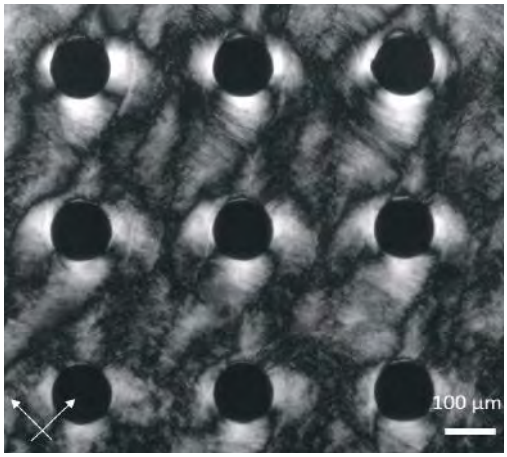
cnrs GDR Groupement de recherche
B2i Bioengineering of interfaces

GDR BIOMIM

Biomimicry and bioinspiration

OBJECTIVES

GDR BIOMIM was established by the Institute of Chemistry of CNRS in January 2020 to unite all French actors working in the field of bioinspiration and biomimicry. It brings together 92 research teams and laboratories with more than 700 researchers and doctoral students, from all over France and with different scientific backgrounds and specializations to address important scientific and societal challenges through solutions inspired by nature. It also aims at creating and promoting internationally a mapping of research activities and initiatives in France and become an innovation support for scientific institutions and public entities.



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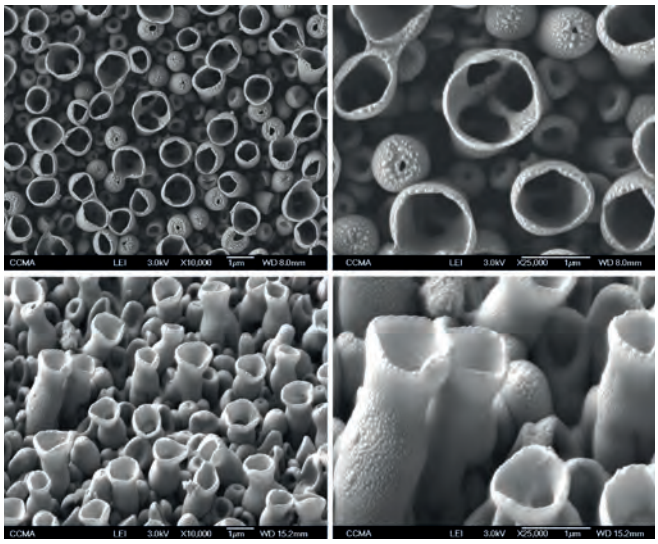
Structuring of collagen mesophases in a microstructured chamber mimicking compact bone.



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Design of a polyaromatic molecular object for its grafting by electropolymerization.

© P. Moretto, Univ. Toulouse

3D reconstruction of *Messor barbarus* obtained with a computerized micro-tomography scan.

THEMATICS

- Feel, experience, perceive
- Biomimetic transformation process
- Displacement, movement
- Structure
- Catalyst, catalytic process, energy and storage
- Bioinspired materials
- Biomaterials

699 RESEARCHERS
INVOLVED IN
92 LABORATORIES

PROSPECTS

FEEL, EXPERIENCE, PERCEIVE

Biosensors and labs-on-chip have great potential for new technologies, especially for health. The design and use of new materials or new detection systems based on biomimetic and / or bio-inspired approaches allow great progress to improve their performance.

BIOMIMETIC TRANSFORMATION PROCESSES

The chemical transformation processes in nature have been optimized and perfected in terms of energy and efficiency depending on the context. This combines the in-depth understanding of the mechanisms of these transformations at different scales (molecular, cellular, complex ecosystem) and the reproduction / engineering of these chemical processes.

DISPLACEMENT, MOVEMENT

The ambition of this axis is to organize a network of laboratories involved in the study of displacement and movement. The research is concerned with understanding mechanisms that make it possible to migrate, flee and conceal or pursue and catch, and finally to move alone or in perfectly coordinated groups. They inspire models and prototypes of sensors, actuators, poly-articulated systems and “hard or soft” robots.

STRUCTURE

Interdisciplinary scientific problems will be addressed through the structural analysis of organized biomimetic systems, hierarchical topologies and tissues, lipid membranes organized in related structures and tunable nano-porous surfaces of superhydrophobic nature. Multi-compartmentalized nanostructures sensitive to biological, chemical and / or physical stimuli will be inspired by organelles and other structures of cell compartmentalization and developed by spontaneous assembly of (bio) molecules.

CATALYST, CATALYTIC PROCESS, ENERGY AND STORAGE

This axis mainly focuses on catalysts, catalytic processes such as enzymatic proteins and bioinspired energy sources such as photosynthesis and energy storage such as biofuel cells.

BIO-INSPIRED MATERIALS

The central challenge is to decipher the structures and mechanisms of biological development in order to best reproduce their main characteristics. Multidisciplinary approaches thus allow the development of biomimetic objects from the molecular scale to three-dimensional surfaces and materials. The field of applications concerns biomaterials, synthetic receptors, sensors, catalysis.

BIOMATERIALS

This axis focuses on biofilms, anti-bacterial substances, bio-contaminants, tissue engineering, bioinspired sensors, 3D bioprinting, drugs and bioinspired materials with therapeutic value.

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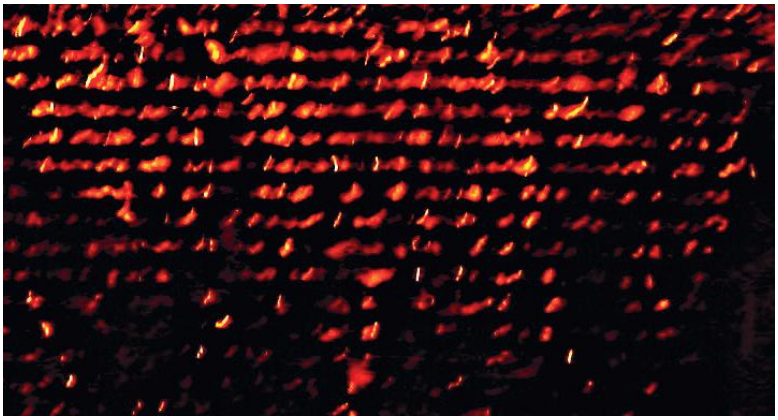
www.gdr-biomim.com

cnrs GDR Groupement de recherche
BIOMIM Biomimicry and bioinspiration

GDR CAVITATION

OBJECTIVES

The objectives of the GDR CAVITATION are to:
– promote the advancement of knowledge of chemical and physico-chemical reaction mechanisms under the effect of acoustic or hydrodynamic cavitation;
– broaden the potential applications of sonochemistry;
– strengthen the interaction between GDR member teams and
– increase the visibility of the French sonochemical community at the international scale



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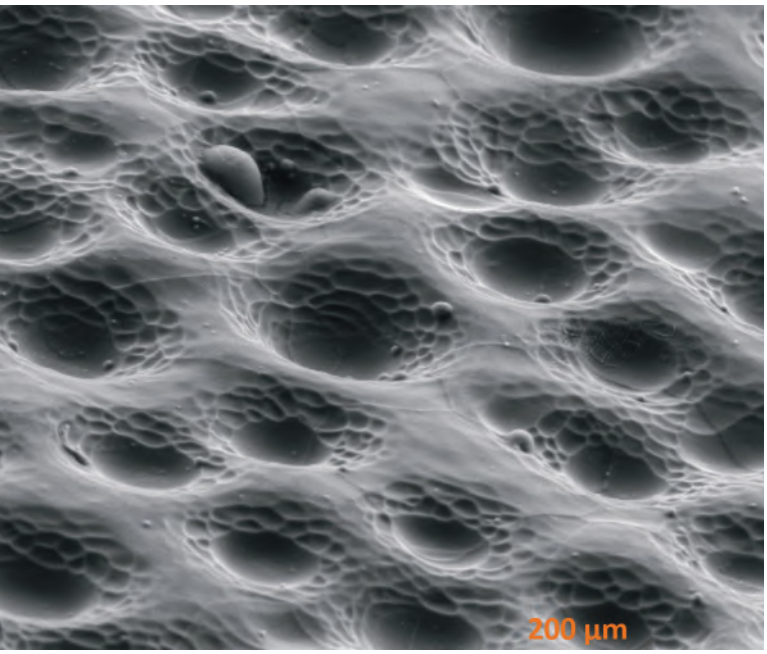
Cavitation bubbles in steady-state waves at 500 kHz.



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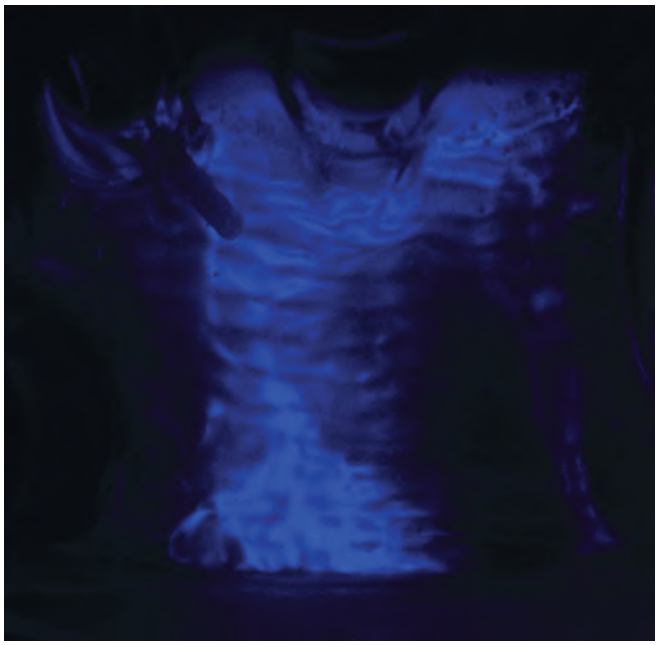
Magnesium surface after ultrasonic treatment.

THEMATICS

- Cavitation: theory and fundamental aspects
- Sonochemical treatment of effluents
- Materials and reactivity
- Valorization of natural products
- Medical applications
- Metrology and tools of measurement and characterization of reactors



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Sonochemiluminescence.

120 RESEARCHERS
INVOLVED IN
33 LABORATORIES

PROSPECTS

Power ultrasound is used in numerous processes, such as homogenization, disintegration, degassing, cleaning, food processing, and medical treatment. In addition, the acoustic cavitation produced by ultrasonic waves brings new solutions in the field of chemistry, allowing the improvement of selectivity and yields as well as the quality of the synthesized products. The chemical effects of ultrasound in liquid media originate from cavitation phenomenon, which is nucleation, growth and implosive collapse of microbubbles formed when a liquid is subjected to an ultrasonic wave. This violent implosion generates extreme conditions inside the bubbles which give rise to chemically active species without the addition of reagents to the medium. For this reason sonochemistry is considered as a part of green chemistry.

The mission of the GDR CAVITATION is to bring together the skills of specialists working in the various fields of cavitation and to define the priorities for scientific activity in the 6 directions of the GDR CAVITATION which are:
– fundamental sonochemistry (sonoluminescence, bubble dynamics, acoustic spectroscopy, modeling);
– sonochemical treatment of effluents;
– sonochemistry of materials (synthesis and reactivity;
– valorization of natural products using the phenomenon of cavitation;
– medical applications of cavitation and
– tools and methods for characterization of ultrasonic reactors.
The scientific perimeter of the GDR has been defined to encourage transdisciplinary exchanges; to strengthen the links between scientific and industrial teams on a national scale; to support the scientific projects of young researchers; to promote the emergence of research projects on a national and international level.

Sonochemistry is an emerging science that is developing quite rapidly around the world. Currently, the world scientific community of sonochemists is structured by two international societies: “European Society of Sonochemistry (ESS)” and “Asia-Oceania Sonochemical Society (AOSS)”. The French sonochemical community is already strongly present in both societies. The objective of GDR CAVITATION is to give even more international visibility to the French research in the field of cavitation through the organization of meetings and the support of international scientific exchanges.

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cnrs GDR Groupement de recherche CAVITATION

GDR CHIRAFUN

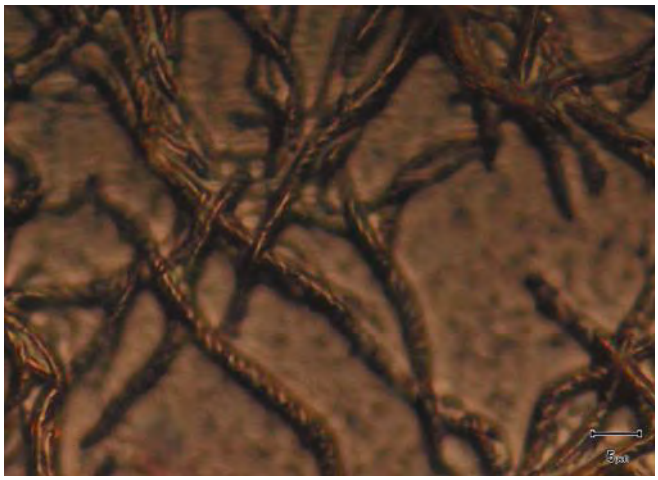
Chirality and multi-functionality

OBJECTIVES

The main goals of the GDR CHIRAFUN are:

– The development of chiral molecular and supramolecular systems.
Chirality will be used both as a structuring tool and as a mean to endow the system with new properties. This will lead to the rational design of a wide portfolio of innovative systems in various fields such as chiral emissive materials, chiral conductors, magnetic or biomimetic materials, polymers, nanoparticles, etc.

– The study of structural and chiroptical properties of simple or complex chiral systems.
These studies aim at establishing new knowledge in chemistry, physical chemistry, and in fundamental physics. They will contribute to the development of advanced experimental and theoretical techniques for the analysis of chiral systems.



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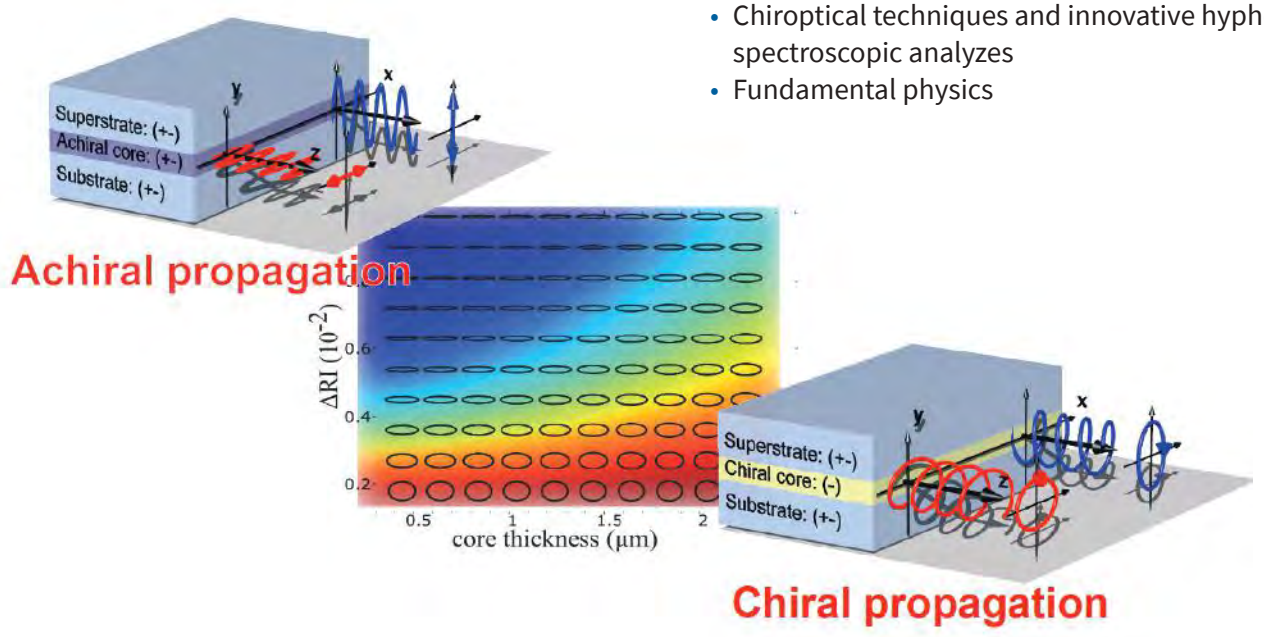
Optical microscopy image of electroactive homochiral supramolecular fibers of a tris(tetrathiafulvalene) derivative.

THEMATICS

- Chiral molecular materials
- Biomimetic systems and chiral supramolecular assemblies
- Chiroptical techniques and innovative hyphenated spectroscopic analyzes
- Fundamental physics

First chiral planar waveguide capable of propagating circular polarizations.



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108 RESEARCHERS
INVOLVED IN
29 LABORATORIES

PROSPECTS

Chirality is an intrinsic property of matter; it is the property of certain three-dimensional objects of not being superimposable to their mirror image. This left-right asymmetry is ubiquitous, from elementary particles, to life-related molecules. Chirality is essential for the proper functions and growth of living systems. It determines the properties of synthetic or natural bioactive molecules, such as active ingredients, odorants, etc. Chirality is a signature of life on earth, but not only. It also has strong implications in fundamental physics and chemistry. Although the fundamental principles associated with chirality are now well established, many phenomena deserve further studies in various fields of research.

Recent significant advances have been made in the field of chiral molecular materials. New concepts currently emerge in opto-electronics, due to the role of chirality in the interaction between matter and light, charges, and magnetic fields. The growing interest of chemists for a wide variety of multifunctional molecular materials (polymers, systems for linear and non-linear optics, electroactive systems, emissive materials, conductors, magnets, nanoparticles, etc.) has given the impetus for numerous studies that shed light on the significant role of chirality in many research fields and their applications.

Chirality is at the heart of biomimetic systems and chiral supramolecular assemblies, their self-organization, recognition processes and their resulting functionality (such as supramolecular catalysis).

The study of these new chiral systems requires the development of unprecedented analytical chemistry and separation techniques such as those based on chromatography or spectroscopy. Chiroptical techniques (circular dichroism, circularly polarized luminescence, Raman optical activity) and time-resolved spectroscopies are therefore closely related to the development of chiral systems and the determination of their structural properties.

Chirality is also a major concept in fundamental physics: origin of life, parity violation, magnetism and spin selectivity in chiral systems are today hot topics in physics and physical chemistry.

The synergy between the different research axes will be an effective means of maintaining and developing a common culture in the community of experimentalists and theoreticians in chemistry, physical chemistry, and physics. The GDR CHIRAFUN project has therefore a unique multidisciplinary character.

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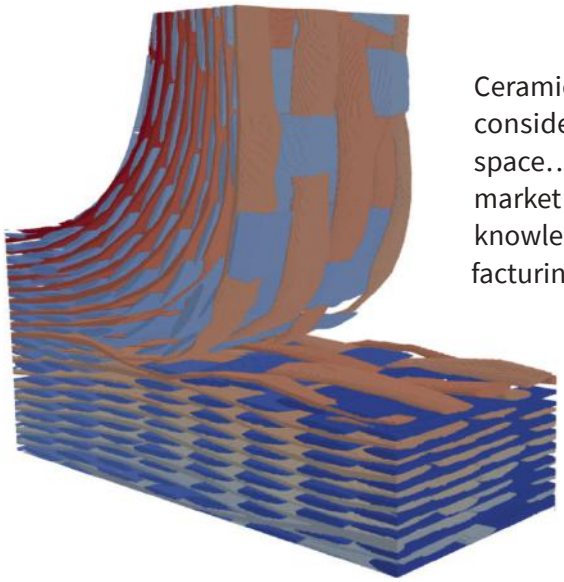
chirafun.sciencesconf.org

cnrs GDR Groupement de recherche
CHIRAFUN Chirality and multi-functionality

GDR (CMC)²

Ceramic-matrix composites: conception, modeling, characterization

OBJECTIVES



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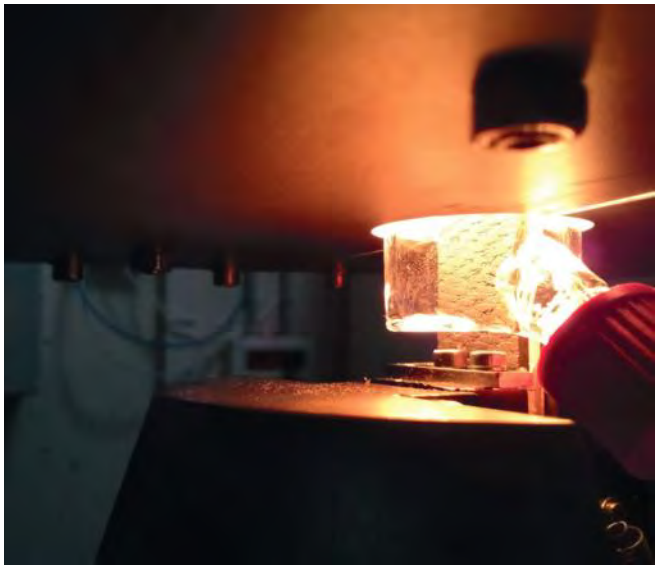
Segmentation of a woven CMC junction for mechanical analysis.

Ceramic-Matrix Composites (CMC) are very high-performance materials considered for very high-temperature applications: energy, transport, space… These materials, still seldom known, have a large potential for market breakup; however, this is only possible with a solid basic scientific knowledge. This research group is dedicated to the study of their manufacturing methods, their structure at all scales and their mechanical, thermal and chemical behavior, including the associated modeling efforts. Research of new applications, new formulations and the progression of knowledge on their behavior are the core activities of the group, which benefits from a strong support from industry and national agencies acting or willing to act in the domain.



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Mechanical testing of a CMC at 800°C under air.

THEMATICS

Towards cheaper, more innovative and easier to produce CMCs:

- Process physico-chemistry
- Process modeling
- Novel processing routes
- Innovative materials

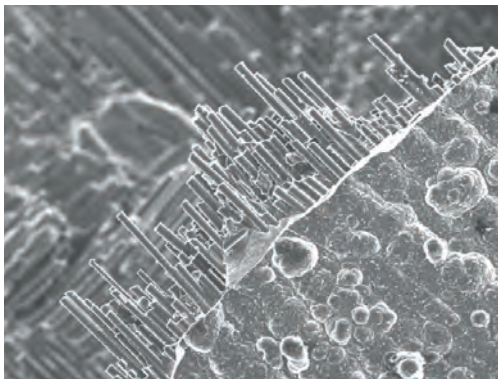
Towards a better certification and integration of CMCs:

- Structural characterization,
- Mechanical, thermal & environmental testing
- Design, modeling
- CMC integration in systems

165 RESEARCHERS
INVOLVED IN
24 LABORATORIES

PROSPECTS

The first axis of the research addresses all aspects of CMC manufacturing and features the following general directions:
– Acquire a better knowledge of the physico-chemistry (broadly speaking) of the manufacturing processes.
– Set up adequate process modeling tools in order to identify optimal parameters.
– Explore new processing routes, in order to reduce costs of existing materials and to create new ones.
– Lastly, imagine new materials looking for novel chemical compositions or novel processes. The industrialization capability of a process has to be considered very early in the “from Lab to Fab” roadmap.



Failure surface of a SIC / SiC composite.

The second axis of the research is the knowledge of the structure and the performances of CMCs, inducing the production of behavior models allowing their optimization and design, as well as on the integration of CMCs in structures. The main directions are:
– a better knowledge of the multi-scale structure of CMCs through the use of multiple characterization tools;
– a better knowledge of the behavior of CMCs under stress and heat flux in aggressive environment, through environmental, mechanical and thermal tests;
– high-fidelity models to describe the behavior of CMCs, and rationalize the design of parts made of such materials and
– a better integration of CMC parts in systems thanks to adequate joining and assembly techniques.

The GDR activity includes workshops, workgroup meetings, scientific colloquia and pedagogical actions. The endeavor of the GDR is to stimulate exchange between research unit members and with industry. Indeed, a strong demand for innovation and increased knowledge arises from national agencies and industrial groups who use or may use CMCs in their applications – some of which are strategic at the national level – and who bring a very strong support to the GDR. Moreover, the French CMC community can strengthen its international visibility with this GDR, in particular towards other leading countries of the domain (Germany, Italy, UK, USA, Japan, China…).

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http://www.gdr-cmc2.cnrs.fr

cnrs GDR Groupement de recherche
(CMC)² Ceramic-matrix composites: conception, modeling, characterization

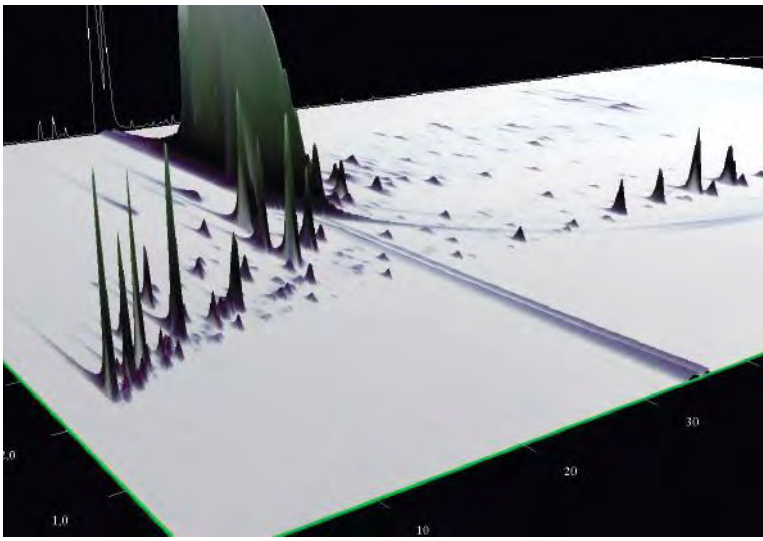
GDR THERMOBIO

Thermochemical conversion of biomass and wastes

OBJECTIVES

The main mission of THERMOBIO GDR is to promote the exchange of knowledge in the field of biomass valorization by thermochemical processes and to federate French researchers involved in this vast and interdisciplinary topic. The scientific perimeter is structured in such a way to respond to main scientific challenges: to better understand the available resource, to innovate with new thermochemical conversion processes, to improve the analysis of conversion products, to model the systems, to define the most appropriate channels that meet economical and environmental criteria.

The GDR's objective is to federate all researchers in this field beyond institutional divisions and to promote new collaborations (ANR and Europe).



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3D view of GCXGC analysis of a lignin bio-oil.

© LRGP Nancy

Gasification pilot.

THEMATICS

- Resource and diversity
- Mechanisms: towards a better understanding of the reactions
- Reactors and processes for biomass conversion
- The multi-scale approach: from molecules to reactors and processes

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Lignocellulosic and algal biomasses.

90 RESEARCHERS
INVOLVED IN
35 LABORATORIES

PROSPECTS

Today, biomass and biomass wastes represent sustainable available resources for the production of chemicals, fuels, additives and materials. Their valorization meets a strong international desire to save resources, to control energy consumption and to fight climate change. The valorization of biomass requires the development of new processes, new catalysts, new reactors and more efficient characterization methods. Indeed, these must be adapted to new systems / fractions that are often very complex and also require the development of modeling methods. At the international level, the valorization of biomass is experiencing a very strong revival of interest in terms of scientific work and the development of demonstrators. All industrial groups are showing a strong interest in bio-resources and some are already offering bio-products on the market, although most industrial projects are still in the research and development phase. The ambitious objectives announced cover many areas such as: bio-fuels, biogas, production of synthons for the chemical industry, production of bio-materials, etc.

The existence of major French projects such as BioTfuel, Futurol, GAYA and Biogreen and many other international projects attest the interest of these sectors.

We have defined four axes that cover the main aspects of researches conducted in this field.

RESOURCE AND ITS DIVERSTY

The actors of the resource will be involved to shed light on available resources and potential applications based on their composition.

REACTION MECHANISMS

In order to define the appropriate channels and improve processes, it is essential to understand the reaction mechanisms that produce complex feedstock such as liquids from biomass (or wastes).
In this axis, modeling tools, model reactions and analysis techniques are discussed among the GDR members.

REACTORS AND PROCESSES FOR BIOMASS CONVERSION

This axis is dedicated to reactors for biomass conversion, and their global integration in the process (reactor / purification synergy), to ultimately develop viable and innovative industrial processes.

MULTISCALE APPROACH: FROM MOLECULES TO REACTORS AND PROCESSES

The challenge is to couple studies on different scales: to include studies on a molecular scale (kinetics, mechanism) in reactor models, to include reactor models in process and process chain models, to use these process chain models to conduct environmental and economical analyses on a regional or even global scale.

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cnrs GDR Groupement de recherche
THERMOBIO Thermochemical conversion of biomass and wastes

GDR CONCORD

Coupling mechanics oxidation diffusion

OBJECTIVES

The objective of the GDR COnCOrD is to establish a dialogue between French teams dealing with high temperature oxidation from different perspectives: chemical and mechanical, experimental approach and modeling. The idea is to motivate a multidisciplinary approach focusing more specifically on oxidation / mechanics coupling. The themes will focus on identifying, understanding and modeling the mechanisms involved in high temperature oxide growth on metallic alloys, with or without an external mechanical loading. Particular attention will be paid to multiscale aspects (spatial and temporal) and the tools required in this kind of study, on an experimental point of view, as well as on theoretical and numerical ones, and the combination between those approaches.

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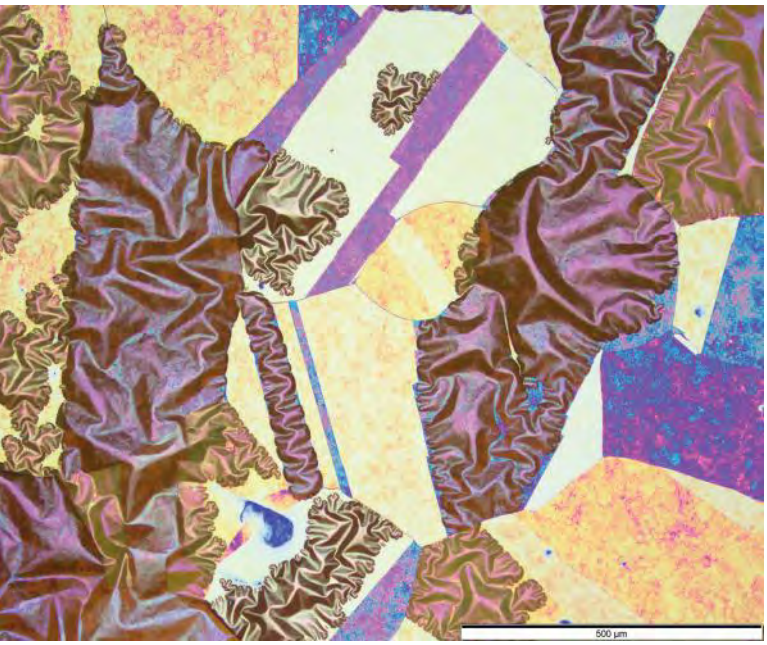
High temperature bending set-up.



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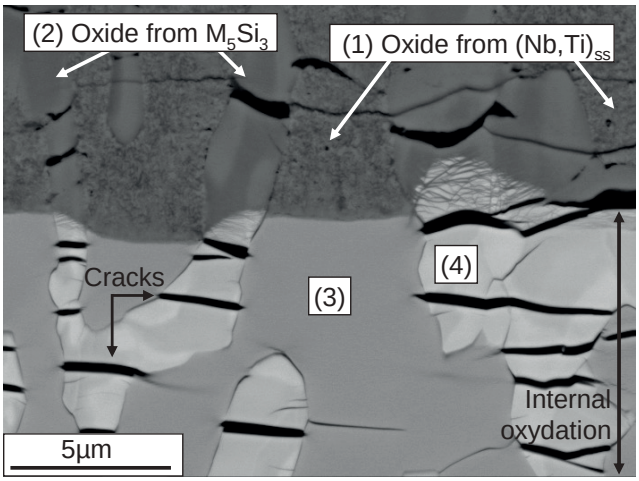
Oxidized surface of copper.

THEMATICS

- Oxidation with external mechanical loading
- Strain genesis during high temperature oxidation of metals
- Experimental measurements
- Modeling / simulation



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MASC type Niobium-based alloy oxidized 24h at 815°C in air. Mechanical fracture of silicide perpendicularly to oxygen flow.

67 RESEARCHERS
INVOLVED IN
15 LABORATORIES

PROSPECTS

OXIDATION WITH EXTERNAL MECHANICAL LOADING

This theme is dedicated to the chemical /physical / mechanical interactions between oxidation phenomena and external mechanical loading, whether applied prior to or concomitantly to oxidation:
– Identification of the influence of some parameters on the coupling between oxidation and mechanical loading through the analysis of existing studies in the community.
– Identification of physical mechanisms acting at the first order in the oxidation / mechanics coupling and attempt of plotting a map describing the oxidation behavior of various materials classes according to temperature and mechanical loading level.

STRAIN GENESIS DURING HIGH TEMPERATURE OXIDATION OF METALS

The aim of this theme is to identify the mechanisms involved in strain genesis and their interactions by:
– listing the potential sources and relaxation terms for each major thermal oxide / metal system and identify the multi-physical couplings that are really significant and
– comparing with experimental measurements and modeling in order to determine the dominant sources of strain according to instant t and spatial location (taking the microstructure into account).

EXPERIMENTAL MEASUREMENTS

Strain generated during thermal oxide growth can be measured at different scales thanks to a large panel of experimental techniques performed *ex-situ* or *in-situ*. The objectives of this theme is to optimize those techniques according to the system under study and the relevant scales, both temporal and spatial:
– optimization of experimental approaches in order to determine on strain / stress in oxide and metal;
– optimization of the investigation tools and methods to highlight diffusion / microstructure / mechanics couplings and
– quantify the critical parameters for damage initiation and their consequences on stress relaxation.

MODELING / SIMULATION

This theme aims to assess the existing theoretical and numerical tools that can contribute to a better analysis of the mechanisms acting in strain development during high temperature oxidation of metals through:
– state of the art of modeling and simulation approaches at a given scale in order to suggest paths towards multi-physics modeling and
– introduction of oxide scale adhesion properties in relation with the microstructure.

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cnrs GDR Groupement de recherche
COnCOrD Coupling mechanics oxidation diffusion

GDR HYDRATES
Gas hydrates

OBJECTIVES

The topic of gas hydrates crosses various disciplinary fields, ranging from astrophysics to geosciences, chemical engineering and molecular sciences. Long considered and examined mainly as an industrial nuisance (plugging of "hydrocarbon pipelines", instability of the ocean floor), these "nanoporous ices" now open up new application prospects (*e.g.* gas storage / separation / capture, secondary refrigeration, water purification, etc.) and new fundamental questions (formation mechanism, natural occurrence in the solar system, impact on planetary atmospheres and climates, etc.). Tackling these challenges requires concerted and multi-disciplinary actions, which are addressed by the GDR.

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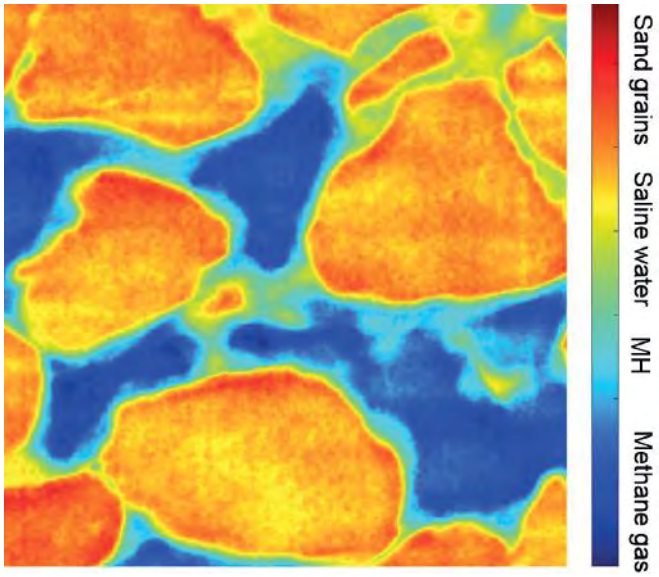
Do gas hydrates occur elsewhere than on Earth?



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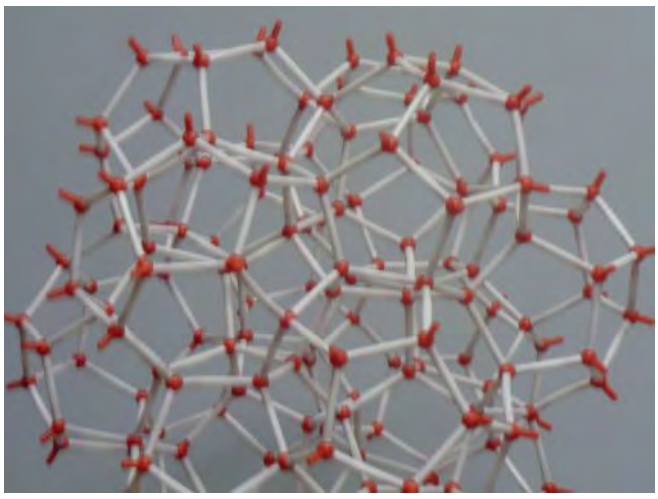
X-ray tomography image (500µm x 500 µm) of an artificial gas hydrate sediment.

THEMATICS

- Molecular sciences and thermodynamics
- Chemical engineering
- Geosciences
- Astrophysics and planetology



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Representation of the water nanocages of gas hydrates.

103 RESEARCHERS
INVOLVED IN
29 LABORATORIES

PROSPECTS

The GDR HYDRATES is based on a transversal axis dedicated to molecular sciences, aiming at providing an in-depth understanding of phenomena at the molecular scale (physico-chemistry, spectroscopy, crystallography, etc.), with the purpose of improving and infering macro-scale behavior (thermodynamic and kinetic poperties, etc.). Such studies are key to the research axis dedicated to chemical engineering and technology, geosciences and astrophysics. Among the major scientific challenges in the field of hydrates (non-exhaustive list), cross-cutting axes have been identified as priorities for their contribution both in terms of fundamental knowledge and impacts for innovation in the energy and environmental fields:

HYDRATE-SUBSTRATE SOLID INTERACTIONS

Under natural or industrial conditions, gas hydrates have strong interactions with substrates (inorganic, organic, (meso)porous, etc.). These interactions control the distribution of gas hydrates in the pore space of gas-hydrate-bearing sediments and in other kinds of porous or mesoporous media. They have an impact on the promoter / inhibitor character of specific solid substrates empirically observed, but poorly understood.

OUT-OF-EQUILIBRIUM THERMODYNAMICS AND METASTABILITY

Hydrates can form with compositions not predicted by classical thermodynamic models. The kinetic properties of crystallization and metastability must be taken into account. To date, the identification of thermo-kinetic couplings is an open question that interests molecular sciences as much as industrial applications, earth sciences or astrophysics.

OCCUPANCY RATE OF GAS HYDRATE CAGES

Hydrates are known for their large capacity to store and selectively capture gas molecules. Our current knowledge of the parameters controlling the occupancy rate of the cages is very limited. However, it is a key parameter for estimating the storage capacity of gases in specific materials, with obvious applications in process engineering, geosciences and astrophysics.

FORMATION UNDER EXTREME CONDITIONS

The conditions encountered in the core of planets or on the surface of comets differ from those encountered in Earth oceans or industrial environments. The formation of gas hydrates under ultra-low or very high-pressures (from the Pa to a few GPa) has been studied very little so far. In addition to their fundamental interest in molecular sciences, geosciences and astrophysics, such studies under boundary conditions open up new prospects for gas storage issues.

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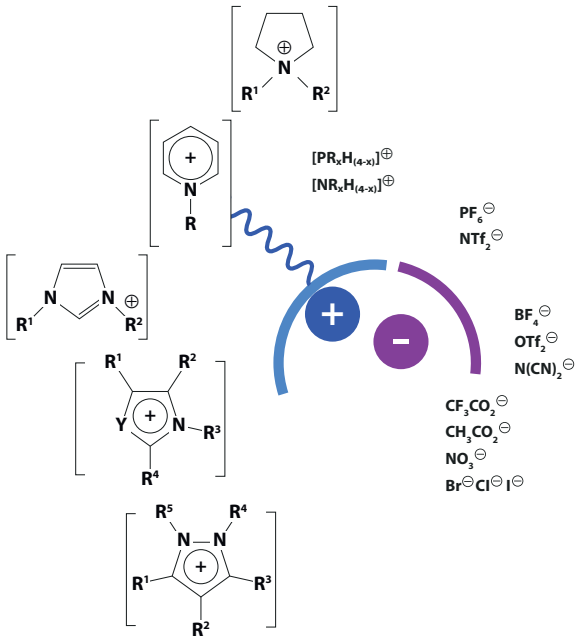
http://hydrates.cnrs.fr

cnrs GDR Groupement de recherche
HYDRATES Gas hydrates

GDR LIPS
Ionic liquids & polymers

OBJECTIVES

The GDR LIPS, created in 2013 and renewed in 2017, displays a strong willing to set up a place of exchange gathering an interdisciplinary, dynamic and visible community at national, european and international level to answer to developments in the field of ionic liquids and polymers. The GDR LIPS joins actors from academic and industrial partners on scientific life and foresight objectives. The first objective of GDR is to implement a significant animation effort through the organization of scientific days and the animation of an online platform. The second objective is the training of young researchers through the organization of a summer school and the allocation of mobility grants. Finally, calls for proposal are set up each year to merge relevant and original research and development approaches.



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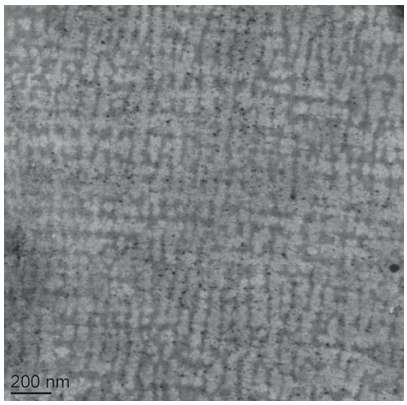
High versatility of combinaisons (cations, anions) of ionic liquids.



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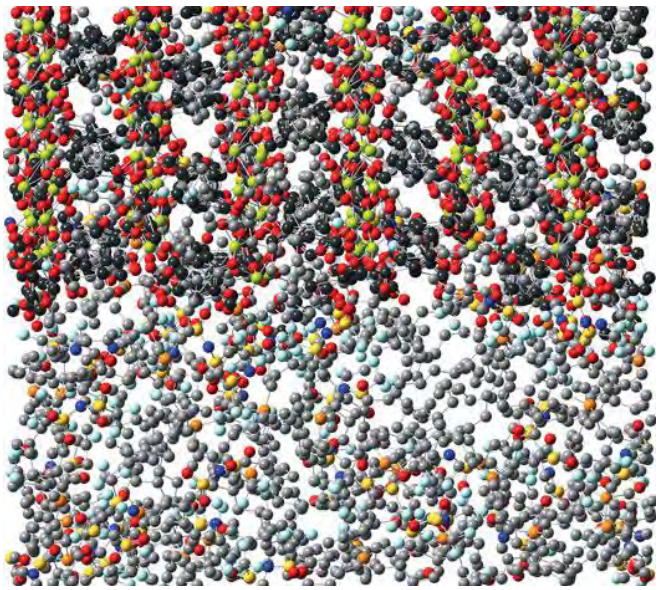
Association of ionic liquids and polymer matrix generating a nanoscale structuration.

THEMATICS

- Molecular design of new ionic liquids and ionic monomers
- Tailoring and characterization of Ils / polymers interactions: from experimental to modeling
- ILs: novel processing aids for polymers
- Polymers and ionic liquids (IL) for advanced materials



© M. Costa Gomes, A. Padua, Laboratoire de Chimie, ENS Lyon

In silico representation of the ionic liquid trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl) imide onto the surface of porous materials.

150 RESEARCHERS
INVOLVED IN
40 LABORATORIES

PROSPECTS

Evolution of the GDR towards an International Research Network 'IRN' owing to:

INCREASING ATTRACTIVITY OF "IONIC LIQUIDS & POLYMERS" TOPIC

The number of publications is still evolving at a prodigious speed testifying to the scientific proliferation of the field.
Interest of young researchers in this topic owing to their attending to summer schools.

CREATE AN INTERDISPLINARY COMMUNITY

Many unresolved scientific issues require the promotion of scientific links between communities.

– Synthesis of specific task ionic liquids for the design of tailored interactions.
While commercially available ionic liquids have already offered a great diversity, the synthesis of specific task ionic liquids remains of great interest for the design of controlled interactions and the use of ionic liquids in combination with a polymer for a specific function.

– Structuring phenomena of ILs at interfaces.
If a fine understanding of ionic liquid and polymer interactions is essential for a relevant combination, this necessarily requires an *ad hoc* characterization of the interactions. Thus, the knowledge of the characterization technics specific to each community, polymer or chemist of ionic liquids should be pooled.

The use of ionic liquids as processing aid still have remained a highly developed area of research for the processing of polymers (natural and petrosourced) by solvent or molten route. Ionic liquids are above all solvents, compatibilizers and even more recently structuring agents. There are significant advances in the construction of polymer / IL and polymer / IL / Co-solvent phase diagrams.

Finally, the eco-toxicity of ILs is an emerging area of research in recent years because this new concept involves the synthesis of bio-based ionic liquids, the regeneration and recyclability of ionic liquids and the analysis of the life cycle.
The synergy between the two scientific communities must be sustained and new career possibilities are opened to young scientists contributing to their professional integration.

EVOLUTION OF THE GEOGRAPHICAL SCOPE TO INCREASE THE INTERNATIONAL DIMENSION OF THE GDR

Strengthen actions to open up to Europe by making sustainable collaborative actions (invitations to international speakers, international summer schools, bilateral or multilateral agreements with international laboratories).

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http://www.gdr-lips.cnrs.fr

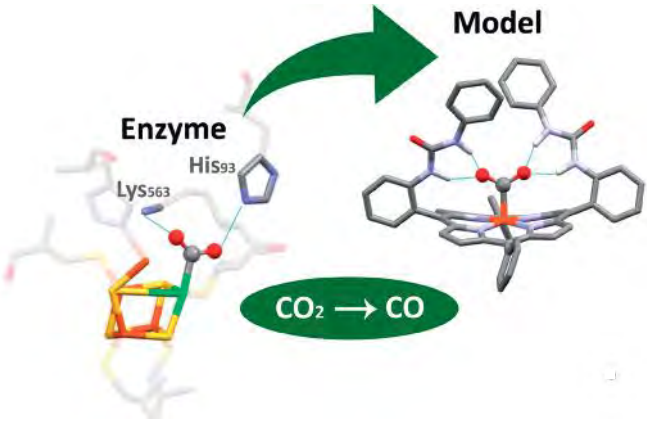
cnrs GDR Groupement de recherche
LIPS Ionic liquids & polymers

GDR MAPYRO
Pyrrolic macrocycles

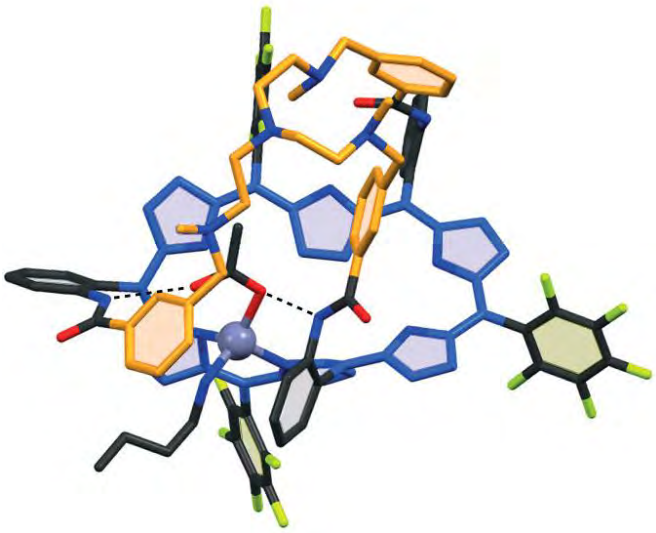
OBJECTIVES

The goal of the GDR MAPYRO is to bring together the various French groups involved in the chemistry of polypyrrolic macrocycles encompassing various specialties such as organic synthesis, coordination chemistry, supramolecular chemistry, homogeneous and heterogeneous catalysis, activation of small molecules, electro- and photoactivation.

This group allows a regular exchange of knowledge and provides solutions to specific problems through collaborations during which researchers can visit another research group to be trained in new techniques and / or practices.



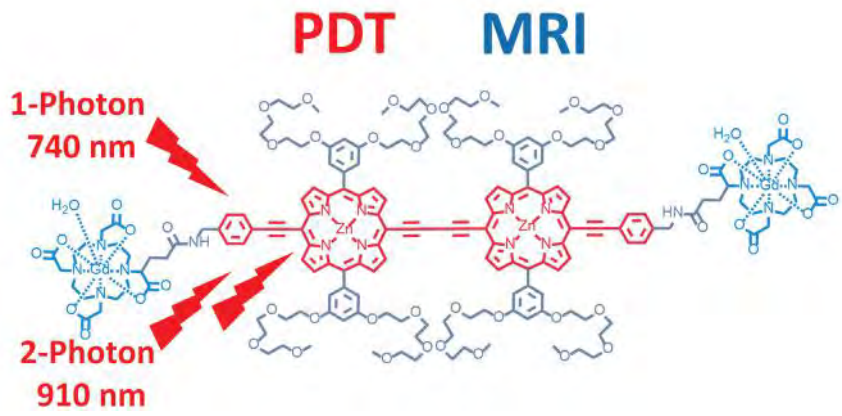
Biomimetic reduction of CO_2



A Capped Hexaphyrin: chiral and Möbius-aromatic metallo receptor.

THEMATICS

- Biomimetic chemistry for the activation of small molecules
- Supramolecular chemistry of porphyrinic assemblies
- Pyrrolic macrocycles in therapeutic chemistry



A functionalized bis-porphyrin for bimodal therapy.

75 RESEARCHERS
INVOLVED IN
23 LABORATORIES

PROSPECTS

Porphyrins and their derivatives are involved in essential processes in the animal and plant worlds. Thus, porphyrin is often referred to as the "molecule of life". Moreover, the in-depth study of the implication of these macrocycles in biological phenomena essential to life on Earth quickly attracted the attention of chemists, generating a large community of cyclic polypyrroles that MAPYRO aims to unite. By structuring the various partners at the national level and by strengthening the international links of many of them, MAPYRO's challenge is to take advantage of pyrrolic macrocycles to find new solutions in three major research areas of significant societal impact.

BIOMIMETIC CATALYSTS FOR THE ACTIVATION OF SMALL MOLECULES

Among the emblematic reactions of this field, the most important are the reduction of dioxygen or carbon dioxide and the oxidation of organic substrates by transfer of oxygen or nitrogen atoms. The study of catalytic mechanisms, the characterization of reaction intermediates, as well as the design of optimized models mobilize a significant force in this Research Group.

SUPRAMOLECULAR CHEMISTRY OF PORPHYRINIC ASSEMBLIES

It is possible to design and study new assemblies produced from cyclic polypyrroles that exhibit specific properties (optical, electrochemical, photochemical, etc.). The properties associated with porphyrinic supramolecular assemblies open up many perspectives for the transmission and storage of information through the switching of systems, the development of self-repairing materials, and the transport and release of therapeutic molecules. Furthermore, the coordination chemistry of new macrocycles (isomeric, contracted, extended, etc.) remains entirely to be discovered, understood and mastered.

PYRROLIC MACROCYCLES IN THERAPEUTIC CHEMISTRY

By their tropism for cancer cells, their ability to coordinate cations, their stability and their photosensitizer properties, pyrrolic macrocycles have long been considered serious candidates in various major therapeutic fields such as anticancer or antimicrobial agents, etc. Thus, in France, several groups are active in the design and development of new pyrrolic macrocycles in the fields of phototherapy, radio-immunotherapy, but also imaging and theranostics.

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https://mapyro.chimie.unistra.fr

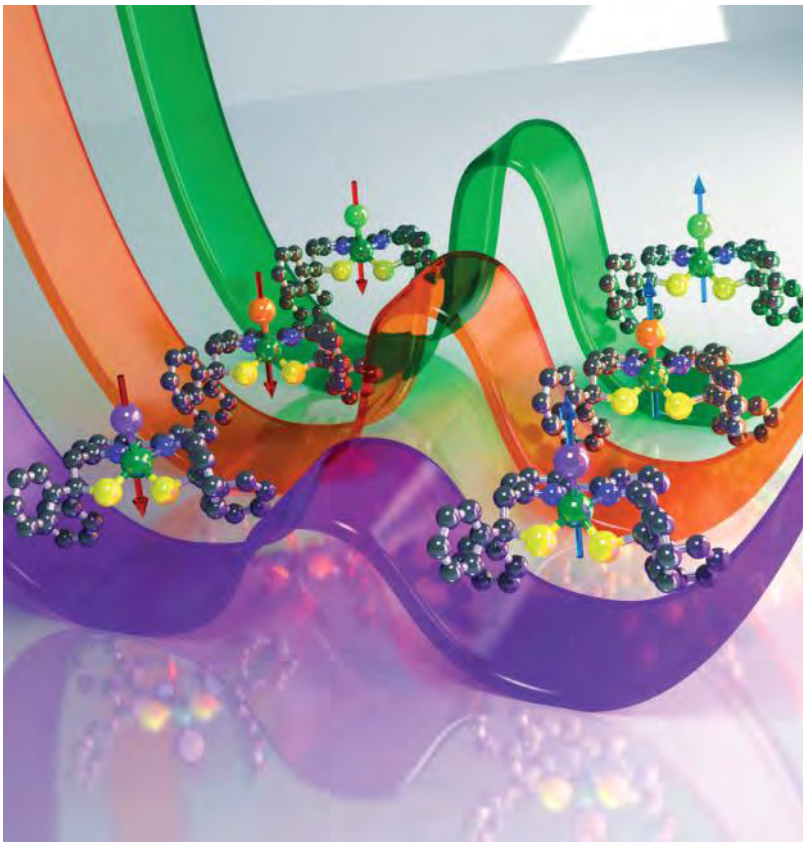
cnrs GDR Groupement de recherche
MAPYRO Macrocycles pyrroliques

GDR MCM2

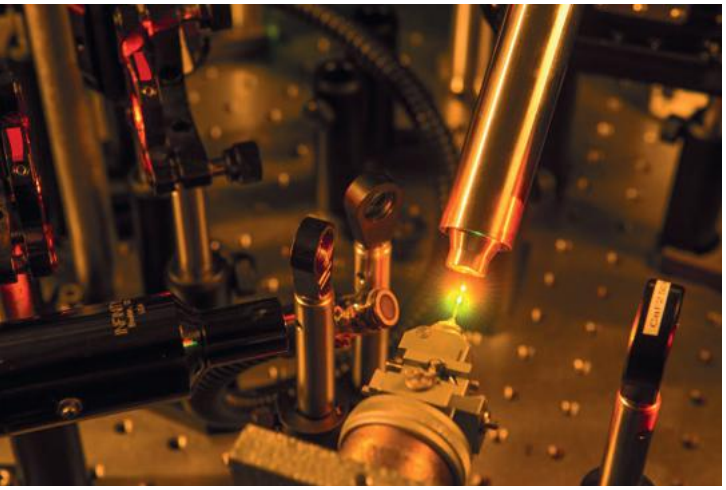
Molecular magnetism and switching 2

OBJECTIVES

For the materials of tomorrow to take their place in everyone's daily life by providing flexibility, functionality and efficiency, it is crucial to design new functional molecules today and to study their behavior. With coordination chemistry at the heart of this approach, this GdR brings together chemists, physico-chemists, theoreticians and physicists from French laboratories and large scall facilities (Synchrotrons, Neutrons, High magnetic fields) within the same community for the development of molecular-based magnetic and switchable materials. These new (multi) functional objects are of interest as MRI contrast agents, for optical and magnetic storage of information, smart pigments, electronics and molecular spintronics…



Molecular engineering and theoretical calculations for the control of magnetic anisotropy in Single-Molecule Magnets.



Time-resolved cristallography and optics.

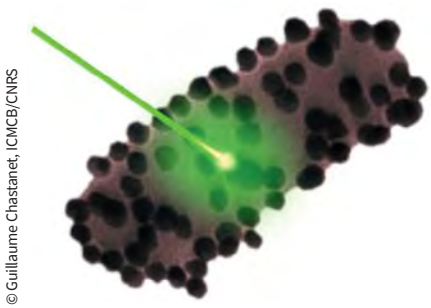
THEMATICS

- Molecular engineering
- Shaping of molecular materials
- Multifonctionnality and hybrid materials
- Molecular electronic and spintronic
- Multi-scale and multi-constrains instrumentation
- Multi-scale theoretical modeling

200 RESEARCHERS
INVOLVED IN
51 LABORATORIES

PROSPECTS

We are currently observing an outstanding growth of molecular magnetism and switching in which the GdR community is greatly involved. This field of research is diversifying both by the approaches to synthesize multifunctional materials and by the nature of the increasingly complex physical processes at work. Real applications are getting closer every day with new magnets at room temperature, magneto-electric couplings, ferro-electricity, smart pigments, biological interest, switchable electronic devices, molecular spintronics etc. All these developments have benefited from the strengthening interactions between chemists, physicists and theoreticians at the core of this GdR. In order to continue this dynamics, it is essential to maintain these interdisciplinary exchanges as well as initiate and develop dialogue with neighboring communities. These exchanges should allow chemists to design new (multi) functional, hybrid, materials with targeted and controlled properties, physicists to explore new topologies and new phenomena, with the support of theoreticians to model and predict behaviors.



© Guillaume Chastanet, ICMCB/CNRS

Photoswitching of nanocomposites.

The structuring of this community, promoting these multidisciplinary dialogues, began in the early 2000s. After almost 20 years of development, this structuring will be perpetuated through the creation of a French association for molecular magnetism (AM^2). The objectives will be multiple. Centered on multidisciplinary exchanges, various actions will be carried out (schools, workshops, mobility, scholarships, annual meeting, meeting with other communities, etc.) to bring this community forward. Special attention will be paid to maintaining the link between fundamental and applied developments. The strengths of the molecular approach will be implemented in poorly explored areas that have emerged in recent years. Meetings with other experts will allow mutual enrichment in the development, characterization and understanding of the materials that will be daily used in tomorrow's technologies.

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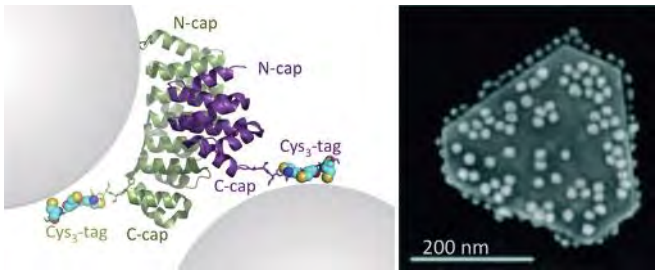
http://www.gdr-mcm2.cnrs.fr

cnrs GDR Groupement de recherche
MCM2 Molecular magnetism and switching 2

GDR MEDYNA

Assembly mechanisms and dynamics of self-organised protein-based complexes

OBJECTIVES

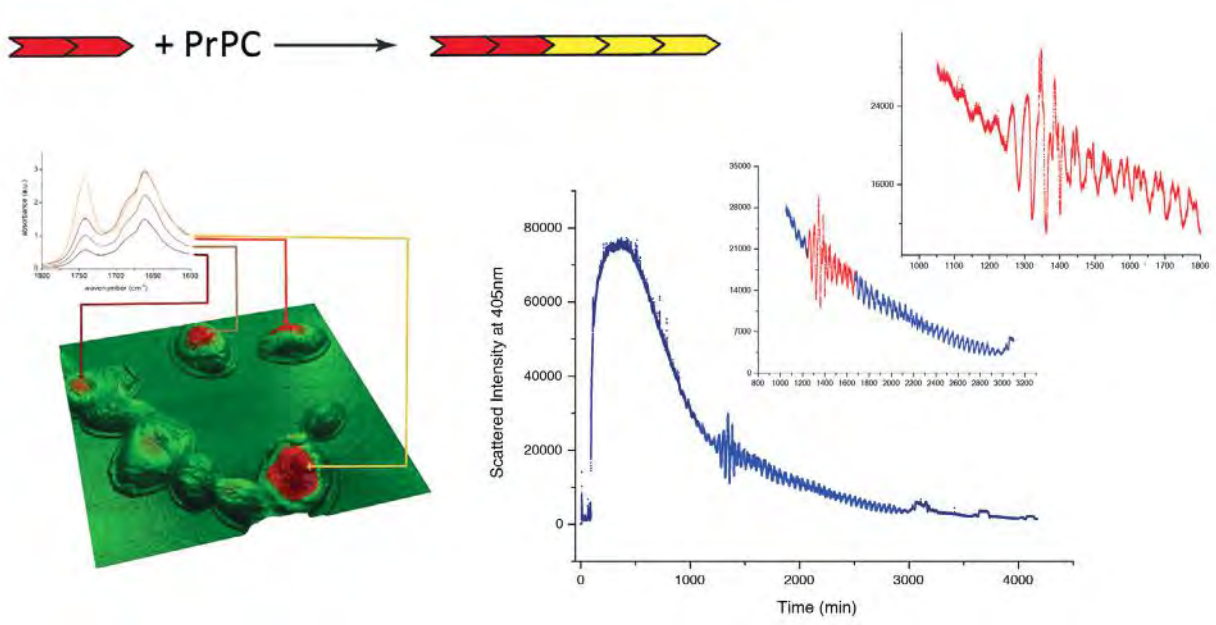


Artifical proteins obtained through combinatory biology followed by directed evolution to create specific molecular recogniton. Right panel, application to the morphosynthesis of nanocrystals.

The objectives of the GDR MéDynA are to:
– bring together French labs studying by diverse means the dynamical pathways by which self-organised protein assemblies or protein-based assemblies form (incl. peptidomimetics);
– forge a common language so as to benefit from the multiple expertise stemming from biology, biophysics, chemistry, physics and mathematics to understand and master mechanisms of protein assembly;
– foster emergence of novel interdisciplinary research projects and
– set up a nationwide interdisciplinary network useful to all researchers, whether at an early career stage (such as graduate students and postdocs) or well established.

THEMATICS

- Biochemistry, biophysics and physico-chemistry of protein assemblies
- Mathematical modeling of assembly processes
- Biomaterials (proteinaceous or proteo-inspired), biomimetic self-assembled systems
- Structural biology, molecular modeling and biomolecular simulations



Fibers of prion protein (PrPC) characterised by AFM coupled to infrared spectroscopy (left panel). The fibers' disassembly kinetics (right panel).

160 RESEARCHERS
INVOLVED IN
35 LABORATORIES

PROSPECTS

MéDynA brings together researchers from multiple disciplines to reach a global understanding of this kind of nonlinear processes, where products do not necessarily stem from an unique preceding state. Each discipline brings unique expertise:

BIOLOGISTS bring protein systems and their wealth of possibilities for self-assembly as well as relevant biological questions.

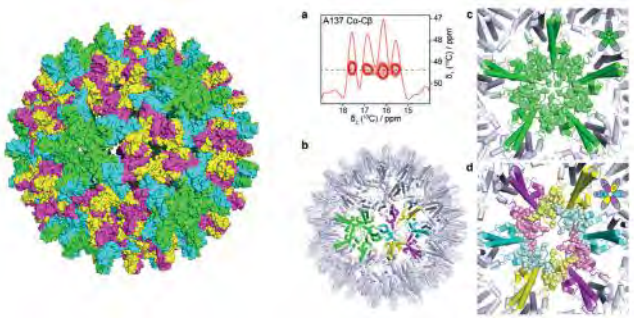
CHEMISTS AND BIOCHEMISTS bring their expertise in experimental characterization of assemblies that can be isolated and stabilised: endpoints of assemblies as well as intermediates with a long lifetime, possibly extended by fine-tuning.

STRUCTURAL BIOLOGISTS bring their expertise in the atomic-scale characterization of equilibrium assemblies and intermediates with a long lifetime.

PHYSICISTS, PHYSICO-CHEMISTS AND BIOPHYSICISTS bring their expertise in rigorous characterization of underlying physical phenomena and generation of physical models accounting for them.

MATHEMATICIANS bring modeling of processes based on assimilation of all data generated by the other disciplines, but also molecular modeling at the interface between chemistry and structural biology.

MéDynA creates a multidisciplinary scientific community for young researchers, but also for senior researchers. It is a starting point for creating a French network where all will discover the importance of working with researchers from other disciplines on this common problem. Confronting other fields and debates in plenary meetings will serve to foster ties between researchers who do not normally meet one another and hopefully allow maturing collaborations. The added value of these exchanges will mainly depend on the will to go towards fields unknown to the researchers participating in these meetings.



Self-assembled viral capsids. Molecular details ruling assembly can be monitored down to the atomic scale, notably by NMR spectroscopy, X-ray crystallography and cryo-electron microscopy.

DEFINING A COMMON LANGUAGE BETWEEN SCIENTISTS FROM SEPARATE FIELDS

One of the essential goals of MéDynA will be to forge a common language, without which our discussions will remain shallow. Forging this common language will allow us to benefit from all expertise to tackle the principal challenge in the field: advancing towards control of the mechanisms of protein assembly.

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https://medyna.cnrs.fr

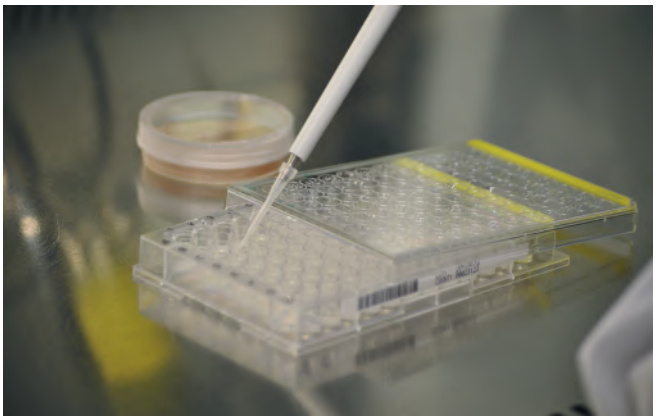
cnrs GDR Groupement de recherche
MéDynA Assembly mechanisms and dynamics of self-organised protein-based complexes

GDR MUFOPAM

Multifunction of antimicrobial peptides

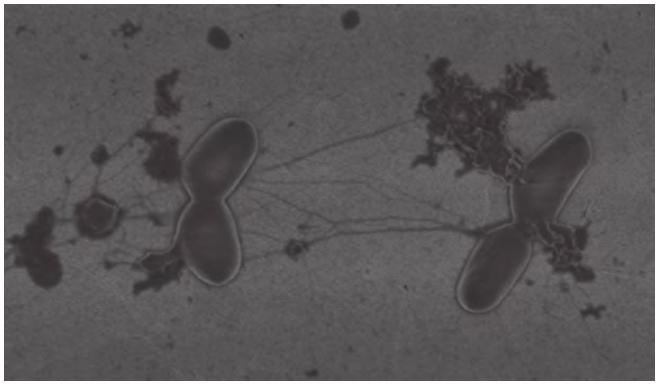
OBJECTIVES

The missions of the GDR MuFoPAM are to:
– bring together the French community working in the field of antimicrobial peptides (AMPs), their multiple biological activities and applications;
– promote synergies between disciplines in order to foster joint innovative and transversal projects and
– develop and promote the multifunctionality of AMPs, especially as a solution to increasing resistance to antibiotics, or for biological activities that are largely underestimated.



© Philippe Bulet, institute for Advanced Biosciences/ INSERM, Grenoble

Antimicrobial assays.

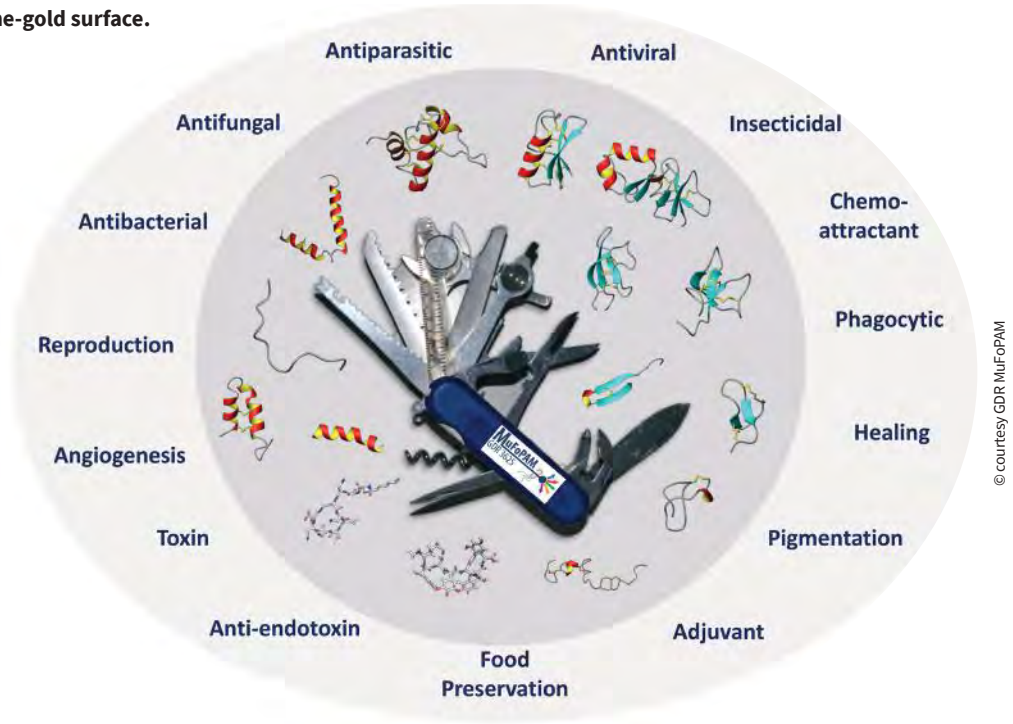


© Vincent Humblot, FEMTO-ST Institute

Dead *listeria* @ temporine-gold surface.

THEMATICS

- Diversity of origins, structures and biological activities
- Microbial resistance
- Microbial ecology
- Vectorization, and surface functionalization
- Valorization strategy



Diversity of AMPs.

© courtesy GDR MuFoPAM

250 RESEARCHERS
INVOLVED IN
48 LABORATORIES

PROSPECTS

THE CURRENT CONTEXT

Antibiotic resistance is a major public health problem, that forcasts more than 10 million deaths per year in 2050, higher than deaths associated with cancer. Given these alarming data, several action plans to fight antibiotic resistance have been initiated at global, European and national levels. Among the objectives, the research and development of new alternatives to antibiotics.

AMPS: ONE OF THE ALTERNATIVES TO ANTIBIOTICS

One of the most promising alternatives to antibiotics, less conducive to the rapid acquisition of resistance, lies in the identification, improvement and / or development of AMPs. These peptides are naturally produced by any living organism colonized or infected with a pathogen, or during an inflammatory process.
The fight against antibiotic resistance is part of a unique health approach, named “Global One Health”, and brings together researchers involved in human, animal and / or environmental health. The activity of GDR MuFoPAM is fully in line with this integrative and multidisciplinary approach since it brings together teams involved in these three areas of research.

OUR ACTIONS

AMPs are an inexhaustible natural resource of promising antibiotic therapy molecules. Each day brings an enrichment of knowledge on new AMPs, as well as on their multifunction and on the understanding of their mechanisms of action. The latter are much more subtle than initially expected, with complex interactions not only with membrane structures but also with multiple intracellular targets. In addition to the exploration of biodiversity (diversity of origin, structure, function and mechanism of action), the GDR teams are working to understand the mechanisms developed by bacteria to escape the action of antibiotics. Indeed, understanding the evolution of resistance is essential to prevent its occurrence. In the context of “Global One Health”, the GDR is also interested in microbiota, and especially in the crosstalk between microbiota, hosts, and AMPs. Finally, the GDR teams focus on vectorization of AMPs, and on surface functionalization for both preventive and curative uses with the aim of developing AMPs as therapeutics of the future.

THE CHALLENGE

More than 50 therapeutic peptides are on the market, all targets combined (2018 data). More than 70 AMPs are currently in the pipeline of therapeutic candidates worldwide, including 34 and 27 in preclinical and clinical trials, respectively (2019 data). The challenge that brings together all members of the GDR, involved in basic or in applied research, is to work for the promotion of AMPs as new therapeutic molecules.

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www.mufopam.cnrs.fr

cnrs GDR Groupement de recherche
MuFoPAM Multifunction of antimicrobial peptides

GDR O3

Odorant – odor – olfaction

OBJECTIVES

© Sébastien Fiorucci, ChemoSim/Univ. Côte d'Azur

Development of numerical models based on molecular modeling, maching learning, or structural bioinformatics to decipher the combinatorial code of chemosensory perception.

The mission of the GDR O3 is to study odorants and olfaction through different fields of research. Therefore, the GDR associates biologists, chemists, physicists, computer scientists, philosophers, researchers from human and social sciences around topics that fascinate the public.

The objectives of this GDR are to:
– encourage the emergence of a community to constitute a pole of experts;
– strengthen scientific dissemination around olfaction;
– develop communication and bring out interdisciplinary projects with academic partners and with companies (perfumes, agro-food, pharmacology, etc.) at the national level (ANR…) and internationally (Horizon2020 project) and
– organize scientific meetings.

© Sandra Perez et Jamel Ben Hassine, Univ. Côte d'Azur

Map of complaints from residents in terms of odor nuisance in Chateaurenard.

THEMATICS

- Physiology and psycho-physiology of olfaction
- Odorants as a tool to communicate
- Ingredients, odorants & innovation
- Odors, cultures and society
- Odors & taste
- Odors & health

>150 RESEARCHERS INVOLVED IN 55 LABORATORIES

PROSPECTS

CHALLENGE

The challenge is to promote the different thematics of olfaction in an interactional way, to create emulation and cooperation between researches from the molecule to society, from the odorant compound to its detection by the olfactory receptors, and its perception by the brain. This can imply medical and societal implications in the health and well-being thematics.
The impact of odorants and odors in human and social sciences will be central. The GDR will also be involved in the theme of olfactory learning, olfactory perception, odor hedonics, and compositions.
Industrial aspects will also be taken into account, from raw materials to finished products, for a variety of applications, ranging from fine perfumery to detergents, from plant protection to the food industry or cosmetics. Many GDR O3 teams have strong interactions with the Cosmetic Valley. These close links with the industry favor applications to national (ANR-PRCE) and European calls.

COVID-19 AND OLFACTION

A frequent and early symptom of COVID-19 disease is an alteration of odor perception. Data collected in several countries impacted by the SARS-CoV-2 virus describe the characteristics of these alterations. The causes and consequences of olfactory perception alteration on the patient daily life remain poorly understood, but research is still ongoing. Indeed, several national and international studies carried out by GDR O3 teams and by the GCCR (Global Consortium for Chemosensory Research (https://gcchemosensr.org/), created at the beginning of the pandemic which brings together more than 600 researchers in more than 50 countries in which many GDR teams have participated, have already been published[1] or are still in progress[2]. These studies aim at better understanding the olfactory disorders induced by the COVID-19.

DISSEMINATION OF SCIENCE

A new website is being developed to better meet the expectations of the public in terms of information but also to better federate the actions of the GDR teams, training courses, calls, etc.

TRAINING

Training is one of the main objectives of GDR. Thematic schools have already been organized and some others are scheduled.

1 Gerkin *et al*. 2020; Pierron *et al*. 2020; Parma *et al*. 2020; Iravanl et al. 2020…

2 https://form.crnl.fr/index.php/146862?newtest=Y&lang=fr

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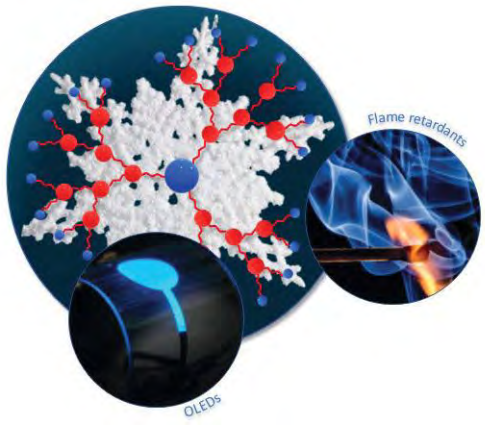
cnrs GDR Groupement de recherche
O3 Odorant – odor – olfaction

GDR PHOSPHORE

OBJECTIVES

Among the elements of the periodic table, phosphorus occupies a unique position as a bridge between the living and non-living world, in the cycles of organic and inorganic matter of our biosphere. These multiple roles are also found in human-developed chemistry and applications of phosphorus molecules extend today from materials science, nanotechnologies and catalysis to life sciences. This multiplicity of fields and applications is covered by the research teams involved in the GDR PHOSPHORE.

The main objectives of the GDR are to:
– contribute to the national emergence of a cluster of experts in phosphorus chemistry;
– develop new skills and encourage the emergence of joint research themes;
– organize and encourage scientific meetings and training actions;
– facilitate the dissemination of scientific knowledge to industry and the general audience and
– contribute to the training of future researchers and entrepreneurs in this field.



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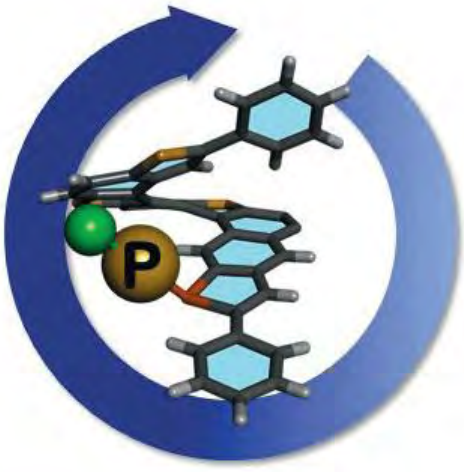
From the molecule to flame retardants, optoelectronics…



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Catalysis: efficient and environmentally benign chemistry.

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Cancer cells treated with Rapamycin for two hours observed in structured illumination microscopy.

THEMATICS

- Nanosciences and material science
- Catalysis – methodologies and applications
- Bioactive molecules and applications

46 RESEARCHERS
INVOLVED IN
32 LABORATORIES

PROSPECTS

The main objective of the GDR PHOSPHORE is to gather French research teams specialized in phosphorus chemistry and involved in the understanding of structure-property relationships of innovative phosphorus compounds, with a view to applications in materials science, catalysis, agrochemistry and medicinal chemistry. While the core of this GDR is centered on chemistry, its interdisciplinary nature makes it possible to envisage essential advances in the fields of physics, engineering sciences and biosciences, answering major economic and societal challenges. At the same time, the GDR aims at sharing knowledge, know-how, equipment and techniques among the network members and to increase visibility of the field in the scientific community.
The three scientific axes of the GDR PHOSPHORE and their challenges are briefly presented below.

NANOSCIENCES AND MATERIALS SCIENCE

Design and synthesis of multifunctional, inexpensive and environment-friendly materials is of great importance as they find applications in everyday life. Heteroatoms in functional materials play a determinant role as they allow the generation of new assemblies or the fine tuning of physical properties. The research teams involved in the GDR use phosphorus chemistry for the development of inorganic, organic and even organometallic molecular precursors for the synthesis of advanced materials with defined properties (electronic, optical, magnetic, mechanical…). For example, inorganic phosphorus-based polymers have been shown to be highly effective flame retardants for textile industry. Moreover, the insertion of phosphorus atoms in oligomers or Π-conjugated polymers yielded fluorescent dyes that can be incorporated in light-emitting diodes and solar cells. Phosphorous derivatives also play an important role for the environment. Polymers based on phosphines or phosphonates can be used for the removal of heavy metals from polluted soils and water purification.

CATALYSIS – METHODOLOGIES AND APPLICATIONS

Catalysis is one of the essential pilar for the development of eco-compatible processes, the industrial production of raw materials and products with high added value. It fulfills the needs of pharmaceutical, flavor and fragrance and agrochemical industries and represents a major economic and societal challenge. In the field of homogeneous catalysis, phosphorus-based ligands and organocatalysts are of great interest and utility. They may also find niche-positions in some peculiar applications. The GDR research teams are developing approaches to new phosphorus organocatalysts and ligands. They are studying their properties and investigating novel structural designs, while focusing on the most ambitious and challenging catalytic applications, with the aim to control both reactivity and stereoselectivity.

BIOACTIVE MOLECULES AND APPLICATIONS

In the living world, phosphorus is a major element acting in many cellular pathways. Phosphate backbone is the structural link of DNA or RNA nucleobases. Reduced species such as phosphonates are mimics of phosphates. The replacement of an oxygen by a carbon atom provides access to compounds with increased metabolic stability. Many therapeutic agents have a phosphonate functional group, and so do anti-cancer drugs and agents against parasitic or bone diseases. The GDR teams are involved in research targeting diseases with a high societal impact such as cancer, inflammatory diseases, neurodegenerative diseases, and they propose new therapeutic approaches using original phosphorus compounds.

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https://gdrphosphore.sciencesconf.org

cnrs GDR Groupement de recherche PHOSPHORE

GDR PES
Photo-electro stimulation

OBJECTIVES

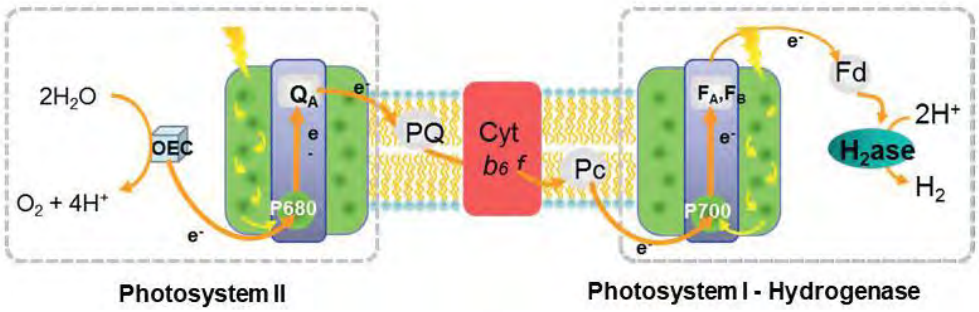
© courtesy of Jean-François Bergamini

Image of photoinduced electroluminescence at BiVO4 anodes.

The objectives of the GDR PES are to:
– build a community on topics about photoelectrostimulation, that is all the phenomena where the joint action of electrons and photons may induce a controlled modification in a molecular system or in nanomaterials and thus a modification of its properties;
– federate on these topics various scientific communities (electrochemists, photochemists, theoreticians) that have few opportunities to interact in scientific meetings;
– organize meetings (conferences, workshops, schools) dealing either with the whole topic or with specific aspects (instrumentation, modeling, synthesis…) and
– generate new collaborations through sharing of complementary expertise.

THEMATICS

- Synthesis of new photo- or electroactive molecules
- Design and characterization of molecular nanomaterials
- Modeling processes involved in photo or electrostimulation
- Developing new setup coupling photo and electrochemistry



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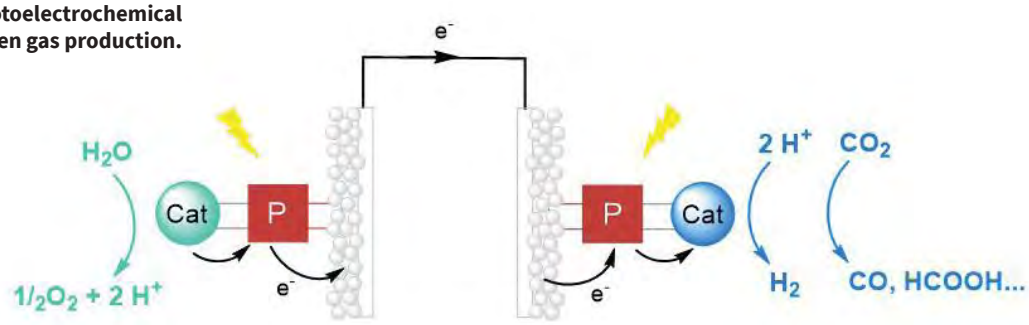
Example of a bioinspired photoelectrochemical cell for hydrogen gas production.



200 RESEARCHERS
INVOLVED IN
49 LABORATORIES

PROSPECTS

SCIENTIFIC CONTEXT

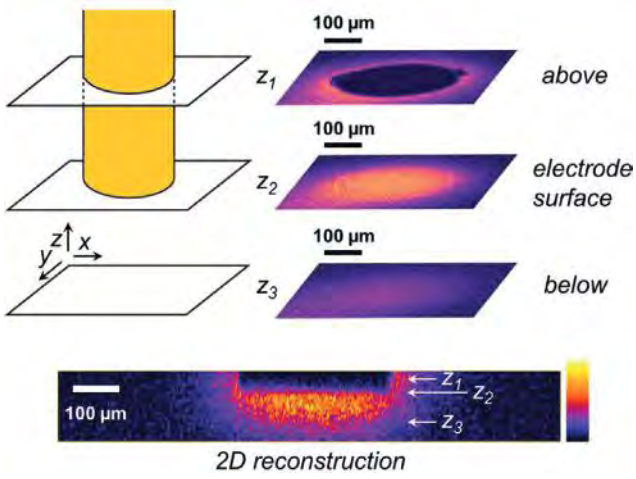
Numerous issues imply a synergy between photochemistry and electrochemistry, like in green energy storage and production (hydrogen, photovoltaic cells coupled with batteries or electrolysers), pollutant detection and treatment (photoreduction of CO_2, photooxidation of toxic compounds). Some applications with high societal impact require complementary skills in these two fields, while they did not meet each other very much up to now. Besides, the resolution of complex issues like those involving biological mechanisms or material ageing in batteries require the coupling of analytical techniques *in situ* to provide information *in operando*. The implementation of this coupling relies on a strong expertise to overcome technological and scientific locks. PES GDR precisely aims at giving its members the necessary skills, both theoretical and experimental. Favoring the development of new materials that can be photo- or electrochemically activated is also a main target. Applications span the information storage, the controlled activation of chemical reactions, the enhancement of existing properties or the creation of new ones in materials.

TRAINING ASPECTS

Stress will be put on training, especially through the organization of thematic school. Scientific communication will be widely open to young researchers (PhD, post-doc) in all meetings organized by the GDR. Many exchanges between partner laboratories will be supported to allow the skills enhancement of PhD and young searchers. Pluridisciplinarity will be encouraged through inter-GDR meetings.

INTERNATIONAL

Interactions with international collaborating networks in the topic will be encouraged, by associating them to scientific or training meetings.



Fluorescence intensity profiles at various distances from the electrode obtained by confocal microscopy.

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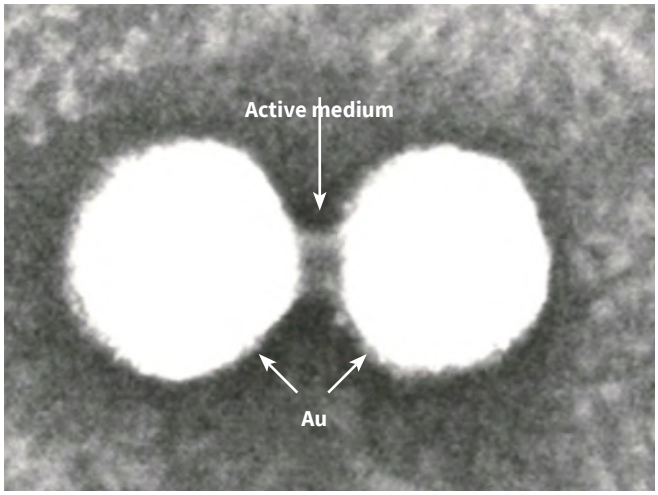
cnrs GDR Groupement de recherche
PES Photo-electro stimulation

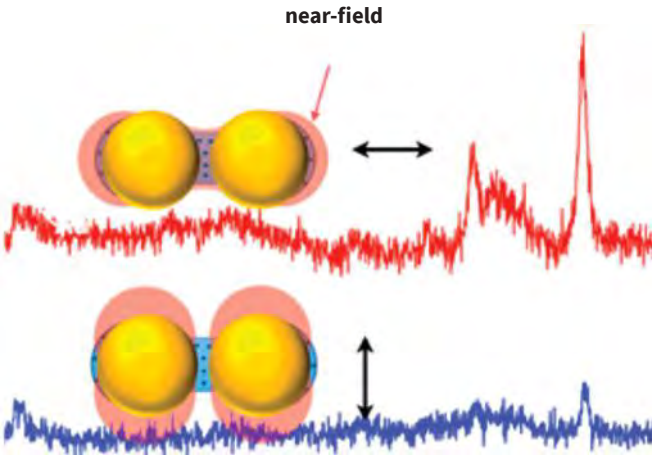
GDR ACTIVE PLASMONICS

OBJECTIVES

Plasmonics is a vast field of scientific and technological study exploiting the light / matter interaction, with many applications in energy, nano-medicine, the environment, enhanced spectroscopies, nano-optics, sensors, art… In this context, the GDR Active Plasmonics leads its scientific community through two complementary approaches:

– either a modification of the physical and chemical properties of molecules via the excitation of surface plasmon or
– the control of optical properties via a local environment or stimulable molecules.

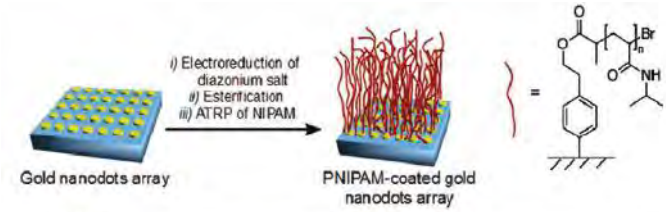


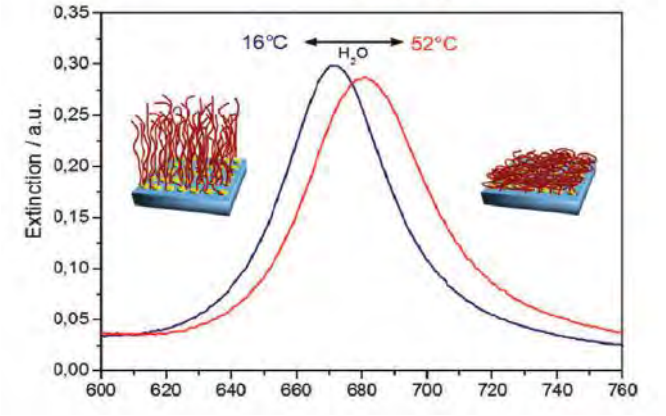


Scheme and SEM image of a typical gold/polymer.

THEMATICS

- Tunable plasmonics
- Plasmonics and chemical reaction
- Plasmonics and physical transformations
- Towards integrated plasmon devices





Extinction spectra of a thermosensitive polymer-coated gold nanoparticles going from 16 to 52 °C versus the temperature.

150 RESEARCHERS
INVOLVED IN
20 LABORATORIES

PROSPECTS

In order to structure the actions and missions of the GDR and more precisely define their outlines, we have divided the scientific themes of interest for the GDR according to the following four major axes.

TUNABLE PLASMONICS

The objective is the modulation and control of optical properties of hybrid plasmonic structures, in a reversible manner. We are interested in the tunability of plasmonic properties via an active dielectric medium (inorganic, organic, solvents, molecules, etc.), or a plasmonic coupling (core / shell, dimers of nanoparticles –NPs-, or coupling between NPs and a metallic substrate…). We are also interested in auto-tunability (via electron injection).

PLASMONICS AND CHEMICAL REACTION

This theme is devoted to the induction of chemical transformations via plasmon excitation. Among the transformations envisaged, we are particularly interested in chemical reduction reactions, surface functionalization, structural modifications, polymerization, catalysis.

PLASMONICS AND PHYSICAL TRANSFOMATIONS

Inductive plasmonics can also induce and control physical effects. We are interested in thermally activated phenomena (thermoplasmonics), optically activated effects (photoelectric effect, nonlinear optics, photo-voltaic,…), but also acoustic (generation of phonons induced by plasmon excitation). The electronic effects linked to the generation of so-called “hot” electrons, often at the origin of these physical (but also chemical) transformations, are also an important aspect discussed. This will focus on the mechanisms linked to this effect, which have not been developed experimentally.

TOWARDS INTEGRATED PLASMON DEVICES

This axis concerns the design and production of various submicronic devices that are always more efficient, combined with plasmonic engineering. We are thus interested in active plasmonic sensor type components (including SPR techniques – plasmon resonance surface-, enhanced spectroscopies such as fluorescence, infrared spectroscopy and Raman scattering), integrated active devices (optical, thermal, electronic…).

In terms of repercussion, the development of transduction systems, ensuring a conversion or transfer of signals (optical, acoustic, etc.) into a signal of an electrical nature, would represent a major societal aspect, for example in the field of energy, medicine, and environment. Through the 4 axes proposed, the GDR attempts to take important steps in understanding the photo-induced phenomena of hot electron transfers between organic and inorganic systems.

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website under construction

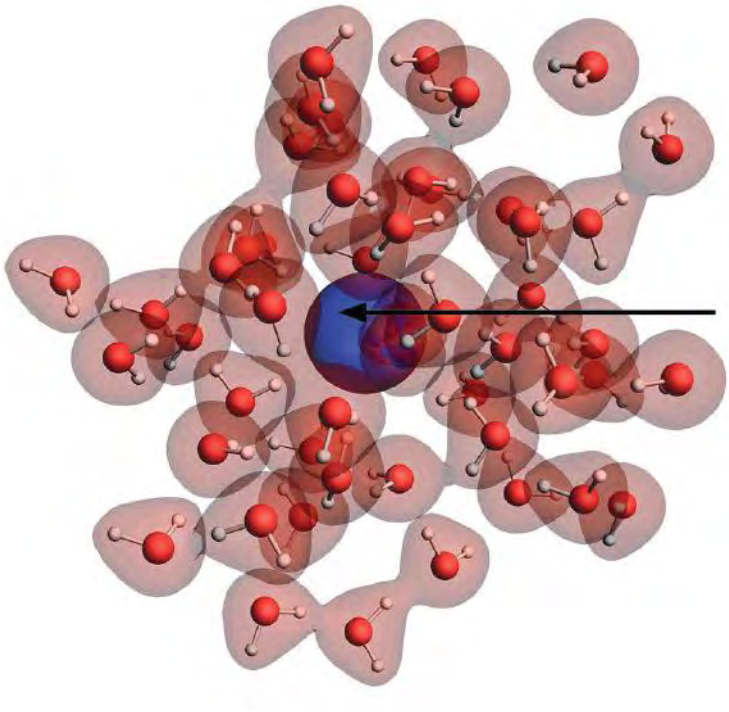
cnrs GDR Groupement de recherche
Plasmonique Active

GDR NBODY

Quantum n-body problem in chemistry and physics

OBJECTIVES

The research network aims to bring together the community working on the quantum N-body problem, mostly from the viewpoint of quantum chemistry, but also including the viewpoints of condensed-matter physics, nuclear physics, and mathematics. The idea is to foster the development of new computational methods in quantum mechanics, the transfer of these methods from one discipline to another, and their efficient computer implementations. To reach this goal, the research network organizes interdisciplinary conferences and workshops. It is also particularly involved in training students and researchers via the organization of several interdisciplinary international schools.



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Quantum calculation for the system I-$(H_2O)_{50}$

THEMATICS

- Quantum chemistry
- Condensed-matter physics
- Nuclear physics
- Mathematics

$$E^{\mathrm{w}}_{\mathrm{c},J}[n^{\mathrm{w}}] = \mathscr{E}^{\mathrm{w}}_{\mathrm{c},J}[n^{\mathrm{w}}] + \sum_{K\geq 0} \mathtt{w}_K \sum_{I>0} (\delta_{IJ} - \mathtt{w}_I) \frac{\partial \left(\mathscr{E}^{\mathrm{w}}_{\mathrm{c},K}[n^{\mathrm{w}}]\right)}{\partial \mathtt{w}_I} + \sum_{K\geq 0} \mathtt{w}_K \int d\mathbf{r} \frac{\delta \mathscr{E}^{\mathrm{w}}_{\mathrm{c},K}[n^{\mathrm{w}}]}{\delta n(\mathbf{r})} \left(n_{\Phi^{\mathrm{KS,w}}_J}(\mathbf{r}) - n_{\Psi_J}(\mathbf{r}) \right)$$

© Emmanuel Fromager, Université de Strasbourg

Development of a density-functional theory for excited states.

100 RESEARCHERS
INVOLVED IN
37 LABORATORIES

PROSPECTS

We are witnessing a remarkable evolution of quantum chemistry at the international level. New approaches based on methods coming from different fields are proposed. This is so for example for wave-function approaches in which new methods overcoming the limits of the current methods are developed. For example, CASSCF calculations with active spaces corresponding to about 50 electrons in 50 orbitals can now be performed. New wave-function representations coming from Physics *(Tensor Network)* are used and provide a much deeper picture of the physical contents of the wave function. The development of stochastic approaches is also very active. For example, the FCI-QMC method introduced a few years ago allows one to sample active spaces that were previously beyond reach. The development of deterministic variants of the FCI-QMC method, such as the selected configuration interaction, is also a very active research field. For all these methods, high-performance computing implementations are crucial. Very efficient implementations adapted to the architecture of current supercomputers, involving in particular massive parallelism, have to be developed. Regarding systematic calculations of numerous molecular systems, we are witnessing a spectacular development of *machine learning* techniques. At a more fundamental level, it is now proposed to use *machine learning* for selecting the most important configurations in configuration-interaction calculations.

Beyond wave-function methods, one can mention the evolution of green-function techniques, a central tool of physicists, and their application to quantum chemistry which progresses. In the same spirit, one can also point out *embedding* methods including environment effects similarly to DMFT methods. Regarding DFT, one can mention the combination of wave-function methods with short-range density functionals in order to correct for the incompleteness of basis sets and include dynamical correlation at low computational cost.

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Super computer CURIE.

This booming activity around *ab initio* computational methods requires mobilizing various methodologies which are not well known yet by all. The NBODY research network has the mission to structure these developments with strengthened interactions between chemists, physicists, and mathematicians.

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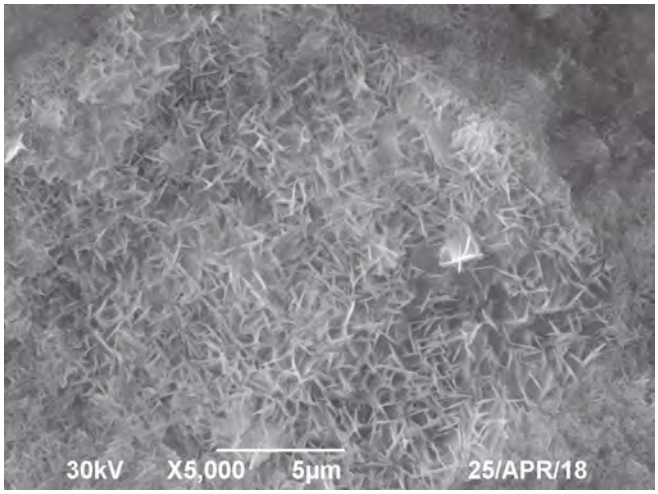
cnrs GDR Groupement de recherche
NBODY Quantum n-body problem in chemistry and physics

GDR PROMETHEE

Hydrometallurgical processes for integrated management of primary and secondary resources

OBJECTIVES



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Scanning electron microscope (MES) image of α-$Co(OH)_2$

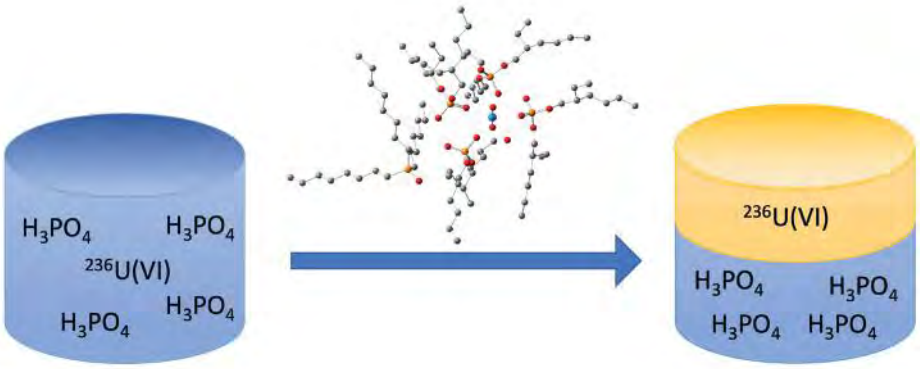
The need for mineral raw materials has been constantly increasing. Some metals, qualified as "strategic", present supply risks that could strongly impact French and European industrial sectors for several decades. Thus, the development of efficient, innovative and competitive hydrometallurgical processes, to extract these elements from depleted or complex resources, from primary mines or from recycling, is becoming a necessity. The aim of the GDR Promethee is to continue structuring, developing and integrating hydrometallurgical research into its environment.

THEMATICS

- Thermodynamic and physical chemistry modeling of hydrometallurgical processes
- Development of disruptive and innovative processes
- Integration aspects – recycling and circular economy environment

© Frédéric Maligne, CNRS

Experimental reactor.



© Marie Le Page, Mostefa/LRGP/ENSIC

Recovery of uranium contained in concentrated phosphoric acid by liquid-liquid extraction.

140 RESEARCHERS
INVOLVED IN
27 LABORATORIES

PROSPECTS

Hydrometallurgy is currently facing many challenges, such as:
– the supply risk of strategic metals;
– the necessity to operate new mines (secondary flows, urban waste, etc.) or
– the need for more efficient and environmentally friendly processes.

The GDR Promethee aims at designing new extraction processes that will meet current and future challenges by taking advantage of synergies between three complementary research themes.

HOW TO DEVELOP RELIABLE MODELS TO UNDERSTAND AND OPTIMIZE PROCESSES?

Thermodynamic and physical chemistry modeling in hydrometallurgy are powerful tools for better understanding the implementation and optimization of processes. However, these approaches require a high level of complexity, since they are based on the description of systems in which many reactions can take place, with sometimes few or no data available. Many challenges remain to be overcome in order to achieve a detailed description of the solid phases (resins, precipitates, colloids) and of the concentrated liquid phases (aqueous phases, organic phases, ionic liquids), as well as the transfers of matter at the interfaces.

HOW TO INNOVATE, INTENSIFY AND OFFER DISRUPTIVE PROCESSES?

Many technological challenges persist in the chemistry and physical chemistry associated with hydrometallurgical processes and more particularly in leaching processes as well as in separation and purification steps. Indeed, these processes are more complex when depleted primary resources are used or for recycling (complexity of multiphasic materials). The skills of the members of the GDR will be an asset for better understanding the physical and chemical phenomena that take place in these processes, to intensify them, make them less energy-consuming and adapt them to new sources of raw materials.

HOW TO INTEGRATE HYDROMETALLURGICAL RESEARCH INTO AN ECONOMIC, SOCIETAL, INDUSTRIAL AND ECOLOGICAL ENVIRONMENT?

The development of hydrometallurgical processes aims at enabling the extraction and recovery of metals, in particular strategic and / or critical metals, on which our societies are based. Thus, the role of the GDR will be to have a more global vision, by:
– integrating aspects related to the “Circular Economy” and the socio-economic environment through the involvement of humanities and social sciences;
– communicating with civil society, consumer of mineral resources and an essential part of the recycling chain through collection and
– intensifying and developing exchanges and collaborative projects with industrial stakeholders, directly concerned by the issues related to the supply of mineral resources.

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https://gdr-promethee.cnrs.fr/index.php/fr
https://www.linkedin.com/groups/13955197

cnrs GDR Groupement de recherche
Promethee Hydrometallurgical processes for integrated management of primary and secondary resources

GDR RAFALD

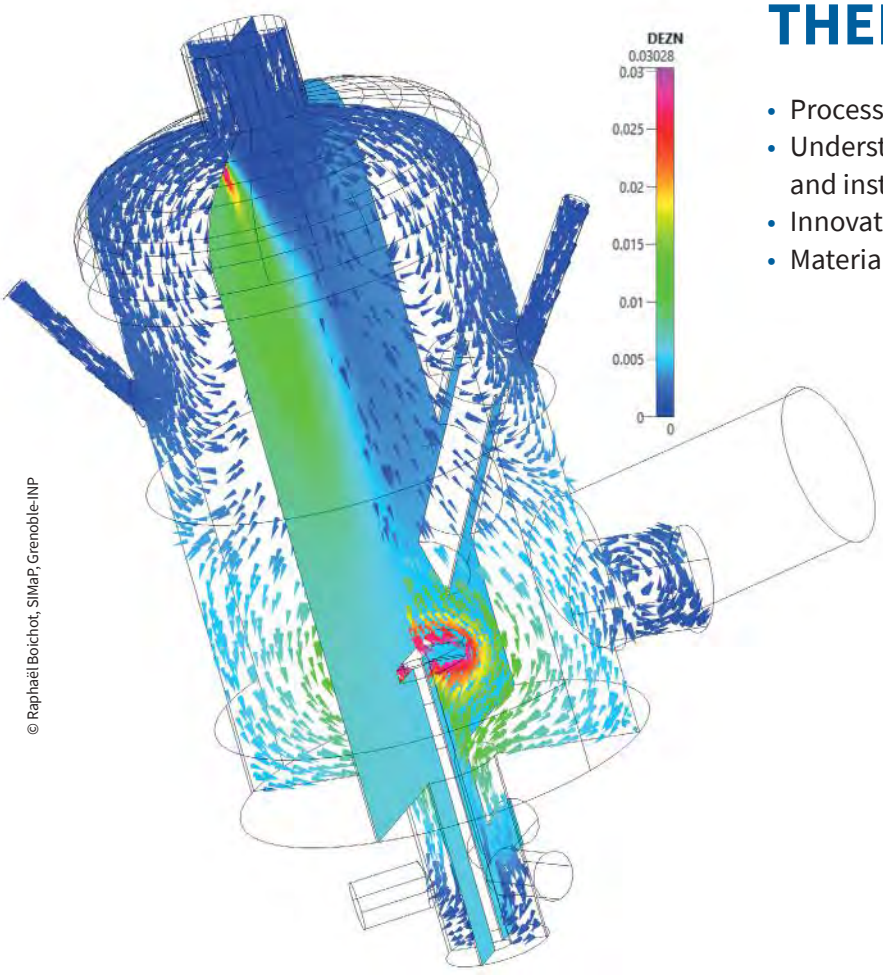
Network of researchers involved in atomic layer deposition

OBJECTIVES

The aim of the RAFALD research group is to strengthen the links between the teams of the ALD community (*Atomic Layer Deposition* process for the deposition of very thin and conformal films from gaseous precursors) in France and to extend them to new users from the entire scientific community. It aims at germinating new projects, proposing a vision of the future of materials and processes, in a spirit of "architectured materials" based on targeted performance specifications. The ambition is to bring together knowledge from the various "historical" applications (microelectronics, energy) and extend it to other fields. The annual workshop of the same name federates the French community of industrial users and researchers using the ALD technique, with the participation of more than 100 people.

THEMATICS

- Process and precursors chemistry
- Understanding of growth mechanisms and instrumentation
- Innovative processes and reactor development
- Materials in emerging fields



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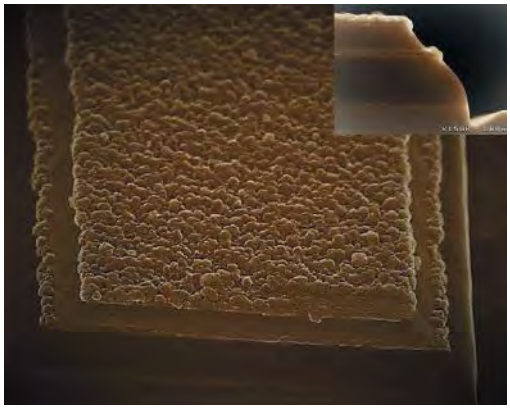
Transient aspects of velocity vectors (colored according to the gas temperature) and diethylzinc precursor into an ALD reactor.



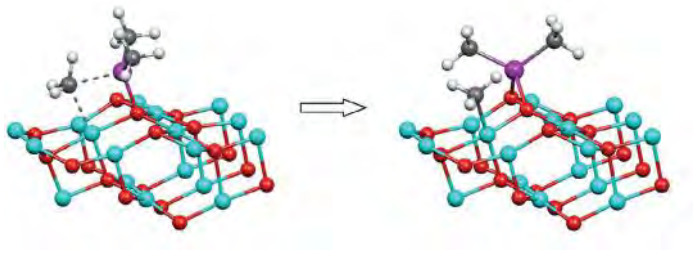
© Rémi Vallat, Christophe Vallée, LTM / CNRS, UGA, Rémy Gassilloud, CEA-LETI

Controlled selective TiO_2 deposition on TiN vs SiO_2

120 RESEARCHERS
INVOLVED IN
26 LABORATORIES

PROSPECTS

The RAFALD community is pursuing its mission to propose processes for the elaboration of increasingly high-performance materials, and with new functionalities. While applications in the field of microelectronics occupy an important place, the GDR laboratories are also involved in new application areas of ALD. Materials (oxides, nitrides, metals, sulfides...) applied to renewable energies (fuel cells, photovoltaics...), to medicine and biology (biosensors, implants, membranes for the detection of biomolecules…), to technical textiles or to the environment (water treatment, sensors and gas filters...) are developed. The manufacture of two-dimensional materials (hBN, transition metal dichalcogenides) and MOFs (metal-organic frameworks) by ALD are also growing fields.



© Alain Estève, LAAS/CNRS

Dissociative chemisorption process of TMA (TriMethylAluminium) reacting with CuO(11-1) surface.

The strategies of the RAFALD community in these major application areas are based on the following axes:

– Precursors chemistry, with the emergence of new precursors for innovative processes such as ALE (Atomic Layer Etching), and the study of precursor evaporation dynamics. These studies can be made more efficient with the development of very low cost / high flow reactors for the systematic screening of precursors.

– The development of innovative processes and support towards industrialization: high throughput ALD or FAST ALD including SALD (Spatial ALD); selective ALD (Area Selective Deposition , ASD); ALD on powder or infiltration of porous organic materials; MLD (Molecular Layer Deposition) for the deposition of organic and hybrid molecular layers; as well as the associated multi-physical modeling.

– The understanding of growth mechanisms based on advanced characterizations (*in situ*, *operando* and *ex situ*), the development of model experimental systems and devices, and the contribution of modeling.

Finally, the GDR RAFALD wishes to get closer to research federations and GDRs focused on applications in order to publicize the technique, broaden the community and contribute to the development of ALD.

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http://rafald.org

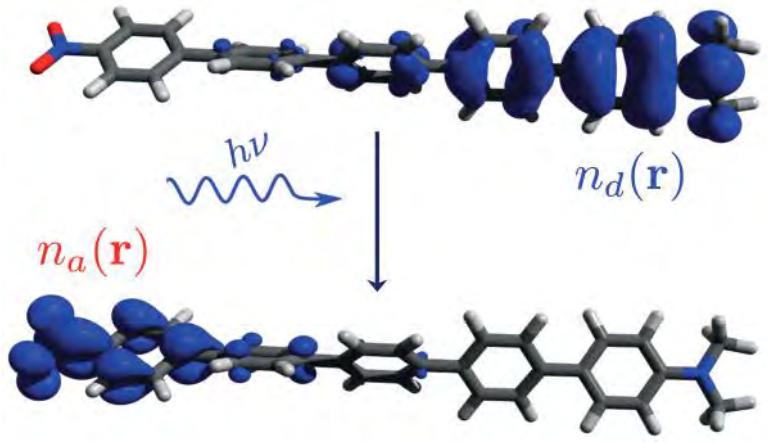
cnrs GDR Groupement de recherche
RAFALD Network of researchers involved in atomic layer deposition

GDR RFCT

French network for theoretical chemistry

OBJECTIVES

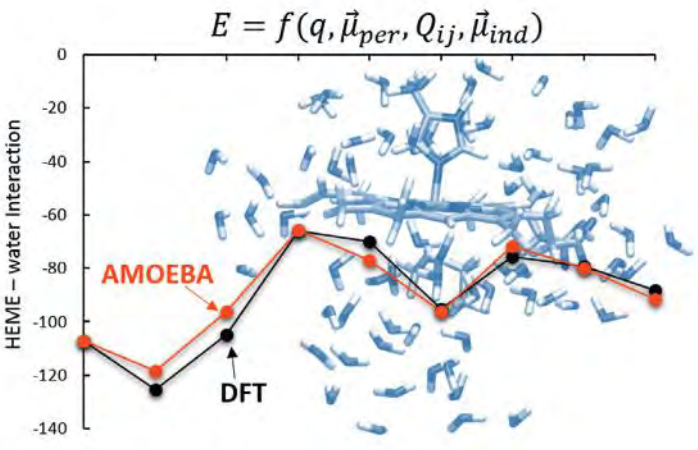
The RFCT was created in 2010 (and renewed twice in 2014 and 2018) and gathers theoretical chemists working in more than 50 different academic research laboratories all over France. This scientific community uses a wide range of common modeling tools to investigate numerous systems on the atomic and molecular scale. Its members work in many different fields such as chemistry, physics, biology and materials science. As a consequence, theoretical chemists can be found in all the sections of the CNRS Institute of Chemistry.



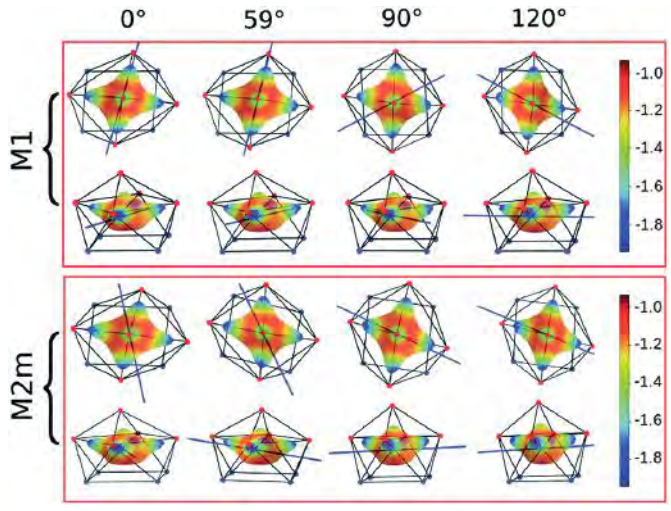
Molecular orbitals for the electronic transition in a donor-acceptor system.

THEMATICS

- Animating the scientific life of the community (financial support for conferences, alternating National Meeting and Forecast Meeting, Gaston Berthier Thesis prize)
- Training young researchers (both theoricians and experimentalists) with theoretical chemistry tools
- Promoting the software and methodological tools that are developed in french research groups (archival storage, support for initiating collaborations between research groups)



Interaction energies of the heme cofactor with droplets of water molecules computed with AMOEBA force field and DFT.



Electrostatic potential for lanthanide-based molecular magnets.

500 RESEARCHERS
INVOLVED IN
50 LABORATORIES

PROSPECTS

In 2022, the GDR RFCT will turn into a Research Federation on Theory, Modeling and Atomistic Simulations (ThéMoSia).
ThéMoSiA is a federation project covering several subject areas that aims at gathering all the researchers in France who develop or use methodologies ranging from quantum mechanics to mesoscopic simulations, with a common interest for the atomic scale. It lies at the intersection between numerous fields of research and application. Its members unite around the use and development of theoretical tools, in order to address the current and future scientific challenges. The goal of ThéMoSiA is to support researches on various scales, to promote knowledge sharing, to create bridges between methodologies, and to help the advent of new concepts. This project comprises three main axes:

RESEARCH

Numerous actions have already been initiated by the GDR in order to help start scientific collaborations or support the organization of scientific meetings. We also want to increase exchanges between members of our community during Forecast meetings that will tackle specific issues, and the National meeting that gathers all members, both taking place every year alternatively.

SOFTWARE LIBRARY

The goal of the software library is to offer a long term solution for the storage of softwares related to the ThéMoSiA research fields that are developed in french laboratories (wether they are designed for research or teaching purposes). We aim to promote these softwares by offering easily accessible storage place (in a open-access perspective) which will help the reproduction of results produced by these softwares. The library will also help setting up training sessions for researchers willing to learn how to use the softwares it contains.

TRAINING

The training part of the project comprises 5 goals. Setting up online training tools, training sessions for master and grad students *(Label de chimie théorique)*, organizing summer schools, training of the software users by the developers (with the collaborative call for proposal), and specific training sessions for the softwares stored in the software library.

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@RFCTheo

cnrs GDR Groupement de recherche
RFCT French network for theoretical chemistry

GDR RNA

RNA as a tool and a target for medicinal chemistry and chemical biology

OBJECTIVES

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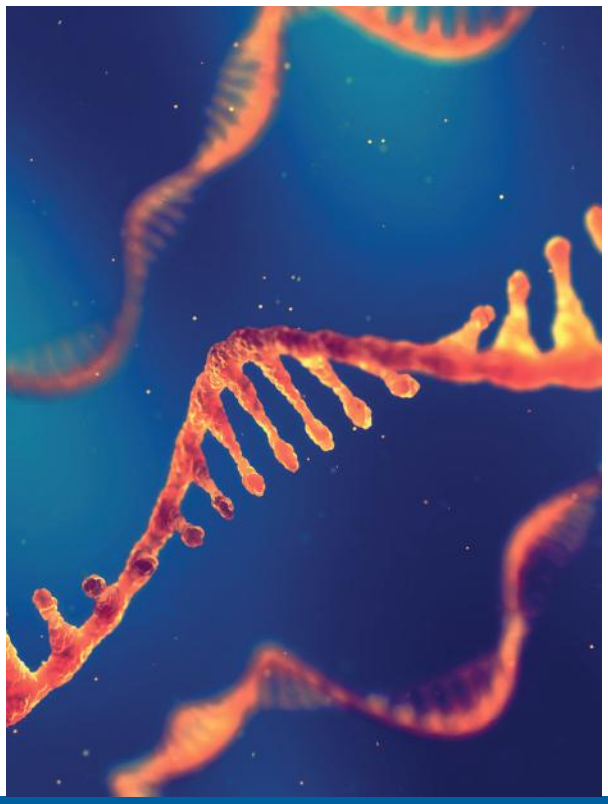
Several disciplines ranging from chemistry, molecular modeling, analytical chemistry, biochemistry, structural biology and cell biology are involved in the study of RNAs of therapeutic interest.

GDR RNA will allow to coordinate and federate the research efforts led by the teams working in the field of RNA targeting and RNA-based tools development. This GDR aims to foster national collaborations and to give to the RNA field the visibility it deserves in order to position French research as a European leader. A better structure and visibility of this community can also lead to strong valorization actions, either through the creation of start-ups or the reinforcement of industrial collaborations. The launch of new collaborations will also enable the development of innovative and long-term fundamental projects.

THEMATICS

- Design and synthesis of tools: from small molecule RNA ligands to modified RNA oligonucleotides
- Study of interactions: development of biochemical and biophysical tools for the understanding of interaction mechanisms at the molecular and cellular level
- Therapeutic applications: *in vitro* and *in vivo* models

RNA is a macromolecule essential for a number of biological processes.



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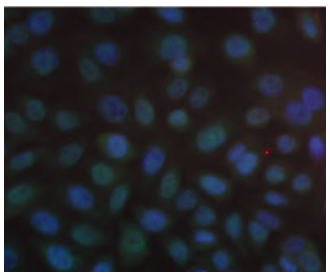

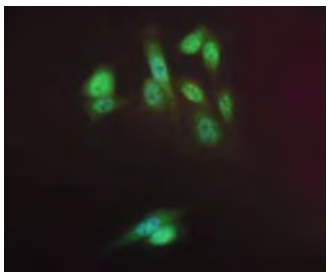

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Untreated cells overexpressing oncogenic miRNAS

Inhibition of cancer cells proliferation and expression of targeted protein

The study of the molecular mechanisms governing the functioning of RNAs or their ligands is essential in order to design more efficient tools.

130 RESEARCHERS
INVOLVED IN
25 LABORATORIES

PROSPECTS

The activities of the GDR RNA are focused on RNA research at the interface of chemistry, biochemistry, biophysics, cell biology and structural biology. They will allow the development of new therapeutic tools, with potential applications in therapy, and of new methodological tools in chemical biology, in order to better understand the molecular and cellular mechanisms in which RNAs are involved.

DESIGN AND SYNTHESIS OF TOOLS: FROM SMALL RNA LIGAND MOLECULES TO MODIFIED RNA OLIGONUCLEOTIDES

Targeting therapeutically relevant RNAs can be carried out using oligonucleotides that recognize a specific RNA sequence and therefore present a very high level of efficiency and specificity or using small-molecule ligands capable of interfering with the structure and / or function of the targeted RNA. Examples of structure-specific ligands (e.g., G-quadruplex RNA, bacterial riboswitch) have been identified and studied. The two approaches are therefore complementary and can converge for an efficient targeting strategy applicable to a large number of targets.

STUDY OF INTERACTIONS: DEVELOPMENT OF BIOCHEMICAL AND BIOPHYSICAL TOOLS FOR THE UNDERSTANDING OF INTERACTION MECHANISMS AT THE MOLECULAR AND CELLULAR LEVEL

The discovery of effective tools for targeting structured RNAs from a therapeutic point of view and the study of the biological mechanisms in which these RNAs are involved require a large amount of information. A close connection between the design and synthesis of ligands and expertise in biochemistry, biophysics and structural biology is therefore essential for the development of efficient and specific targeting strategies. All these studies will improve our knowledge of all parameters necessary to understand and rationalize the choice of targeting tools to be synthesized. Establishing these connections, also thanks to the network supported by the GDR, would be a relevant improvement for the success of research projects in the field.

THERAPEUTIC APPLICATIONS: *IN VITRO* AND *IN VIVO* MODELS

The tools designed and synthesized (oligonucleotides and small molecules) must then be validated *in vitro* and *in vivo* for their application in medicinal chemistry or chemical biology. In order to carry out these biological studies, it is thus necessary to develop appropriate study tools and models. The GDR RNA network will allow the necessary interactions to set up new collaborations towards more efficient studies.

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cnrs GDR Groupement de recherche
RNA RNA as a tool and a target for medicinal chemistry and chemical biology

GDR SFN – FRANCE

The french solar fuels network

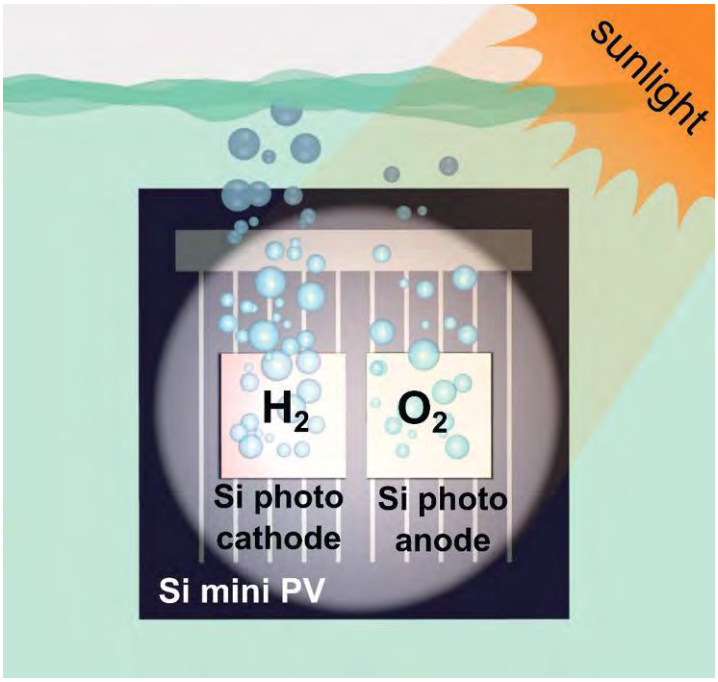
OBJECTIVES

The objectives of the GDR SFN-FRANCE are to:

– Gather experts in the field within a dedicated Research Group to promote exchanges and initiate collaborations between teams with complementary skills.

– Bring together expertise in materials science, molecular chemistry and biochemistry through the use of concepts and approaches (nanosciences, bio-inspiration, light capture and energy conversion, catalysis, reaction mechanisms), and the sharing of methodologies and tools (electrochemistry, photochemistry, advanced and coupled characterization methods, modeling and simulation).

– Enable the development of innovative processes in the field of solar energy.



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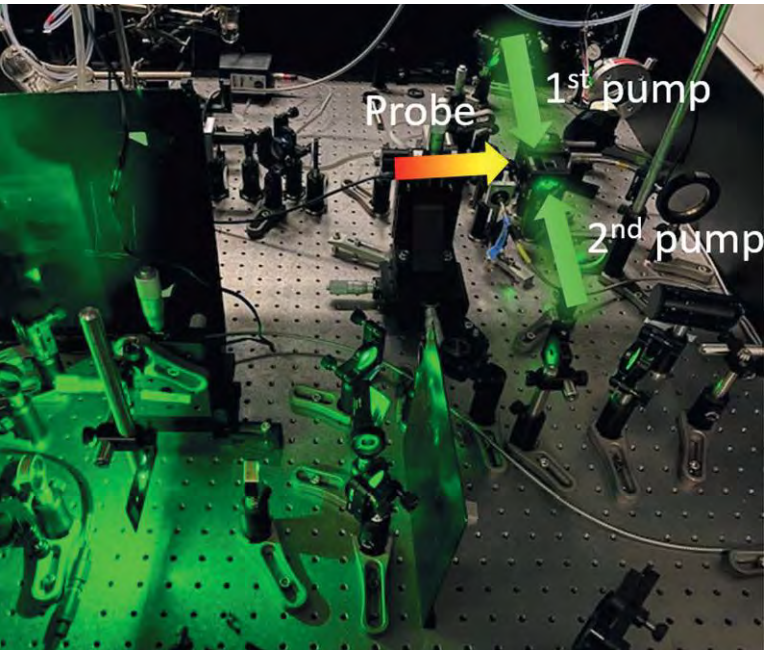
Silicon-based photoelectrochemical cell for hydrogen production from water and solar energy.



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Probing charge accumulation with advanced pump-pump-probe spectroscopic techniques.

THEMATICS

- Materials chemistry & nanosciences
- Molecular & bioinspired approaches
- Enzymatic systems
- Theoretical approach & modeling
- Chemical engineering & system integration
- Advanced characterizations & methodologies

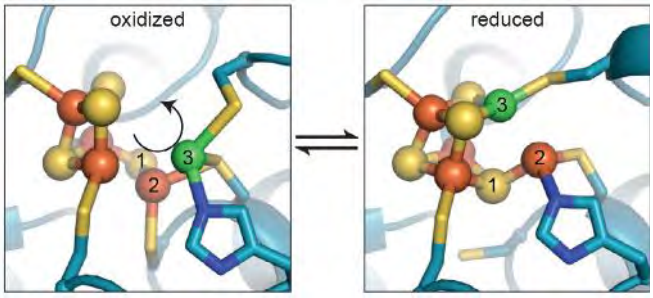
130 RESEARCHERS INVOLVED IN 55 LABORATORIES

PROSPECTS

Over the last five years, research efforts dedicated to the production of solar fuels have been significant on an international scale and are gradually taking shape with the emergence of innovative approaches in bio-chemistry, molecular chemistry and materials science, but also with significant advances in the characterization and modeling techniques for these systems. Meanwhile, a new step is being taken at the European level with the SUNERGY initiative, which is helping to define the European roadmap to meet major scientific and technical challenges of the energy transition. The GDR SFN-France, as a support to this action, must be the privileged place for French researchers to exchange on the field, thus allowing synergies and a common response to future European calls for projects.

Over the period 2016-2020, the GDR Solar Fuels has contributed to these efforts, by, on one hand, enabling structuring of the French scientific community in the field, and on the other hand, initiating new inter-team collaborations, with already very promising results. This new dynamics is extremely positive for our community and must be continued for the period 2021-2025.

The steering committee of the GDR Solar Fuels, in charge of the scientific animation of the network, is composed of the management and coordinators of the thematic axes. The organization of annual residential meetings, gathering the participants of the GDR, is central for the network animation. The annual solar fuel days are an important meeting and exchange place for the community, very interdisciplinary by nature. Young researchers are particularly highlighted during these days, giving them the opportunity to present their vision of the future of solar fuels, as they will ultimately lead the development efforts in this field.



Structural reorganization of the actif site of the CO-deshydrogenase enzyme, selectively reducing CO_2 to CO.

Gathering diverse but complementary expertise to exchange around a common scientific objective, the development and diffusion of solar fuels, this is the purpose of GDR Solar Fuels.

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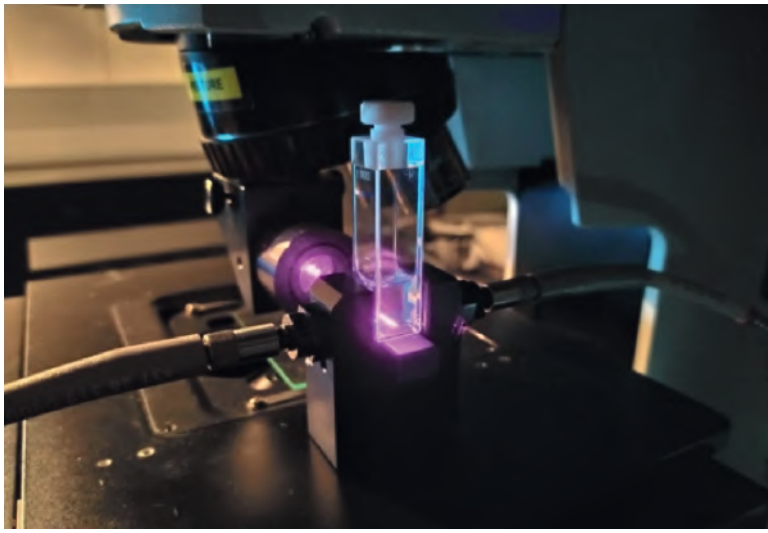
cnrs GDR Groupement de recherche
SFN – FRANCE The French solar fuels network

GDR SOLVATE

Solvation: advances in theory and experiments

OBJECTIVES

The importance of solvent effects has continuously pushed the boundaries of knowledge, in fundamental research as well as for technological applications. An essential mission of the GDR SolvATE is to bring out the general solvation question as a fundamental, interdisciplinary field of chemistry and chemical physics. We wish to promote exchanges among French researchers, theorists and experimentalists, who study the influence of solvent at the molecular level for the understanding of chemical processes, from complementary points of view. The organization of this dynamic community in a network of laboratories gives it an identity and leads to the emergence of cutting-edge projects involving partners outside the academic world as well.



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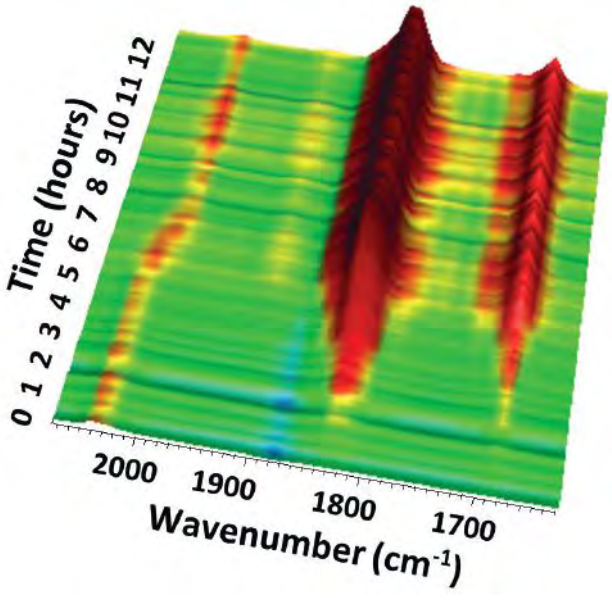
Simultaneous analysis by UV-Visible absorption and Raman scattering of an aqueous solution.



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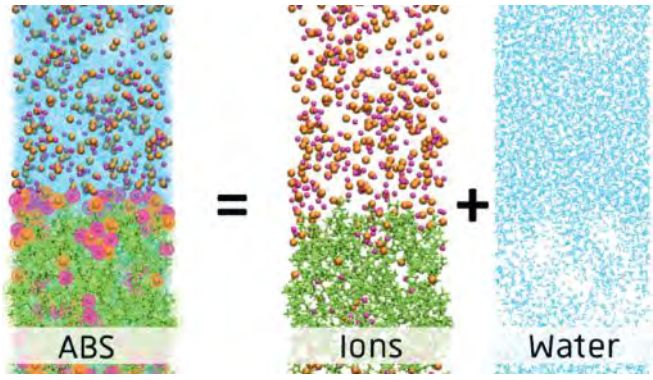
Kinetic study (ATR-IR) of the synthesis of α-alkylidene carbonate from the catalytic coupling of CO_2 with 2-methyl-3-butyn-2-ol.

THEMATICS

- Solvents in chemistry; towards a sustainable future
- Solvation and interfaces / surfaces, nanoconfined media
- Solvation in systems of interest in the biological and pharmaceutical field and for food processing



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Ionic liquid-based aqueous biphasic systems: molecular dynamics simulations.

100 RESEARCHERS
INVOLVED IN
37 LABORATORIES

PROSPECTS

The main objective of the GDR SolvATE is to promote the knowledge of the phenomena related to solvation in order to respond to well identified scientific challenges, including the optimization of industrial processes. The strength of this project lies in the interplay between theory and experiment and in the implementation of interdisciplinary approaches, leading to the development of original methodologies.

The GDR scientific project revolves around three research themes.

SOLVENTS IN CHEMISTRY: TOWARDS A SUSTAINABLE FUTURE

Developing fundamental research to clarify the effect of solvents on chemical reactivity will open important perspectives for technological and industrial applications. The interaction of specialists in the field will lead to new strategies to respond to societal needs for environmentally friendly processes.

SOLVATION AND INTERFACES / SURFACES, NANOCONFINED MEDIA

The chemical processes taking place at interfaces / surfaces and in nanoconfined environments reveal specificities that can be used to design a new chemistry in solution. The presence in this network of researchers is key to promote new interactions and the development of novel technologies (distillation, extraction, development of materials, electrochemistry, etc.).

SOLVATION IN SYSTEMS OF INTEREST IN THE BIOLOGICAL AND PHARMACEUTICAL FIELD AND FOR FOOD PROCESSING

From fundamental research to process design, our researchers are working to bring innovative insights into biological phenomena that are sensitive to the environment, to enable the development of biocompatible technologies and original analytical approaches.

HIGHLIGHTS

Since the creation of the GDR, a priority theme has emerged and generated new dynamics, that of deep eutectic solvents, and specific actions have been mounted around this innovative subject. Another theme that has brought us new synergies is that of solvation at solid-liquid interfaces, with possible interactions with other communities (electrochemistry, energy). Finally, important theoretical developments are underway in the field of calculations of free energies of solvation and the development of efficient force fields.

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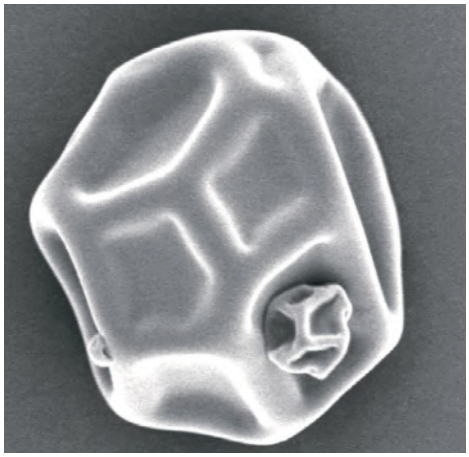
solvate.cnrs.fr

cnrs GDR Groupement de recherche
SolvATE Solvation: Advances in Theory and Experiments

GDR SLAMM
Driving soft matter

OBJECTIVES

SLAMM is a joint Research Group between CNRS and INRAE. SLAMM gathers within the same structure laboratories associated with the Department TRANSFORM of INRAE and laboratories associated with CNRS from three institutes: Chemistry, Physics, and Engineering and Systems. SLAMM Research Group presents a strong multidisciplinary character. Its mission is to gather different fundamental and applied research communities involved in the study of the behaviour of complex fluids at different length and time scales. The first objective of the SLAMM research group is the scientific animation in the area of Soft Matter, a highly active community in France, still loosely structured.



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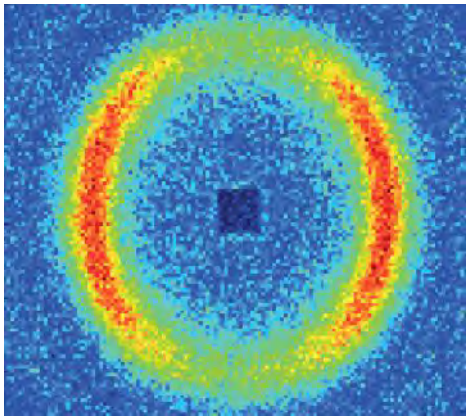
Micellar case in powder grain.



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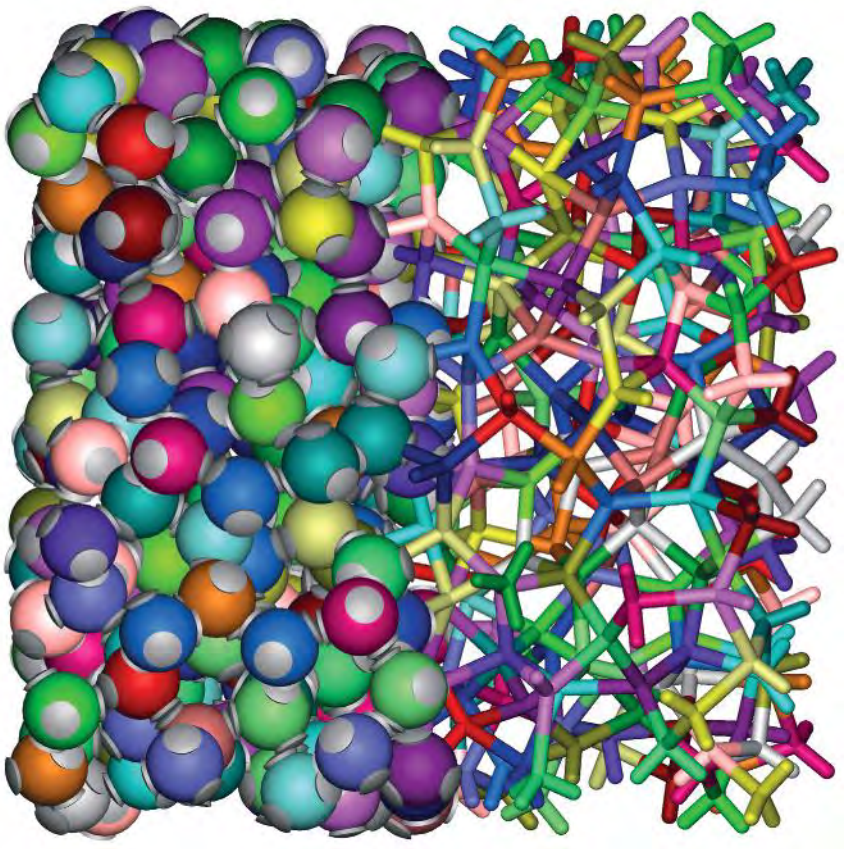
2D neutron scattering profile.



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Fluids of patchy particles.

THEMATICS

- Interactions and assembly in volume and at interfaces
- Transport and diffusion
- Multi-scale structuration
- Deformations and destructuration under mechanical stress

300 RESEARCHERS
INVOLVED IN
40 LABORATORIES

PROSPECTS

SLAMM proposes to characterize, rationalize, model, and predict the complex behaviors of soft matter, at equilibrium and under the effect of solicitations, with two main motivations:
– identify universal behaviors, common to many experimental systems and
– answer more specific questions related to applications, complex fluids being indeed omnipresent in everyday life (food products, cosmetics, sludges, paints…), and at the heart of many industrial fields, such as food, coatings, or enhanced oil recovery.

SLAMM brings together physics, chemistry, food and bioproduct sciences, and chemical engineering in a single structure, with a rich community of around 300 researchers from about 40 laboratories. The main missions of SLAMM are the structuring and scientific animation of this community through:
– sharing of scientific knowledge,
– the provision and circulation of useful information to researchers,
– the catalysis of multidisciplinary interactions and
– opening to the industrial world.

To carry out these missions, SLAMM relies on regular scientific meetings organized in several formats:

– thematic workshops addressing current topics, scientific and / or technological questions such as: *Transport and diffusion in soft matter*; *Are proteins colloids / polymers like any other? Rheological behaviour at large deformations*, with presentations by SLAMM members and invited lectures given by international speakers;

– annual plenary meetings which allow one to initiate exchanges between young and confirmed researchers by combining animated poster sessions, short scientific presentations and plenary lectures. The organization of round-table discussions allows one to assess methodological aspects[1], as well as access to large measurement instruments and their contribution[2];

– training is covered by online courses-conferences on transverse techniques or concepts *(e.g. electrostatic interactions in soft matter, scattering techniques, NMR for soft matter)*.

1 *Measurement methods for a heterogeneous sample: sampling and representativeness*

2 *Users synchrotron radiation and Upgrade SOLEIL horizon 2025: What do you expect from the upgrade in your research topics*?

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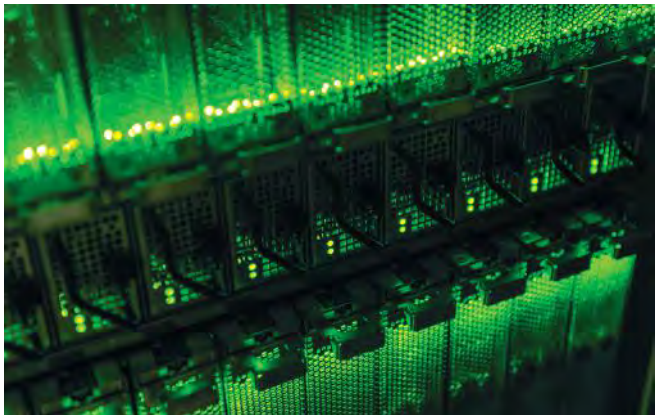
cnrs GDR Groupement de recherche
SLAMM Driving soft matter

GDR SNMS2

Natural substances: methods and strategies of synthesis. Tomorrow's challenges

OBJECTIVES

The objectives of the GDR SNMS2 will be to encourage exchanges between several communities of scientists interested in multi-step organic synthesis, theoretical chemistry and computer science. Questions concerning data management, a crucial point related to the laboratory notebook, and experimental prediction will be addressed. Through the setting up of interdisciplinary scientific meetings and training actions, we will seek to develop skills and encourage the emergence of related themes. Finally, we will seek to facilitate spreading of scientific and technical knowledge among teams, and towards industry and society.



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Computing nodes of the Jean Zay supercomputer capable of executing 13.9 10^{12} operations per second.

THEMATICS

- Strategies towards an ideal synthesis
- Total synthesis & machine learning

© Laurence Médard, CNRS Photothèque

Laboratory book for reporting dauly experiments.

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Experiment in lab: usual device for organic synthesis.

190 RESEARCHERS
INVOLVED IN
26 LABORATORIES

PROSPECTS

Within the framework of total synthesis, and organic synthesis more broadly, the learning machine can be used to perform different tasks.

RETROSYNTHETIC DISCONNECTIONS

A program can propose retrosynthesis for a given molecule. To train such a program, a large corpus of reactions is required. Historically, these approaches began in the 1960s with Corey's LHASA program, based however on pure retrosynthetic logic. Other programs can help with disconnection, by identifying the most bridged cycles that Corey believes should be disconnected first. Today, the learning machine should be able to improve its ability to solve increasingly complex problems.

PREDICTING THE FEASIBILITY OF REACTIONS

A program can predict the feasibility of a given reaction and its main products. Such a tool also requires a large corpus of reactions to train it. It could be coupled with data from molecular modeling and theoretical chemistry.

AUTOMATED EXPERIMENTAL RESEARCH OF REACTION CONDITIONS

For a given synthesis step, the identification of reaction conditions allowing to reach a sufficient yield or selectivity may require a large number of experiments. Automated exploration of reaction conditions (solvents, catalysts, additives, process variables) can save researchers a lot of time and allow them to focus their efforts on other tasks with higher added value such as retrosynthesis. This exploration of the reaction conditions can be driven by a machine learning program. Such a program requires much less data than the two previous ones, because it learns as the experimental trials are carried out using a synthesis automaton, or to carry out reactions in parallel, to speed up data generation and thus the optimization process.
Access to data is essential to be able to train machine learning programs.

LABORATORY NOTEBOOKS are a very important source of data of "successful" and "failed" reactions, which is a very positive point for machine learning algorithms to learn efficiently, unlike databases and articles, which contain a large majority of "successful" reactions. Finally, in addition to these experimental data, data from theoretical chemistry, such as calculated activation barriers, could also be used, in particular to predict the feasibility of reactions.

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Website in construction

cnrs GDR Groupement de recherche
SNMS2 Natural substances: methods and strategies of synthesis – the challenges of tomorrow

GDR SYNTH FLUX

Organic, inorganic and macromolecular synthesis in continuous flow

OBJECTIVES

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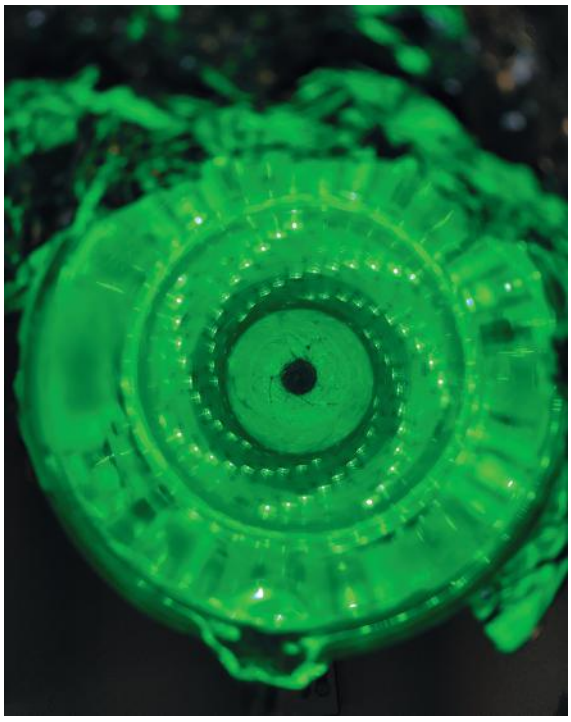
Device for synthesis in continuous flow.

Unlike other sciences that have revolutionised their concepts in recent decades, synthetic chemistry has been using roughly the same tools since the 1950s, especially the reactor. Today, there is however an alternative technology to these batch macroreactors: the miniaturised continuous flow reactors.

Created in 2019, the GdR Synth Flux aims at federating emerging continuous flow chemistry laboratories and to promote this technology. Particularly, it creates bridges between process engineering, analytical and synthetic chemistry, formulation and automation, and even autonomization, in order to think about the chemistry of tomorrow.

THEMATICS

- Fine chemistry (methodology, medicinal chemistry, scale-up)
- Nano-, macro- and supramolecular objects and systems (nanoparticles, polymers, formulation)
- Tools and methods (reactor design, in-line analysis, autonomization)



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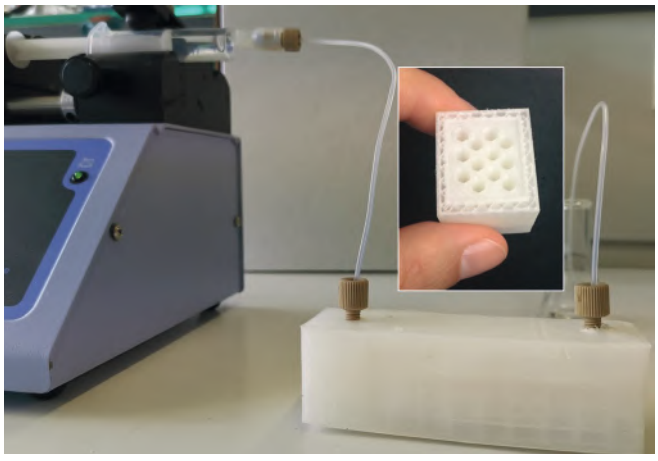
Tubular photochemical reactor.



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Flow microreactor manufactured by 3D printing and cross section.

150 RESEARCHERS
INVOLVED IN
28 LABORATORIES

PROSPECTS

POLYMERS
Chain lengths distribution and average chainlength (key parameters orienting the properties of polymers) are strongly affected by concentration and temperature gradients within the reactor. Continuous flow reactors allow homogeneous transfer conditions during synthesis, while enabling the use of extreme operating conditions, in order to significantly increase monomer conversion rate, the average molar mass and a better control of chain growth.

NANOMATERIALS
The introduction of micro- and milli-fluidic techniques has revolutionized the synthesis of nanomaterials, affording better control of operating conditions and better reproducibility. Continuous flow offers a solution of choice for the production of new nanomaterials with multiple applications.

FORMULATION
The formulation of emulsions has not escaped the boom in microfluidics. Research has been carried out to understand phenomena related to their stability or the development of particles and complex structures. Indeed, multiple emulsions are often the “matrix” for obtaining microcapsules or vesicles and research aimed at developing pharmaceutical or cosmetic applications is constantly increasing.

PHARMACEUTICAL CHEMISTRY OF THE FUTURE
Continuous flow devices offer integrated systems for the discovery and production of bioactive molecules while reducing the number of intensification steps. The flexibility of these devices allows different analysis tools to be connected to them for real-time reaction monitoring. In addition, the system is fully computer-controlled and advances in artificial intelligence (via ‘machine learning’) should make possible, in the near future, to have fully automated or even autonomous systems for drug discovery.

NEW FLOW REACTORS
The accessibility of CAD and 3D printing makes it easy to produce reactors with geometric characteristics specifically adapted to target reactions. These custom-built reactors allow a selective intensification of physical and chemical processes.

TRAINING
While batch reactor production is rather simple, continuous flow production requires a higher level of technical expertise. The development of flow synthesis is therefore a unique opportunity to boost local industries and increase their innovation potential.

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https://gdrsynth-flux.cnrs.fr

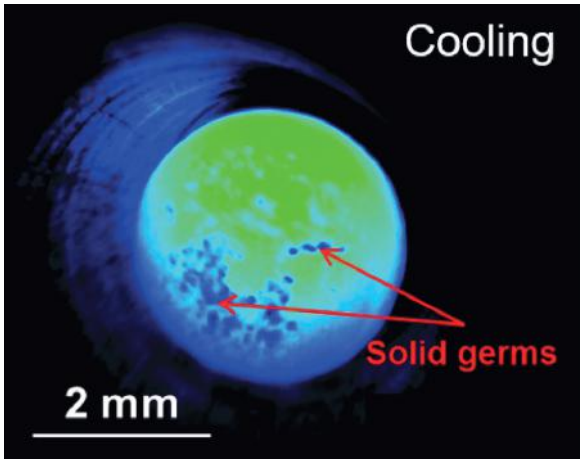
cnrs GDR Groupement de recherche
Synth Flux Organic, inorganic and macromolecular synthesis in continuous flow

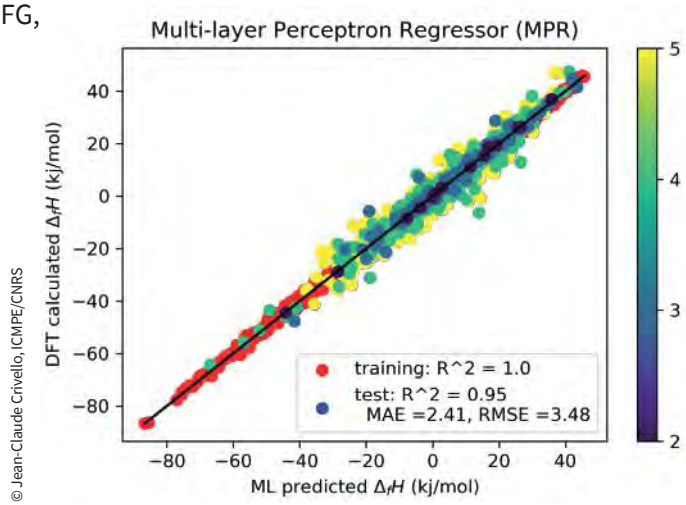
GDR THERMATHT

Materials thermodynamics at high temperature

OBJECTIVES

GDR THERMATHT was initially created with the objective of bringing together, federating and structuring the French community active in the field of thermodynamic data acquisition. The GDR scope goes actually far beyond data acquisition, opening itself to *ab-initio* calculations, Calphad modeling and more broadly to modeling of materials as well as their synthesis and transformation processes. The GDR also aims at promoting the discipline of thermodynamics, which involves the organization of 3 thematic schools and short training courses, through actions to open up to other communities in France (metallurgy, GDR Glass, etc.) and to abroad (DFG, APDIC, ThermoCon in the USA).





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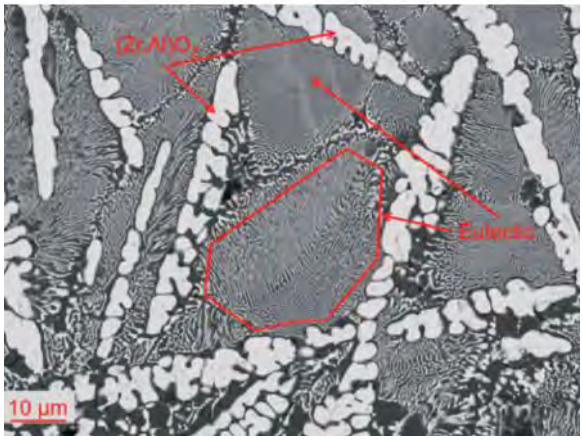
Coupling DFT calculations and machine learning to predict enthalpy of formation.



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Liquid Al_2O_3-ZrO_2 drop in levitation and its final microstructure. ATTILHA installation at CEA-Saclay.

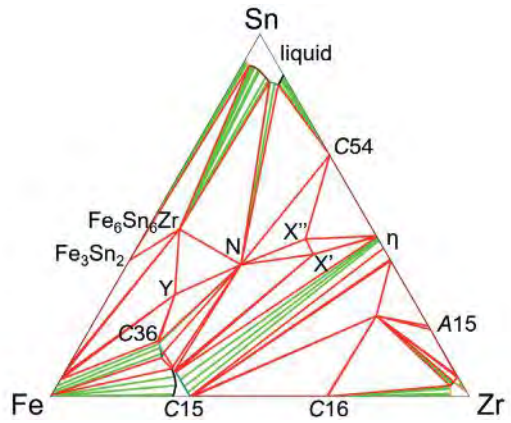
THEMATICS

- Thermodynamics of glasses
- Ultra high temperature measurements
- Calculations
- Metallurgy
- Silicon carbide

160 RESEARCHERS
INVOLVED IN
40 LABORATORIES

PROSPECTS

For several years now, we have seen the emergence of digital techniques in materials science, with of course modeling which is becoming more and more quantitative at all scales, the design of alloys but also the advent of artificial intelligence that supports the development of new materials. These three directions highlight the critical need for reliable energy data and models on which calculation can be based.



Isothermal section of Fe-Sn-Zr system @ 900°C.

The acquisition of thermodynamic data, through experience or *ab-initio* calculation, will therefore remain an important topic for decades to come. Much remains to be done, especially on refractory and ultra-refractory materials for which measurements are difficult but essential in many respects. One could cite as an example calcium aluminate which is a key compound in earth science and planetology as well as for industrial applications such as aluminous and Portland cements. Their thermodynamic properties at very high temperature (T> 2000K) are not well known and uncertainties exceeding 40% are frequently observed. Taking into account minor or trace elements in metal alloys, hitherto largely neglected, is becoming increasingly important with the aim of always better controlling and optimizing properties.

Historically, the Calphad method was developed on the basis of simple parametric energy models of practical interest but not representative of physics. The current trend is towards the development of so-called third-generation thermodynamic bases whose energy models are more firmly anchored in physics. It is for example important that heat capacities be compatible with the model of Einstein or to determine a model allowing an adequate and continuous description of the vitreous solids, between liquid and the crystal.

The perimeter of GDR THERMATHT was that of the bulk thermodynamic properties of phases. Interactions with other communities have highlighted a lack and therefore a need to make an effort on other thermodynamic quantities such as interfacial quantities or those associated with diffusion. Here again, process modeling requires the use of these quantities and therefore an effort in terms of measurement, understanding and modeling.

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http://www.thermatht.fr

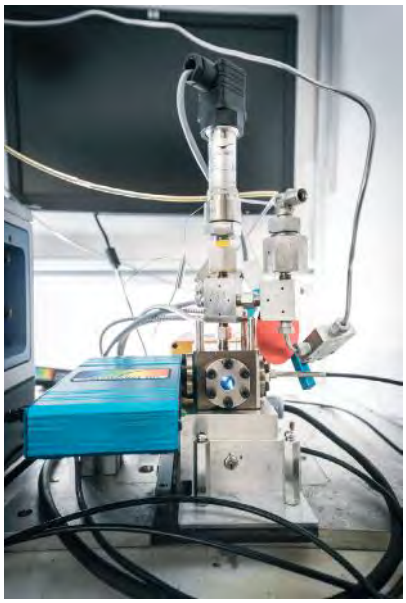
cnrs GDR Groupement de recherche
THERMATHT Material thermodynamics at high temperature

GDR THERMO

Molecular thermodynamics and methods

OBJECTIVES

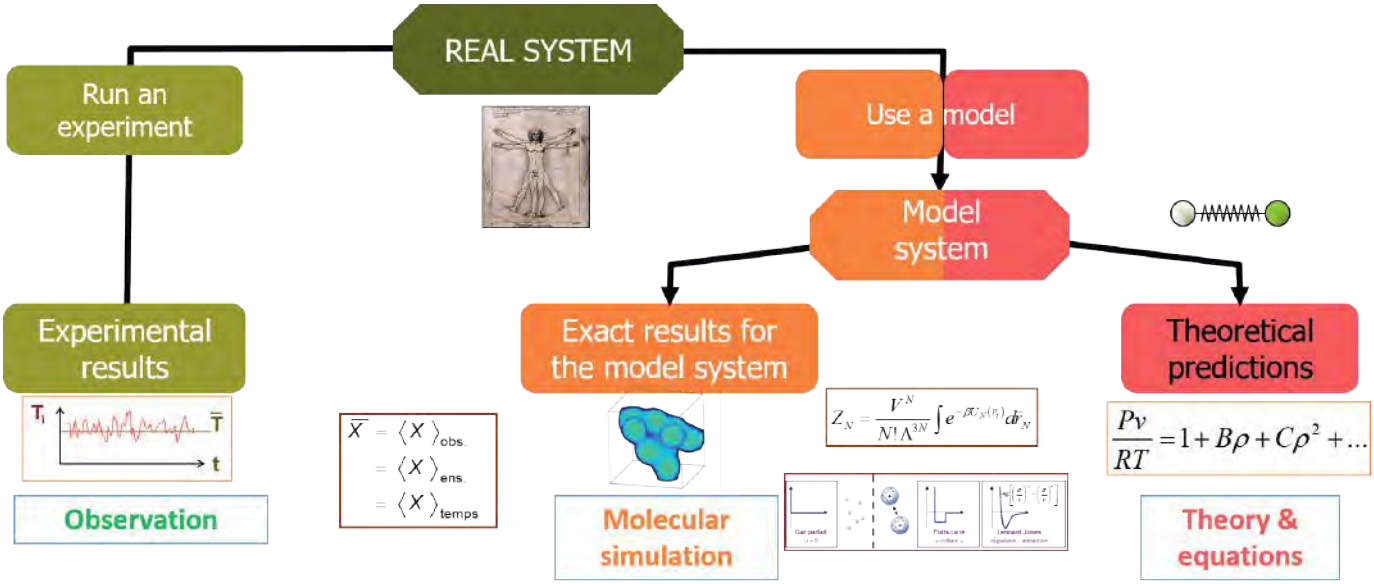
The objectives of the GDR THERMO are to:
– animate the community around molecular and process thermodynamics, energetics and nonequilibrium thermodynamics, in collaboration with existing academic societies;
– support and promote activities around modeling and experiments;
– propose interdisciplinary topics in relation with thermodynamics;
– organize platforms including experimental devices and modeling tools, with the aim to improve methods and develop new techniques;
– give thermodynamic classes to students and professionals and
– animate a club of industrial partners.



Viscosity measurements.

THEMATICS

- Molecular thermodynamics
- Thermodynamic properties
- Equilibrium thermodynamics
- Energetics
- Nonequilibrium thermodynamics

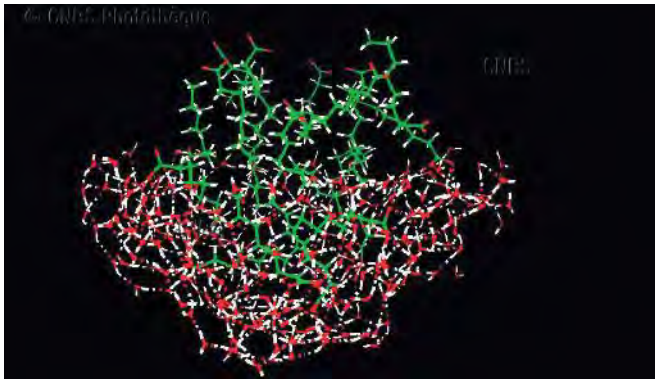


Thermodynamics merges experiments, theory and simulation.

80 RESEARCHERS
INVOLVED IN
24 LABORATORIES

PROSPECTS

Since 2012, the GDR THERMO aims at federating communities of thermodynamicists dispatched in several fields, like chemistry, chemical engineering, energetics of physics. Within each field, they already meet in events organized by scientific societies, like SCF, SFGP or SFT. These institutions are also invited to events organized by the GDR, often on a 2-day basis, with a special teaching action in favor of students.



Molecular simulation of a liquid mixture.

Research activities of the members of the GDR aim at getting physico-chemical datas, by using experiments and molecular simulations, as well as at developing thermodynamic models for material systems in various physical states (solid, liquid, gas, supercritical, …) of pure components and mixtures. We also promote multiscale approaches and theoretical developments using Thermodynamic 1st and 2nd principles via various concepts related to statistical thermodynamic, exergy, entropy production, finite time thermodynamic, nonequilibrium thermodynamic, or nonextensive thermodynamic.
The following research fields are nonexhaustively covered:

– investigation of new chemical families (ionic liquids, deep-eutectic solvent), development of technological fluids for substituting existing fluids ruled out by the REACH regulation (solvents, absorbents, coolant, calorific fluids, hydraulic fluids, lubrifiants), electrolytes used in in electrochemical devices (fuel cells, battery, supercapacitors), for dissolving or enhancing properties (polymer plastifiers, cellulose dissolvant), for manufacturing supported liquid membranes or gels;

– study of complex, heterogeneous or nanostructured systems: investigating and understanding phenomena, developing manufacturing processes, exploring stability of systems, multiscale modeling and

– study of large scale integrated systems, within the scope of energy transition: dynamics of the sysem trajectory, process and supply chain energy and exergy analysis, energy dissipation, free work.
Perspectives of the GDR are foreseen to concern new fields where thermodynamic is at work: biological systems, from cell to the whole living body, or social systems and economics.

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THERMO Molecular thermodynamics and methods

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