General outline of the project

On the basis of the **actual skills** of the Labex members and the **current trends** in the field of materials, the proposed research program will still be based on the investigation of functional and structural materials, photonic devices and process development (not explicitly considered as a research axis in the previous project, but present in a lot of projects). It will be structured around four research themes and two large experimental and numerical platforms gathering all accessible facilities concerning characterization and processing routes on the one side and processes and materials modeling on the other. It integrates some **emerging research themes**, which have not yet been supported by the Labex as the elaboration and study of metamaterials and waveguide arrays, 2D materials, heterogeneous graded materials (HGM), hybrid materials and nanostructures for various applications, the experimental and numerical investigation of “smart” composite materials and the use of plasma for surface treatment or hydrogen storage. The outline of the project is presented in the table below. The new themes include some research topics that are emerging within the different laboratories, for which at least one laboratory develops already high-quality international research and leadership, and which were not considered in the previous SEAM project.

Axe	A Functional materials	B Structural materials	C Photonic materials &devices	D Surfaces& Interfaces / Processes
Old themes	A1 – Diamond and carbon-based (nano) materials A2 – Inorganic and hybrid nanomaterials	B1— Microstructure optimization for enhanced mechanical properties B2—Smart structural materials	C1—Photonic crystals & hybrid materials C2—Integrated Micro and Nanophotonics	D1 —Surface functionalization D2 — Elaboration and Transformation
New themes	A3 – Low Dimensional Materials and Devices	B3—Heterogeneous Graded Materials (HGMs)	C3 —Metamaterials	D3 — Surface treatment D4— Printed and Flexible Electronic
Platforms	Characterization—Platforms, clean rooms			
	Multiscale Modeling of Materials and Processes			

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A. Functional Materials

A.1 Diamond and carbon-based (nano)materials

This sub-axis gathers researchers who elaborate diamond at different scales (macro, micro or nanoscale) or who analyze carbon-based materials or nanostructures (CNTs, C60, graphene). ***Some new associations of carbon-based materials leading e.g. to the elaboration of heterostructures will also be explored, as the use of some of these materials, such as graphene, for energy storage.*** Applications concern mainly photonics (with axis C) and electronics, including power electronics and molecular electronics, detectors, etc. The main motivations for the investigation of carbon-based nanostructures and diamond are to elaborate them with varying purity and structure depending on the application, to produce them in large scale and to make them amenable to a vast variety of (electro-)chemical and physical treatments prior to their use as components in high-tech devices.
For diamond, LSPM, in collaboration with ITODYS, LPL, MPQ, will continue to focus on overcoming the scientific and technological bottlenecks that are still preventing diamond from playing a central role in the field of electronics (especially power electronics), in optoelectronics or photonics, particularly the inhibiting dislocation propagation in bulk diamond, the fabrication of diamond active/passive multi-layers and color centers networks for photonic structures.

A.2 Inorganic and hybrid nanomaterials

The main objectives of this sub-axis are to establish a clear link between the structure of metallic, oxide, semiconductor **nanomaterials** (ultra-thin layers, quantum boxes, nanoparticles, nano-structured bulk materials) and their **physical properties** (electronic, magnetic and optical), including also superconductivity, photonics, and multiferroïcity. The ultimate goal is to elaborate **new devices** from these new functionalities. The efforts will be pursued first to produce **new inorganic or hybrid nanostructures** by chemical or physical routes, then to optimize deposition techniques to produce thin films, functionalization for surface coating or powder compaction to produce nanostructured bulk metals and ceramic**.** The large available elaboration and characterization facilities offered by the SEAM Labex will allow exploring more widely the vast application field of such materials.
The elaboration of these nanomaterials and nanostructures, as well as the investigation of the coupling effects (such as magneto—electrical, magneto-mechanics) will be pursued, by tentatively introducing more and more the possibility of **predicting the effective properties and coupling effects of the studied nanostructured materials**, in connection with the researchers from axis B who develop such modeling tools for composite materials at various scales.

A.3 Low Dimensional Materials and Devices

New emerging physical phenomena such as exotic electronic phases, spintronic… are originated from **low-dimensional materials** (LDM) for which various orders of electron matter are competing. In close collaboration between physicists and researchers involved in the elaboration and characterization of nanomaterials (A1, A2 and C Axes), the following topics will be addressed:

Transport properties: Two dimensional dichalcogenides, such as WSe_2, hold new and interesting electronic and spin transport properties. A fully electrical controllable spin-valve, for example, can be conceived by connecting individual WSe_2 flakes with ferromagnetic and local gate electrodes. Effort will be focused on 2D Van der Waals heterostructures, based on the stacking of graphene, hBN, WSe_2 monolayers. High electrical conductivity and low thermal conductivity of 2D dichalcogenides make them particularly suitable for thermoelectric applications.

Local electronic properties: Interest will focus on the doping of LDM and on their interface with organic molecules or metallic nanostructures. Doping allows tuning the electronic band structure and chemical reactivity of the materials and can thus be exploited for devices as sensors. The interaction between doped materials and organic molecules or metallic nanostructures will also be investigated.

Low energy electronic dynamics: In LDM, interacting degrees of freedom such as the charge, spin, orbital, and lattice, give rise to a rich variety of collective orders: spin liquids, density waves and superconductivity (SC) are few striking examples. Detecting and controlling these orders and their collective motion is an emerging field with potentially far-reaching applications in terms of material design and enhanced functionalities such as superconductivity with higher critical temperatures.

B. STRUCTURAL MATERIALS

Because of more and more demanding performances, structural materials need to be studied under more and more **severe conditions** (thermomechanical loading conditions or chemical environments); Thus, not only their mechanical response needs to be investigated, but their physical and chemical characteristics also need to be simultaneously characterized, their coupled properties must be predicted and some efforts should be put on the control of their elaboration processes. All the aspects concerning material science have to be present, from the elaboration to the evaluation of their lifetime and recycling processes, through modeling and development of characterization tools, and this requires the aggregation of complementary competences to lead to significant progress.

B.1 MICROSTRUCTURE OPTIMIZATION FOR ENHANCED MECHANICAL PROPERTIES

This classical preoccupation of all researchers in mechanics of materials will rely within the Labex on

• The multi-scale investigation and modeling of the behavior of materials in plasticity, damage and fracture, based on the use of (i) original experimental techniques (in situ mechanical testing within SEM/XRD/AFM, large strain mechanical tests and strain field measurements, high resolution X-ray diffraction for stress field measurements and (ii) multiscale modeling procedures ranging from *ab initio* to finite element simulations, which can be applied to the study of all heterogeneous materials (metals, composites, ceramics, elastomers, solid foams) by taking into account the microstructural organization of composing phases, which can be determined experimentally. Starting collaborations between ITODYS, LSPM and MSC explore e.g. the development of **new composite materials for civil engineering**. **The developed models will also be validated on other materials, such as magnetic thin films, for which the mechanical resistance also is of primary importance**.

• The development of **nanostructured structural materials**, from nanopowders, based on the use and development of the unique LSPM elaboration and transformation platform comprising very high pressure devices, severe deformation and compaction (HIP) techniques, in order to further **develop (new) metallic alloys or composites** with ultrafine grains or multiphase arrangements with improved coupled properties. This part should greatly benefit from the collaboration with other teams of the Labex involved in elaboration and characterization of nanopowders (A axis mainly).

B.2 SMART STRUCTURAL MATERIALS

This sub-axis is a natural extension of B1, since the design of structural materials with improved mechanical properties can be extended with the addition of other functional properties, making the material “smarter” from the view point of its thermal, magnetic or electrical properties, or capable of resisting to severe environments with improved corrosion, friction resistance or biocompatibility. The project HEMA (selected in 2018), which involves researchers from LSPM, ITODYS and MPQ aims at developing **multifunctional High Entropy Alloys** (HEA) (with appropriate surface treatments for their use in severe mechanical conditions or biomedical applications).This will be performed in association with D axis for the development of new surface treatments and elaboration processes, and with the characterization platform to characterize the coupled mechanical and functional properties.

B.3 HETEROGENEOUS GRADED MATERIALS (HGMS)

If all the skills are now gathered within the Labex to elaborate, characterize and model more and more precisely, all kinds of finely architecture materials for coupled structural and functional applications, the general development of new multifunctional HGMs with superior or even disruptive properties (among which some bio-inspired ones) will necessitate going one step further by developing systematic materials multicriteria selection methods. However, this is not an easy task since some properties are intrinsically conflicting. In that context, the accent will be put on the use and the **development of numerical optimization procedures**, such as e.g. the topological optimization, classically used for the development of honeycomb geometries for mass reduction, to design new composite or hybrid materials or structures (like the pantographic structure, used in a growing number of applications) for combined properties. ***These tools developed for the design of structural materials will then be used for the design of functional hybrid nanostructures or photonic metamaterials, in addition to the numerical tools developed to simulate the electromagnetic, plasmonic, optomechanical or optoelectronic effects*** *(see below).*On the experimental side, **interface engineering and interface-related phenomena** such as strain gradient and back-stress buildup and their effect on the global properties are critical issues which will also be explored.

C. Photonic Materials and Devices

The goal of the axis is the development of **devices for the emission, detection, manipulation, storage of photons** in various regimes (classical, quantum, single object, collective phenomena). It contributes to the fundamental and applied research in the fields of optics, quantum physics, materials science, and semiconductor devices. It is a very active field at the international level as well as within the Labex. It takes advantage of the know-how in material science, modeling, fabrication, characterization making the strength of the Labex. Indeed, a large variety of material platforms for optics and optoelectronics is now available including III-V semiconductors, Si-based materials, diamond, graphene, oxides and photosensitive hybrids, π-conjugated organics, metallic nanoparticles… The design and the fabrication of these devices will fully exploit the cutting-edge instruments and modeling tools available within the Labex. Based on the strong collaborations already established, the axis will concentrate its efforts on three main research directions:

C.1 Photonic crystals & hybrid materials

Organic photonics and dielectric nonlinear photonic crystals, photosensitive oxides and hybrids for reversible laser microstructuring and photovoltaic (LSPM and LPL), Molecular plasmonics and surface enhanced Raman scattering (ITODYS), actively controlled hybrid photonic chips, arrays of waveguides and resonators (topological photonics, new functionalities...)

C.2 Integrated Micro and Nanophotonics

Optically and electrically injected quantum light sources, sources for dense coding of information (exploiting high-dimensional degrees of freedom), nano-optomechanics (high-speed Atomic Force Microscope, sensors, collective phenomena), mid-IR electrically injected OPO, devices for the generation of classical and quantum frequency combs for massively parallel communications.

C.3 Metamaterials

Nanostructured surfaces, also called metasurfaces when they allow the emergence of macroscopic properties otherwise unattainable, can not only facilitate the integration of optical functionalities in photonic circuits, but also replace bulky components which are today based on the propagation of light in free space. For the control of light, the frontier of research is to bring several of sub-micron semiconductor resonators into interaction with each other, in order to explore collective photonic phenomena and applications from optical manipulation and computation to quantum devices. Also, foam (liquid and solid) properties, their optimization to control sound propagation up to the design of metamaterials will be explored (biomimetic foams are being explored by MSC and ITODYS).

D. SURFACES & INTERFACES/PROCESSES

A lot of research projects inside the Labex are concerned with **surface (or interfaces) problems** (elaboration of thin films, functionalization of surfaces, grain boundaries within metals, …). Up to now, the main developments have concerned the nanostructuration of surfaces for functional applications and the wettability. These subjects will be continued, in connection with various investigations on functional and structural materials, but the program will also be extended to the very active research field of **printed electronics** and to more fundamental aspects concerning the understanding of the basic mechanisms, based on the interaction of an atom and a surface, active in surface nanostructuration. This axis will naturally include surface treatment. Additionally, research concerning elaboration and transformation of materials already present, will move further in the direction of new processes such as **additive manufacturing,** for which metal powder behaviour will be explored, as well as for polymers, non-Newtonian flows, unstable or turbulent flows, contact lines motions, extrusion flows, etc.. For such new processes, some specific efforts have also to be made on the process optimization, especially by numerical simulations.

D.1 SURFACE FUNCTIONALIZATION

ITODYS will continue to federate original research on sensors and biosensors using **functionalized nanostructured surfaces**. LSPM, LPL, MSC and MPQ will join ITODYS for specific studies.

The control of surface properties also is of utmost importance for fluid-solid interactions and intervenes in many practical situations (anti-wear, antifouling, anti-icing, etc.) where **wetting or adhesion between a liquid and a solid** are involved. Aspects which will be developed include:

(i) Complexities in wetting on simple surfaces and simple wetting on complex surfaces. Functionalization of hard or soft surfaces includes chemical coating, at macro to nano-scales, or the fabrication of micro- or nano-texturations, both dramatically changing the wetting and adhesion properties. The novel aspect will be to combine chemical and textural aspects, with the possibility of dynamically controlling the local wettability by external stimuli (temperature, pH). Also, the wetting of complex fluids on solids is an active and largely unexplored area, despite its relevance to industrial applications: ink jet printing relies on the use of liquids that contain colloids, salts, polymers, etc. As far as we know, knowledge on the wetting of such fluids is empirical. The expertise available in the Labex offers the opportunity to extend it significantly.

(ii) Wetting coupled to phase transition: the study of the influence of freezing processes on liquid spreading is driven by practical issues of frost formation on airplanes and windmills, but also on additive 3Dprinting. In simple situations of drop spreading, the liquid pinning seems to occur as soon as the speed of the solid front expansion overcomes the speed of liquid spreading. Strategies have to be developed to control and delay this freezing.

D.2 Elaboration and Transformation

The elaboration and transformation platform of the Labex is very rich and comprises plasma reactors (for e.g. diamond elaboration), facilities for soft chemistry (for the nanoparticles synthesis), for thin films elaboration, for nanostructuration, and possibilities of transformation through chemistry, or thermo-mechanical treatments. It is well distributed within LSPM, ITODYS and MPQ and has contributed to the success of several projects. It also comprises new equipment such as 3D printers for polymers (in P7 and P13) and a Hot Isostatic Pressing device allowing the post-processing of pieces fabricated by additive manufacturing. All these processes need to be optimized but they are already available for the design of multifunctional materials, or the development of a new alloying concept (HEA). This axis can thus lead to the development and to the validation (through the use of models and mechanical characterization) of **new multi-materials or new assembly techniques, which will have some potential applications for ecological constructions**.

D.3 Surface treatment

In terms of surface treatment, apart from the nanostructuration performed at ITODYS, some efforts should be made to develop cleaner and more effective surface treatments for enhanced surface and mechanical properties of metals. This has recently started with the use of microwave plasma in connection with mechanical surface texturing and classical thermal treatment to oxidize titanium alloys. This “multifunctionnalization” of surfaces will combine the expertise in mechanics for the control of the mechanical properties and the expertise in chemistry for the surface modification.

D.4 Printed and Flexible Electronic

This topic has developed recently within the Labex, with 2 structuring projects (P2M in 2016 and MECAMAG in 2017). It typically uses common printing equipment for defining patterns on material and creating electrical devices on various substrates, such as gravure, offset lithography or inkjet. Electrically functional electronic, magnetic or optical inks are deposited on the substrate, creating active or passive devices, such as thin film transistors, capacitors, coils, resistors.

Depending on the application, the accent is put on the printing method or on the investigation of the properties of the materials (substrate or deposited material) and of the response of the created device. The ongoing SEAM projects concern the development of the technique to print **functional materials on fibrous substrates** (for the manufacturing of smart devices such as active textiles) on the one side, and the optimization of **nanometers magnetic systems deposited on flexible polymer substrates** (for the development of flexible magnetic fields sensors, magnetic memories and high frequency devices) on the other side. In this case, the focus is made on the understanding of the influence of large strains (of the substrate) on the properties of the device. In both cases, a better understanding of the interactions between the substrate and the deposited material is essential.

E. PLATFORMS

E.1 MODELING AND SIMULATION

Finally, the efforts initiated in terms of modeling will be pursued to be able to use the different parts of the multiscale chain in more and more applications, but already, the strong, consistent, multidisciplinary and large expertise spectrum allows addressing almost all the issues that are encountered when working on **material design, investigation and elaboration**. The research activity performed at LSPM on the modeling and simulation of material elaboration processes will be associated with great benefit to the theoretical and numerical investigations performed at MPQ, MSC and ITODYS to **quantitatively** take into account the functional and structural constraints when developing elaboration processes. Examples of studies under way are the comparison between fracture and wetting dynamics, or the comparison of plasticity in foams and crystalline materials. Similarly, the models developed on fluid surface interaction will be combined with the models describing structural materials developed at LSPM in order to investigate the chemical, physical and structural changes of materials and their consequences on the behavior of the materials when used under specific conditions related to targeted applications.

E.2 INSTRUMENTATION

The platforms will also be developed so that they remain in the forefront of progress and can thus train students to the **highest level of technology**. This notably involves the structural characterization of materials (SEM, TEM, XRD), surface characterization (XPS), characterization of the mechanical, rheological and magnetic properties of materials, plasma reactors, tools for the development and production of materials, clean rooms for the development of devices, etc.
In the next 5 years, the following state-of-the-art instruments will become available to all members:

- **An environmental high resolution TEM** (MPQ) dedicated to the study of the structure dynamics of materials in well-controlled liquid and gaseous environments which opens immense fields of investigation in material synthesis, electrochemistry, catalysis, but also for structural materials.
- **A thermal-mechanical physical simulator** (Gleeble® machine, LSPM), whose testing and simulation capabilities include welding and additive manufacturing simulations, hot ductility, study of embrittlement and crack susceptibility.
- A new time resolved coherent **Raman scattering spectroscopy platform** at MPQ dedicated to the optical manipulation and real-time visualization of electronic and structural properties of materials as well as chemically sensitive imaging of molecules and nanoparticles. Combination of spectroscopic investigation techniques with rheological measurements are also under development at MSC (correlation between microscopic structure and macroscopic properties).
- The first dry cooled **scanning probe microscope (SPM)** developed in the world is currently installed in the Labex (MPQ). The goal of this new instrument is to achieve measurements at the sub-nanometric scale, either by scanning tunneling microscopy or atomic force microscopy, at low temperature (10K) without He consumption. It will couple light with SPM measurements to explore photo-induced phenomena at the atomic and molecular scale.