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FRANCE 2030

Exploratory Priority Research Programme and Equipment

Call for proposals

"DIADEME: Integrated devices to Accelerate the Deployment of Emerging Materials"

CLOSING DATE TO RECEIVE THE LETTERS OF INTENT: **15 JUNE 2023** AT 11:00 AM (CET)

CLOSING DATE OF THE CALL FOR PROPOSALS: **17 OCTOBER 2023** AT 11:00 AM (CET)

Consultation page for the call for proposals
https://anr.fr/PEPR-Explo-DIADEM-AAP

Contents

Summary

The DIADEM PEPR aims to transform, in the long term and in-depth, the way we address Materials Science in France, particularly to accelerate its development through synergies between the scientific themes guided by artificial intelligence, which impact, “from the idea to the object”, each stage of the innovation chain. This call for proposals intends to promote this multidisciplinary approach through methodological Interdisciplinary Research Proposals (IRPs) backing major scientific themes that were substantially strengthened by the national materials community.

This call for proposals focuses on two themes, one on the “Accelerating the discovery of innovative and sustainable materials for a Green Deal”, the other on “Accelerating the mastery of synthesis and shaping processes”. This call for proposals aims to elicit project proposals from structures organised in consortia and covering one of the aforementioned themes.

The call for proposals will be carried out in two stages:

- A first mandatory stage to pre-select the consortia. At the end of this stage, a limited number of consortia will be selected for each theme. If necessary, PEPR directors will facilitate the establishment of the consortia. The scientific scope of the proposals will also be approved at the end of this stage.
- The second stage will consist in submitting to an evaluation conducted by an international panel the proposals that were pre-selected in stage 1.

For projects lasting up to 4 years maximum, the expected proposals must address only one theme. Aid recipients are research institutions, and higher education and research institutions. Companies and foreign institutions may act as Partner Institutions within the proposals but will not receive any funding for their involvement. International cooperation is very much an option. The aid granted for each proposal amounts to between €800k and €1 million, for a maximum of €12 **million** for this call.

Keywords

Materials, Processes, Accelerated Discovery, High-Throughput Characterisation, Screening, Database, Artificial Intelligence, Modelling, Numerical simulation, Sobriety.

Important dates

The submission dossier must absolutely be electronically submitted before:

CLOSING DATE TO RECEIVE THE LETTERS OF INTENT: 15 JUNE 2023 AT 11:00 AM (CET)

At:

https://france2030.agencerecherche.fr/PEPR-Explo-DIADEM-AAP-lettre

The submission dossier must absolutely be electronically submitted, including the documents signed by the legal representative of each partner before:

CLOSING DATE TO SUBMIT THE PROPOSALS PRE-SELECTED IN STAGE 1: 17 OCTOBER 2023 AT 11:00 AM (CET)

At:

https://france2030.agencerecherche.fr/PEPR-Explo-DIAD__EM-AAP-dossier

OTHER IMPORTANT DATES

1st stage results: late July 2023
Starting date for proposals selected after evaluation: 1st quarter of 2024

ANR Contacts

For any question regarding the call for proposals: PEPR-DIADEM@anr.fr

SCIENTIFIC PROJECT MANAGER: MARION PATTE

PROGRAMME DIRECTOR: DOMINIQUE DALOZ

Please read carefully and thoroughly this document as well as the instructions available on the submission for the letters of intent:

https://france2030.agencerecherche.fr/PEPR-Explo-DIADEM-AAP-lettre

and for the full proposals:

https://fra nce2030.agencerecherche.fr/PEPR-Explo-DIAD_EM-AAP-dossier

For any question: PEPR-DIADEM@anr.fr

1. Background and objectives of the call for proposals

1.1. Background

Materials substantially shape the competitiveness of an industry through innovation which, under the Green Deal, must now more than ever be part of a virtuous path integrating economic, environmental and societal aspects. The DIADEM Exploratory Research Programme and Equipment (PEPR) pushes for an ambitious programme to accelerate the design of better-performing materials, which are sustainable and stemming from non-critical and non-toxic raw materials, and their arrival on the market, thus contributing to France's economic development. Such a programme must integrally combine modelling, numerical simulation, artificial intelligence (AI) methodologies, synthesis/screening technology and high-throughput characterisation. The objective is to identify new materials in response to given specifications, with a speed unattainable in the purely experimental process, where breakthroughs are often unpredictable. This acceleration requires the integration of teams/centres of excellence that bring together experimental platforms for synthesis and combinatorial formulation, shaping and high-throughput characterisation combined with multi-scale digital modelling, data mining and machine learning tools or, more generally, with adapted AIs.

The programme relies on a network of platforms intended to increase the materials identification cycle by two or five times - from 20 years to between 4 and 10 years. Ideally, these platforms will assemble:

i- Combinatorial and/or high-throughput synthesis of materials. The various methods of additive manufacturing are key to quickly develop new materials (metal, ceramics, possible bio-sourced polymers) but also new architectures, sometimes even evolving under the influence of a stimulus, as in the case of 4D printing. Surface engineering often becomes a must to achieve the desired final performances. Very special attention will be paid to the synthesis of new architectural, hybrid, bio-inspired or non-bio-inspired materials to optimise their structural or functional properties. Scaling up these laboratory syntheses will help introduce novel and faster industrial processes with low environmental impact.

ii- High-throughput chemical, structural (Large Soleil and ESRF instruments) characterisation, usability metrics (optical, magnetic, mechanical, corrosion resistance, etc.), use of sensors associated with *in situ* or *operando* characterisation, which are essential for high-throughput access and collection of massive amounts of data, particularly under extreme conditions.

iii- Numerical simulation and processes of materials. Multi-scale simulation tools, from *ab initio* to the macroscopic scale, including AI approaches, will be easier to use, interoperable and integrated into workflows to enable automatic and/or high-throughput calculations.

iv- Databases intended for AI storage, management and exploitation. Experiments and modelling will be increasingly automated, the resulting data will be structured in databases under a strategy to be decided (connection to local existing databases or

launch of a national database), AI tools specifically developed to improve their exploitation.

These 4 types of platforms, but above all their synergy (DIADEM HUB), will give rise to the ability to renew innovation in Materials Science.

1.2. Objectives of the call for proposals

This first DIADEM PEPR call for proposals aims to encourage the emergence and development of **Innovative Research Proposals (IRP)** intended to address the two themes of this call.

The proposals will be carried out in two stages:

1st stage: a first mandatory stage to pre-select the consortia through the submission of a letter of intent. If necessary, DIADEM PEPR directors will facilitate the establishment of the consortia. The scientific scope of the proposals will also be approved at the end of this stage

2nd stage: it will consist in submitting the proposals that were pre-selected during stage 1 of this call for proposals. The proposals will be subject to an evaluation by an international panel.

1.3. Role played by PEPR directors

PEPR directors are responsible for drafting the document setting out the objectives, scientific scope and themes of the call. They ensure that the call is consistent and complementary with the 17 targeted projects.

During stage 1, PEPR directors will be tasked with pre-selecting the consortia, if required, by facilitating the establishment of the consortia from proposals submitted separately.

PEPR directors may support project coordinators seeking to submit a proposal. Applicants to this call for proposals are strongly encouraged to contact PEPR directors as soon as possible to confirm if the theme and development considered for the proposal fall under this call for proposals. PEPR directors will also act as intermediary between the project proposals from the consortia and operational platforms to determine the best way to access them (subcontracting or partnership), but given the status in setting up the platforms, their use is not mandatory for this call for proposals.

For the next call for proposals in 2025 and 2026, DIADEM platforms should be routinely included in the proposals submitted.

2. Themes of the call and expected proposals

2.1. Themes

The DIADEM PEPR aims to transform, in the long term and in-depth, the way we address Materials Science in France, particularly to accelerate its development through synergies

between the scientific themes guided by artificial intelligence, which impact, “from the idea to the object”, each stage of the innovation chain. This call for proposals intends to promote this multidisciplinary approach through methodological Interdisciplinary Research Proposals backing major scientific themes that were substantially reinforced by the national materials community.

This call for proposals consists of two themes:

- **A theme focusing on “Accelerating the discovery of innovative and sustainable materials for a Green Deal” leading to applications for major transitions** (towards low-carbon energy and transports, frugal digital technology, and medicine of the future). These proposals must help strengthen the methods to accelerate the discovery of new families of materials of interests, by combining, if possible: interaction design, synthesis and high-throughput characterisation aspects, and data processing through artificial intelligence. When possible, these proposals should consider sobriety requirements regarding the use of critical (or toxic) raw materials, which should be substituted.

- **A theme focusing on “Accelerating the mastery of synthesis and shaping processes” to build or strengthen France’s technological sovereignty.** The objective here is to propose proposals to accelerate the development of 1D, 2D, 3D and 4D processes, particularly by combining approaches on numerical simulation, instrumentation, *in situ* monitoring and data processing through artificial intelligence. The idea is to push for machines with increased autonomy, even independent, and for the digital twin of sovereignty processes.

These proposals will therefore **cross disciplinary boundaries**. As illustrated by biology, creating a new discipline that combines Materials Science and Data Sciences requires overcoming thematic obstacles. This call for proposals is therefore a great opportunity to establish completely new consortia, both from a thematic and organisational point of view, by relying on the development process described in Appendix 1.

The call for proposals, which is intended for interdisciplinary research proposals, will focus on two main themes:

Theme 1: interdisciplinary research proposals to accelerate the discovery of materials for a Green Deal.

Under this theme, interdisciplinary proposals combining the numerical design of materials (e.g., the use of multi-scale simulation tools, from *ab initio* to the macroscopic scale), synthesis and high-throughput characterisation, processing the data generated from artificial intelligence approaches, will be favoured. With regard to the characterisation of materials, high-throughput approaches will focus on the chemical composition, structure (particularly Large Soleil and ESRF Instruments), micro/mesostructure and usability. A major issue will be to delve into complex phase diagrams, both in terms of chemical composition and assembly (coordination geometry, ligands, etc.). To do so, multi-scale modelling must be included in the optimisation loop within increasingly independent laboratories. Synthesis robotisation, and *in situ* and post-synthesis characterisation is one of the main objectives of the DIADEM platforms. The proposals selected will be challenged to adapt these tools to address specific scientific and technological issues. In addition to this robotisation, the development and use of sensors associated with *in situ* and *operando* characterisation is essential for high-throughput access and to collect

massive amounts of data associated with metadata, particularly under extreme conditions. Drawing upon the increased automation of synthesis, special attention will also be paid to the discovery of novel nano-structured, structured, composite and hybrid materials, to optimise their structural or functional properties. Monitoring the surfaces and interfaces within these multi-materials will be a main focus. As for the synthesis, this means discovering new avenues for chemical reactivity at interfaces by exploring extended, and eventually unexpected, precursor zones. As for the properties, confinement effects and properties being transferred at interfaces will be used to generate multi-materials with multi-properties.

Beyond the accelerated discovery of novel materials, using Artificial Intelligence will allow Materials Science to reduce the environmental impact of our research and development sector. First and foremost, the development of bio-inspired, bio-sourced and recycled materials must be draw on the methodological developments implemented in the field of biology. In addition, the use of non-critical resources, decreasing thermal budgets and recycling are major challenges, but still little explored when searching for new materials. The proposals selected must include this sustainable development and eco-design aspect for innovative materials. The accelerated discovery of novel materials is a first step towards scaling up these laboratory syntheses to new and faster industrial processes with lower environmental impacts. While remaining an exploratory PEPR, DIADEM cannot ignore this vital aspect when it comes to the various transitions that are underway.

Theme 2: interdisciplinary research proposals to accelerate the mastery of synthesis and shaping processes.

This theme aims to develop a holistic approach to synthesis and shaping process integrating numerical simulation, *in situ* and *operando* instrumentation, data processing through artificial intelligence to optimise complex processes more efficiently. The design and development of digital process twins is the way to demonstrate how this approach is efficient.

New features will emerge from couplings at interfaces within multi-materials, adding another degree of complexity and emphasising the need to use artificial intelligence. Two approaches will be favoured: a bottom-up approach based on architectural strengthening with basic components, and a top-down approach using material pixelation techniques.

The first approach will be based on three options: Additive Manufacturing, self-organisation and multi-layer production. The various additive manufacturing methods are key to developing different types of materials (metals and alloys, ceramics, possible bio-sourced polymers, composites) but also new architectures (including compositional gradient), and sometimes even evolving under the influence of a stimulus, as in the case of 4D printing. The self-organisation of materials with specific morphology and size helps monitor porosity at large scale, including nanoscale, leading to diverse fields of application. Technologies for thin film deposition, from monatomic two-dimensional layers to thick film, have reached a great level of maturity, including those of complex hybrid inorganic materials. Deposition processes vary to be adapted to these different scales. From now on, the objective is to develop multi-tier architecture from various compositions, and/or through additional deposit methods, and/or processes hybridisation.

The second top-down approach, which is complementary to the first approach, aims to locate samples within 3D or 2D macroscopic materials. This is the case for lithography or removal techniques, which define areas of interest within graded materials. Another non-destructive option aims to locally anneal a possible amorphous compound to create libraries of 2D or 3D crystallised samples.

Ideally, the preferred processes will be those in line with a sobriety approach, in terms of use of

resources and, also, the environmental impact. Generally, eco-design must be included in the definition of new processes and the life cycle of the materials manufactured must be fully analysed.

Interdisciplinary research proposals must address, **in the two areas above**, the scientific themes and techniques listed below. This list stems from the aforementioned challenges, the approach developed from the submission of DIADEM in July 2021, and the extensive community consultation conducted between October 2022 and January 2023. Over a thousand people took part in this consultation through the mobilisation of various authorities.

Among the different options to present these themes, PEPR directors opted for methods whose generic character can cover a wide range of applications, particularly to support major transitions (towards low-carbon energy and transport, frugal digital technology, and technologies for the medicine of the future). Similarly, to the development of DIADEM, having various materials and functions is not an issue, but an asset.

Scientific themes and techniques to be addressed in Interdisciplinary Research Proposals (2024 DIADEM CALL FOR PROPOSALS)

Numerical design

Numerical design of materials and processes

- atomic scale modelling (DFT, Monte Carlo, molecular dynamics, etc.)
- thermodynamics modelling for microstructure monitoring
- kinetic modelling for ageing monitoring
- structural topology optimisation
- non-equilibrium process modelling
- digital twins for processes and architectures
- high-throughput calculations

Materials property modelling

- electromagnetic property modelling
- electrical and thermal conductivity property modelling
- mechanical properties and corrosion resistance modelling
- mechanical, electrical and thermal conductivity and coupling at interfaces
- prediction of properties yet unmeasured

Materials high-throughput synthesis	Materials development and shaping processes (1D, 2D, 3D, 4D)
• high-throughput screening, synthesis automation and robotisation including *in situ* structural and chemical analyses • high-throughput sensors of synthesis parameters: precursors, geometry, thermodynamic conditions, pH • 2D compositional and microstructural gradient materials • 3D compositional and microstructural gradient materials through additive manufacturing • localised annealing/irradiation pixelation • materials with high compositional entropy: metal alloys, inorganic compound, polymers • hybridisation at unit cell, (nano-)particles and assembly scale • bio-sourced and bio-inspired materials	• high-throughput sensors & instrumentation of process parameters • additive manufacturing, synthesis and surface engineering, and solid integration of nano-objects • process pixelation • sobriety as a major parameter to implement processes • monitoring of interfaces and interphases in multi-materials • multi-scale porosity monitoring • relationships between microstructure and processing parameters

Materials characterisation

- measurement automation and robotisation
- high-throughput sensors for characterisation environment
- functional characterisation
- multi-scale structural characterisation
- multi-scale imaging
- measurement pixelation (including non-local properties such as ionic, electronic and thermal conduction)
- acceleration of degradation processes and their characterisation

Databases & Artificial Intelligence

- data mining
- metamodeling and metadata: design, synthesis, shaping, function
- optimised descriptors from synthesis to ownership

- correlational analysis of multiple and heterogeneous data
- learning through heterogeneous data crossing
- materials database as input for life cycle assessments

2.2. Main proposal characteristics

The proposals submitted must be in line with the general approach of the DIADEM PEPR. Thematic overlaps with other PEPRs (national acceleration and exploratory strategies) would be beneficial, but the idea is not to replace the proposals submitted to the calls for proposals covering these PEPRs.

Proposals must be collaborative, with at least two and up to 5 different research teams from at least two different research institutions or higher education and research institutions. The research teams involved in current Targeted DIADEM Projects may be involved in the partnership covering these projects. In addition to the funded partners, the proposals may absolutely include international partners providing their own funding. The same goes for industrial partners who may not qualify for funding under this exploratory PEPR, but who may be associated with the proposals.

The aid allocated to each proposal shall be between €800k and €1 million. For information purposes, the total aid granted, for this first call for proposals, will be €12 million maximum.

In addition, the breakdown between the two themes will be 2/3 for the theme focusing on "Accelerating the discovery of innovative and sustainable materials for a Green Deal", and 1/3 for the theme focusing on "Accelerating the mastery of synthesis and shaping processes".

Projects may last four years maximum. The proposals expected must:

- "Foster and/or support the transformation of some research stakeholders to strengthen its French attractiveness, European and worldwide development, along with its impact on economy and society" (cf. "Exploratory PEPRs" Call for proposals).
- Producing high quality research to strengthen the acquisition of disciplinary and/or interdisciplinary scientific knowledge to meet current and future challenges.
- Promote the research and innovation developed by the collective involved, to support the transitions wanted by DIADEM and beyond.
- Include data, results and knowledge sharing, in compliance with Open Science. Take part in the scientific events organized by the DIADEM programme.
- Comply with the rules on generation parity and diversity, ethics and the various agreements that may apply to research proposals (e.g., Biological resources— Nagoya Convention).
- Fostering training through research by involving students (all levels).
- Providing for co-supervision in the event of a thesis or post-doc proposal, with supervisors from different research units or institutions, where relevant.

2.3. Partners

Aid recipients are research institutions, and higher education and research institutions. Companies and foreign institutions may act as Partner Institutions within proposals but will not receive any funding for their involvement. International cooperation is very much an option.

3. Review of the proposals submitted

3.1. Selection process

The main stages of the process, for the first stage of this call for proposals, are as follows:

- Submission of the application on the dedicated ANR website,
- The ANR reviews the **admissibility** of the application, under the criteria listed in §3.2,
- For this first stage, the submitted applications must describe:
    - The state of the art and opportunities that the proposal represents,
    - The scientific proposal, its key stages and deliverables,
    - The partners (existing or to be identified) required to conduct the project and necessary for a synergy,
    - The reasoned overall budget and aid requested,

  and include:
    - The best 5 publications, over the last three years, by the teams involved, in line with the proposal,
    - Short CVs for all main investigators.
- PEPR directors will be responsible for reviewing the proposals. They will pre-select the consortia by theme. If required, they will facilitate the grouping of consortia. Where appropriate, they will issue recommendations regarding the content of the proposals to be evaluated in stage 2.

Following the first stage, the call's second stage will begin: the project coordinators selected at the end of the preparatory work and development of the first stage (response in late July 2023) must draft and submit a comprehensive application including a scientific document and an administrative and financial document (cf. date listed in page 5).

The ANR will review if the comprehensive proposals submitted are admissible (cf. § 3.2) before submitted them for evaluation by an international and independent panel. This panel may call on external peer reviewers and may conduct, if necessary, a hearing with project coordinators.

Following its proceedings, the international evaluation panel will provide DIADEM PEPR co-directors with a report including:

1) The marks and comments given to the proposals evaluated, in accordance with the criteria listed in § 3.3.

2) The list of proposals recommended for funding by the panel, based on their quality, evaluated in accordance with the criteria listed in paragraph 3.3.

3) The list of proposals which the panel proposes not to fund due to insufficient quality on at least one of the criteria listed in § 3.3.

Each proposal evaluated will be the subject of arguments justifying its position on one of the two lists. The panel may submit an opinion on the amount of funding requested.

Based on the list ranking the proposals submitted, under the evaluation criteria of the call, PEPR co-directors will identify the proposals that could be funded and the amount that could be allocated to each one, to the French General Secretariat for Investment. The Prime Minister, after receiving the opinion of the SGPI, chooses the recipients and amounts granted. Each proposal shall be the subject of a contract between the ANR and the project coordinating institution, detailing the mutual obligations of both parties.

The members of the evaluation panel and external peer reviewers called upon undertake to comply with the rules of ethics and scientific integrity set up by the ANR. The ANR's Code of Ethics and Scientific Integrity is available on its website. The ANR ensures strict compliance with the rules of confidentiality, the absence of personal connections between panel members or external peer reviewers and project coordinators and partners, as well as the absence of conflicts of interest for panel members and external peer reviewers. If there is a duly noted breach, the ANR reserves the right to take any action it deems necessary to remedy the situation. The composition of the selection panel will be posted on the call for proposals publication website at the end of the selection process.

3.2. Acceptability criteria

IMPORTANT

The applications that do not meet the acceptability criteria will not be submitted to the evaluation panel and will in no way be eligible for funding.

First stage:

1) The letter of intent (5 pages maximum- cf. template provided on the call's publication page, written in French) must be deposited on the ANR submission website before the closing date and time of the first stage (cf. page 4).

Second stage:

1) At the suggestion of possible thematic groupings and/or consortia, the submission dossier for the proposal must be filed in full on the ANR submission website before the call for proposals closing date and time. More specifically, i) the scientific document, ii)

the financial and administrative document in Excel format, iii) the administrative and financial document signed by each Partner Institution and scanned in PDF format, must be filed on the ANR submission website at the time and date listed in page 4.

2) The scientific project document (20 pages maximum + an appendix of 10 pages maximum, written in English) must follow the template available on the call for proposals website and be submitted under unprotected PDF format.
3) Proposals must be collaborative, with at least two and up to 5 different research teams funded under this call.
4) Research teams will come from at least two different research institutions or higher education and research institutions.
5) A single scientific project manager can only be responsible for one proposal, and may not be in charge of one of DIADEM's current targeted projects.
6) The project will last 4 years maximum.
7) The amount of aid requested will be €800k minimum and €1 million maximum.
8) Proposals that could cause significant environmental harm are excluded (application of the DNSH – Do No Significant Harm - principle) by virtue of Article 17 of the European taxonomy regulation.

3.3. Evaluation criteria

a) Letter of intent

- The proposal submitted must **cover** the call listed in § 2.1,
- The proposal must address one of the two themes defined in § 2.1,
- The Project Manager must be known for his/her previous research,
- Quality and complementarity of the consortium to meet the targeted challenges,
- The role played by training through research.

b) Research proposals for funding

To conduct the final evaluation of the proposal, evaluation criteria are provided **to guide project coordinators** in the drafting of their response to the call for proposals.

1) Scientific excellence and ambition:

- Clarity of research objectives and hypotheses,
- Innovative nature, ambition, originality, methodological or conceptual difference of the proposal with respect to the state of the art,
- Relevance of the methodology.

2) **Quality of the consortium, resources deployed and governance:**

- Skill, expertise and involvement of the project manager: ability to coordinate multidisciplinary and ambitious consortia, academic background, international recognition,
- Quality, complementarity and novelty of the scientific consortium with regard to the objectives of the proposal,
- Harmony between the human and financial resources deployed (including those requested under the proposal) with respect to the objectives to be achieved,
- Relevance of the timetable (especially for long-term projects), management of scientific risks and alternative solutions, credibility of the proposed milestones,
- Relevance and efficiency of the governance (steering, organisation, coordination, introduction of advisory boards, etc.).

3) **Impact and consequences of the proposal:**

- Proposal's ability to meet research challenges in the theme selected,
- Economic and societal impacts, contribution to the development of solutions in response to the priority areas of the Exploratory PEPR,
- Strategy to disseminate (*ongoing* and *ex-post*) and exploit the results, compliance with FAIR principles, Open Science and the promotion of scientific culture.

4. General provisions for funding

4.1. Funding

The calls funded under the PEPR are of an exceptional nature and differ from recurrent funding from academic or research institutions.

The funding granted provides additional resources intended for new actions. They can be used to launch innovative research proposals and to fund, for instance, the purchase of equipment as well as expenditure on staff specifically assigned to this proposal and all operating costs.

Eligible expenses are specified in the financial regulations on the allocation of grants under the PEPR initiative. Financial support will be provided in the form of a grant, whose disbursement is made by the ANR for the project coordinating institution, according to the timetable set out in the agreement, over the duration of the project.

4.2. Consortium agreements

A consortium agreement, which may consist of a set of agreements between the Coordinating Institution and each Partner Institution individually, specifying the rights and obligations of each Partner Institution, regarding the completion of the project, must be provided by the Coordinating

Institution within 12 months maximum from the date of signature of the grant agreement. In the event of multiple agreements, the Coordinating Institution guarantees the consistency (absence of contradictory provisions) of this set of agreements.

All Partner Institutions that set resources aside for the Proposal are signatories to this/these agreement(s), even if they do not receive a share of the grant.

This agreement specifies, depending on the type of proposal funded:

- The terms to exploit the results generated at the end of the research and share their intellectual and industrial property,
- The distribution of tasks, human and financial resources, and deliverables,
- The regime for publication/dissemination of results,
- The governance, including the name of the project manager for the Coordinating Institution,
- The promotion of digital educational tools and/or products created.

The Coordinating Institution sends a copy of this agreement, along with any amendments, directly to the ANR.

This agreement will assess the absence of an indirect aid granted to Companies through higher education and/or research institutions.

The absence of this document may result in the end of proposal funding and the implementation of the provisions of Article 6.6 (aid suspension and recovery).

There is no need to draw up a consortium agreement if there is already a framework agreement containing the provisions above binding Partner Institutions. A copy of this framework agreement or a certificate must be submitted before the grant agreement is signed. When the aforementioned agreement expires, if it is not renewed, the consortium agreement will then be required.

4.3. Open Science

As part of the ANR's contribution to the promotion and implementation of Open Science, and in line with the French National Plan for Open Science (NPOS) and International Plan S, recipients of the France 2030 grant undertake to ensure immediate open access to peer-reviewed scientific publications and to adopt, for research data, a FAIR (Findable, Accessible, Interoperable, Reusable) approach in line with the "as open as possible and as closed as necessary" principle. Thus, all scientific publications from projects funded within the framework of this PEPR will be available in open access, under the Creative Commons CC-BY license or equivalent, using one of the three following methods:

- publication in a natively open access journal,
- publication in a subscription journal that is part of a transformative agreement or transformative journal[1],

[1] Definition of a transformative agreement or transformative journal: https://www.coalition-s.org/faq-theme/publication-fees-costs-prices-business-models/

- publication in a subscription journal. The publisher's version or the manuscript accepted for publication will be deposited in the Open archive HAL by its authors, under a CC-BY license, implementing the Rights Retention Strategy (RRS), according to the terms specified in the Special Conditions of the Funding Decision or Agreement.

Furthermore, the Coordinating Institution undertakes to ensure that the full version of these scientific publications (version approved for publication or publisher's version) is deposited in the national Open archive HAL, no later than the time of publication, and to mention the ANR reference of the research proposal from which they result.

The ANR encourages the deposit of pre-prints in open platforms or archives, and to privilege permanent or unique login details (e.g., DOI or HAL Id). In addition, the ANR recommends that priority be given to publications in natively open access journals or books[2].

Finally, the Coordinating Institution agrees to provide, within 6 months after the start of the project, a first version of the Data Management Plan (DMP), under the terms and conditions set out in the Grant Agreement.

5. Terms of submission for this call for proposals

5.1. Content of the submission dossier

The submission dossier shall include all the elements necessary for the scientific and technical evaluation of the proposal. It must be deposited before the closing of the call for proposals, whose date and time are listed in page 4.

IMPORTANT

No additional element will be accepted after the closing for the submission of the call for proposals, whose date and time are listed in page 4.

The documents are to be deposited on the submission website whose address is listed in page 4. To access this service, opening an account first is required (username and password). It is recommended to register as soon as possible to obtain those elements.

First off, the 5-page letter of intent consists of a technical document written in French, including a description of the project planned, under the format provided, with, in appendix, the financial resources (full cost and aid requested), a list of the best 5 scientific publications made by the teams involved, and short CVs of the main

[2] The DOAJ website (https://doaj.org/) lists peer-reviewed open access scientific journals.. The same applies to the DOAB website (https://www.doabooks.org/) but with monographs.

investigators).

The technical document template is available on the publication page of this call for expressions for proposals (see URL in page 4).

Secondly, for all applications selected, the full submission dossier consists of three fully completed documents:

1) The scientific document"", of 20 pages maximum, written in English, which includes a description of the proposed project, under the format provided, with an appended list of scientific publications (10 pages maximum) made in the last 3 years by the researchers/teams proposing the project,

2) The "administrative and financial document", which includes the administrative and budgetary description of the proposal, along with the engagement letters,

The elements of the submission dossier (administrative and financial document in Excel format/ the scientific document and commitment letter in Word format) will be available on the publication page of this call for proposals (see the URL on page 4).

5.2. Submission procedure

The documents of this submission dossier must be sent by the person responsible for the letter of intent, then, if selected for stage 2:

Only IN ELECTRONIC FORMAT:

- Before the closing date of this call for proposals, listed in page 4,
- On the submission website, as recommended in paragraph 5.3.

Prior registration on the submission website is required to submit a proposal.

Only the electronic version of the submission documents available on the submission website when this call for proposals closes will be considered for evaluation.

AN ACKOWLEDGEMENT OF RECEIPT, in electronic format, will be sent to the project manager once the documents are submitted.

NB: The signature of the commitment letters certifies that project partners agree to submit the proposal in compliance with the conditions described in the administrative and financial document as well as the scientific document and its potential appendices.

5.3. Submission advice

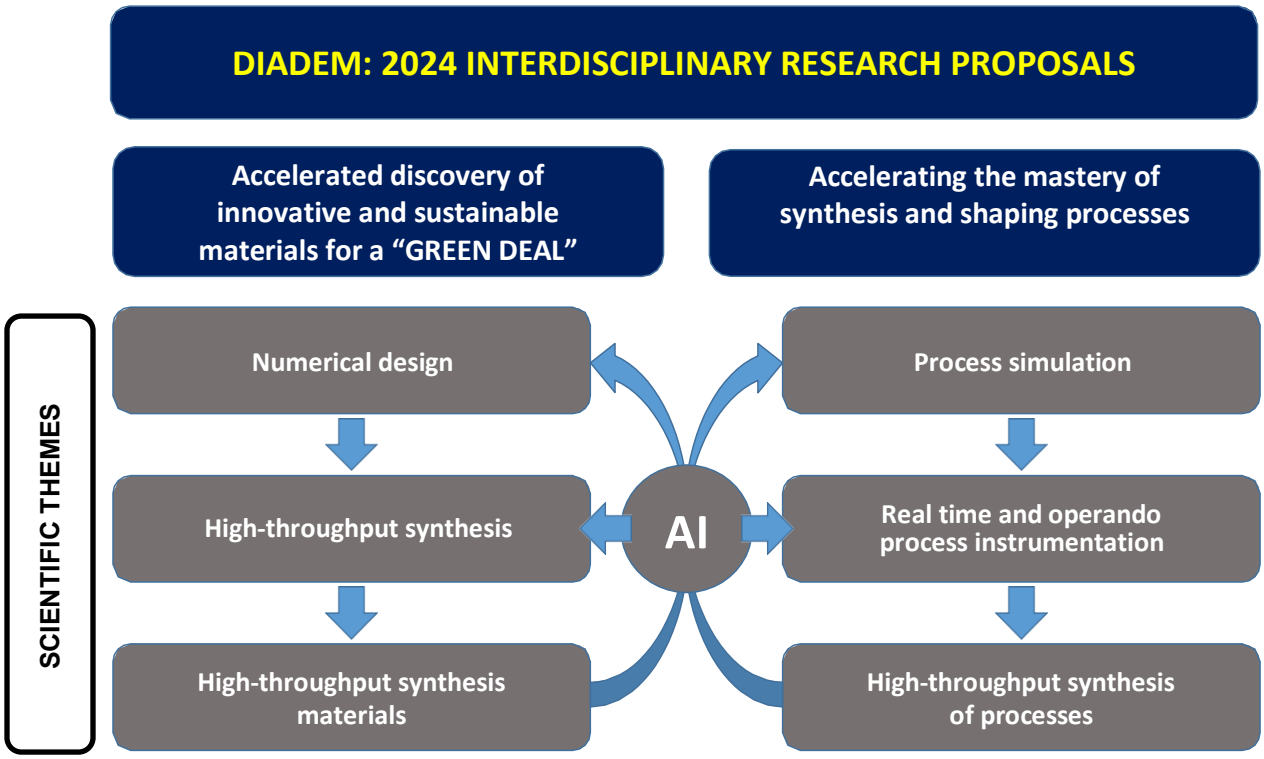
It is strongly advised to:

- Open an account on the submission website at the earliest,
- Not wait until the deadline for proposal submission to enter data online and upload files (please note that the submission deadline must be respected),

- Check that the documents submitted in the dedicated area “submission documents” are complete and consistent with the expected elements,
- Regularly consult the programme’s dedicated website at the address listed in page 1, which includes up-to-date information on its operation,
- Contact, if necessary, the correspondents by email at the address listed in page 4 of this document.

APPENDIX 1 – DEVELOPMENT PROCESS

For both stages of the call for proposals, the proposals must comply with the diagram below. As the total budget allocated for 2024 amounts to €12 million, and each funded proposal ranges between €800k and €1 million, 12 to 15 proposals will be funded. The objective is to ensure that 2/3 of proposals cover the accelerated discovery of materials, and 1/3 the acceleration of processes. The use of AI for all stages of these acceleration processes will be a major criterion for the selection of the proposals.



Interdisciplinary Research Proposals (IRPs) wanted under this call for proposals.

APPENDIX 2 - LIST AND SUMMARIES OF THE TARGETED PROJECTS OF THE DIADEM PROGRAMME

DIAMOND: Data Management and Infrastructures for Artificial Intelligence, Modelling and Optimisation for Material Numerical Design

Summary: The main objective of this targeted project is to develop a digital infrastructure to accelerate the development of materials. On the one hand, it is based on a platform dedicated to simulation codes at different scales, and workflows for automated sets of calculations, including high-throughput calculations and AI-based result processing, and, on the other and, a database infrastructure from both experiments and simulations. For each infrastructure, some use cases arising from ongoing targeted projects were identified to be used as an example and ensure the suitability with user requirements. They apply to MOF-learning, ESRF and FastNano projects. A demonstrator using both infrastructures will be developed, and will focus on the development, through machine learning, of interatomic potentials for atomic scale simulations. The specifications for these infrastructures, and this demonstrator, will be established by calling on task forces with representatives from the main laboratories involved. The code and workflow platform will be developed and implemented at the GRICAD Meso-Computing Centre, and the database infrastructure at TGCC.

ESRF: Accelerated X-ray Materials Characterisation using **ESRF**'s French CRG beamlines

Summary: Through the high-energy X-ray penetration depth of ESRF's new EBS source, French CRG beamlines provide 150 French laboratories with high-resolution multi-scale characterisation through diffraction, scattering or absorption spectroscopy. They develop sample environments for *in situ* and *operando* measurements. Scientific panels, common to both SOLEIL and ESRF, select experiment proposals twice a year. Beamtime can also be purchased by private companies. The DIADEM PEPR programme aims to accelerate the discovery and optimisation of functional or structural materials by speeding up experiments and making data processing more efficient. Based on their experience with advanced materials characterisation, 4 CRG lines propose to conduct the DIADEM/ESRF: D2AM (BM02) and IF (BM32) project by using X- diffraction and scattering in chemistry, physics, surface and materials processing, including historical materials; FAME-UHD (BM16) and FAME-PIX (BM30) for spectroscopy and speciation in biology, chemistry, Environmental Sciences and Geosciences.

Given the renewed performance of the equipment (Equipex+ MAGNIFIX project), the counting time will be reduced by improving the beam and detection. The determining stage will then become sample handling. Further automation, such as screening, measurement and data management, would help increase the characterised samples throughput. Such opportunities were identified in these 4 lines, where automated sample chargers may generate hundreds of samples (SAXS-WAXS and GISAXS-GIWAXS in D2AM, LaueMAX and GMT (XRR, GIXRD) instruments in IF). Simultaneously, novel *operando* devices (HPHT reactors or micro-

reactors, (electro)chemicals, furnaces, electric fields) using faster detectors, constitute another option to speed up studies, particularly for XAS (FAME-UHD and FAME-PIX) characterisation, or SAXS-based screening the conditions of development (D2AM).

Acceleration will also arise from the introduction of a new generation of 2D energy-resolved detectors, where each pixel records a spectrum: such pixel detectors will be developed for Laue (IF) or XAS spectra using highly diluted samples (sub-ppm: FAME-UHD). Once equipped, these 4 F-CRG beamlines will comply with rapid characterisation conditions required to join the “open discovery hub” proposed by the DIADEME programme.

With the arrival of high-resolution 3D imaging and fast 2D detectors, very large-scale worldwide research facilities (TGIR) are subject to a "data deluge" and existing digital tools must be adapted to deal with such issues. In this context, Artificial Intelligence (AI) will conduct a serial assessment of massive and complex data, and materials characterisation at nano-scale.

These tasks require specific digital skills, for which beamline scientists will require to be trained by IA experts. Processing and assessment processes for large data sets must interact if the interoperability required by the users is to be achieved. In order to exchange ideas and practices, these new skills will be mutualised between the beamlines and within the DIADEM programme.

To achieve the objectives set by DIADEM, in terms of rapid characterisation, the current bi-annual mode to access these lines may be insufficient. One final objective of the DIADEM/ESRF project will be to see if other modes, such as BAGs (block-allocated experiments by biocrystallography), may be adapted for the advanced materials community while complying with scientific quality requirements.

METSA SET-DIA: Improving Experiments on scanning electron topographies using direct electron detectors and innovative algorithms

Summary: DIADEM aims to accelerate the development of novel materials in France by integrally combining modelling, numerical simulation, artificial intelligence (AI) methodologies, synthesis/screening technology and high throughput characterisation. METSA is contributing to the fulfilment of this objective by through the optimisation and development of three Scanning Electron Tomography techniques (SET), in such a way that they are faster, more effective and automatic. The three SETs selected are complementary and have a number of points in common: EELS-SET for three-dimensional (3D) chemistry characterisation at nano-scale (EELS: Energy Electron Loss Spectroscopy), Nano-SET and Ptycho-SET for structural characterisation, at nano- and atomic scale, respectively. METSA will rely on (1) the equipment and know-how available, either on the Nanocharacterization Platform (PFNC) on the Minatec campus at CEA-Grenoble, or the NEEL Institute (NEEL) in Grenoble, (2) new equipment purchased, either as part of METSA or outside DIADEM (set up of a new low-

voltage microscope in early 2023 at CEA, and of a new microscope in 2022 at NEEL). The PNFC already masters two of the proposed SET techniques (EELS-SET and Nano-SET), and the METSA project will help increase and automate them by (i) using a new type of Direct Electron Detector (DeD), without noise, sensitive to a single electron and with time resolution, (i) by improving digital 3D image reconstruction techniques using Deep Learning (DL) and parsimony concepts, (ii) by optimising the digital management and processing of large experimental data (use of clusters or graphics cards). The third SET, the ptycho-SET, is completely new, but is in fact a combination of tomography and 2D-ptychography using very similar methods (same detector, scanning, digital processing techniques, etc.) to the other two SETs.

This 'Tomo-Ptycho' combination has already been identified in the case of X-rays, but with nanometre resolution, whereas for METSA, and thus electrons, an atomic scale resolution of several picometers should be achieved. Having rapid and semi-automatic characterisation tools to determine the structure and chemistry of materials should strongly help design and develop novel materials with improved properties. To demonstrate this, the techniques developed will, of course, be applied to a selection of novel materials engineered under DIADEM.

Based on the tools and infrastructures implemented in various DIADEM platforms, the developments conducted under METSA will be accelerated and optimised, the know-know and knowledge acquired may be quickly disseminated nationally through exchanges with the French METSA (Transmission Electron Microscopy and Atom Probe) Research infrastructure (RI). The same name was chosen to underline the connection between this DIADEM sub-project and the RI METSA. When METSA is in bold, the word refers to the DIADEM sub-project.

SOLEIL: Platform for an Accelerated High-Performance Materials Characterisation at **SOLEIL**

Summary: Accelerated SOLEIL materials characterisation

SOLEIL provides a wide range of experimental techniques and sample environments to conduct multimodal materials characterisation. As part of the DIADEM PEPR project, this experimental arsenal will be upgraded to a new level of scientific efficiency for high-throughput characterisation. The different beamlines where this strategy may be best suited are: ANATOMIX, ANTARES, CASSIOPEE, CRISTAL, DIFFABS, GALAXIES, HERMES, MARS, NANOSCOPIUM, PUMA, PX2, PSICHE, ROCK, SEXTANT SWING and TEMPO.

Heading towards high-throughput characterisation

SOLEIL has planned several actions to meet the requirements of the DIADEM project, aiming towards high-throughput characterisation:

i) A new workflow will combine different experiments over a same category of samples, helped by an online data assessment and an AI-based modelling strategy. The workflow will generate a unique Digital Object

Identifier (DOI), which will be saved with the data.

ii) Fast sample chargers, including robotic arms, will progressively be deployed in experimental stations, with, in the long term, the possibility to automate sample transfer under ultra-high vacuum.

iii) A new generation of 2D-pixel detectors will be developed within the project, with large light-sensible material, fast and integrated data processing, and optimised beamline equipment synchronisation.

iv) Automatic data reduction will be implemented directly at the output of the detectors using AI-based software embedded on GPU cards. In addition, powerful data reduction and assessment tools will be available to users as well as advanced numerical simulation codes.

v) The fast mode for continuous data acquisition (FLYSCAN) will be extended to various experimental stations.

vi) New ways to access beamlines are planned, such as BAGs (Block Allocation Group) to provide frequent and guaranteed beam time to a consortium of users, or hubs with specific access.

LIBELUL: LIBS for basic high-throughput analysis

Summary: The accelerated development of materials through the use of artificial intelligence, as proposed in the DIADEM PEPR project, requires developing high-throughput analysis tools in order to develop the databases used. Within this framework, a basic analysis, which aims to assess the fluorescence emission spectrum of the plasma induced by the removal of the material to be analysed by a laser pulse, may be conducted using LIBS (Laser Induced Breakdown Spectroscopy) technology. This technique helps detect the different constituents of a variety of materials (metals, insulators, polymers, etc.) with a great level of sensitivity that can go down to a few ppm for some elements, and is very well adapted to the strategy adopted by the DIADEM project. The LIBELUL project aims to develop two “platform” experiments using LIBS technology. The first platform will consist in implementing a preliminary mapping on very large surfaces with a measuring step of 30?m, requiring targeting high-throughput laser rates (up to kHz). Imaging will be coupled within a single experiment with RAMAN and Luminescence spectroscopy. In fact, **RAMAN** spectroscopy provides information on structural aspects, while Luminescence spectroscopy can also inform on the optical properties of a large number of impurities in their environment and some flaws. The use of artificial intelligence will also be exploited to automatically detect major elements and improve the signal-to-noise ratio, in order to also improve raw data processing. If the first platform is expected to receive the materials to be analysed, the second LIBS platform, on the contrary, is expected to visit the materials high-throughput synthesis site. Therefore, this means developing a mobile and adaptable LIBS platform that may be operated on-site. This second platform will present the best performances combining sensitivity and reproducibility, and will be designed to be easily operable. These two platforms will supplement the basic high-throughput analysis tools of the DIADEME project.

ADAM: Accelerated Design of Architectured Materials

Summary: Because there is an increasing demand for multifunctional materials with enhanced properties, the usual approach to designing materials to optimise their chemistry and nanostructure is interesting but has reached its limits. To overcome them, a complementary approach appears relevant, and consists in taking advantage of the upper scale and the mesostructure, in which materials architecture may be controlled by geometry hybridisation. This approach requires using development and shaping processes for innovative materials, such as 3D or 4D printing. By taking advantage of the recent breakthroughs in artificial intelligence and data mining, the ADAM (Accelerated Design of Architectured Materials) project proposes to discover novel architectured materials (i) with optimised mesostructures for enhanced multifunctional properties, (ii) which represent real breakthroughs with respect to existing materials solutions, (iii) by accelerating, by a factor of ten, the design process. The global proof of concept will be emphasised through three printed architectured materials, in line with the major issues of energy transition and climate change. They are of particular interest in the field of energy, transport of goods and persons, or yet health. For the first two architectured and metal systems, we will optimise their shaping, mesostructures, thermal (conductive and radiative) and mechanic (elasto-plastic) properties by coupling (1) live *in operando* 3D imaging on an instrumented additive manufacturing device, (2) live *in situ* 3D imaging during the deformation of the manufactured architectures, (3) advanced numerical modelling in materials science and structural optimisation, and (4) data mining and artificial intelligence techniques. The third system will be a hydrophilic bio-sourced system developed through printing and optimised to achieve new hygromorphic properties.

A-DREAM: Accelerated development of corrosion-resistant materials

Summary: The A-DREAM project aims to develop a generic approach to accelerate the discovery of corrosion-resistant materials and coatings in extreme environments. To do so, the A-DREAM project proposes an integrated approach using: (i) the digital design of materials/coatings, (ii) the synthesis of these high-throughput materials, and (iii) the implementation of accelerated corrosion tests. Through a digital approach that will include data mining, a CALPHAD-type thermodynamic approach, and corrosion modelling, a wide range of materials and coatings will be analysed to extract targeted compounds for corrosion application. These materials will then be developed through a combinatorial PVD process to quickly synthesize many chemical compositions deposited in thin films over glass substrates. Simultaneously, HEA-type (High-Entropy Alloys) materials will also be developed under the targeted DIAMS project (through conventional or combinatorial additive manufacturing) to be tested in the corrosion devices of the A-DREAM project. Finally, these upper-scale coating developments will be conducted through Cold Spraying technology. All these processes will help cover a panel of compositions and microstructures to identify enhanced compositions of massive materials and coatings, and, on the other and, to study the effect of microstructure on the behaviour of the materials manufactured. These materials will then be tested for corrosion through the implementation of an experimental

device to accelerate the evaluation (by freeing ourselves from long-term immersion testing) of corrosion behaviour by coupling electrochemical techniques and analytical chemistry. This generic approach will be applied if there is corrosion in high-temperature molten chlorides.

AMETHYST : **Accelerated design of polymer materials through artificial intelligence tools, preparation methods and high-throughput characterisation**

Summary: With a worldwide production of around 380 million tonnes a year, polymer materials play a major role in modern society. Indeed, they are used in the manufacturing of numerous everyday products, or as more sophisticated compounds in medicine, diagnostics and fine chemistry. However, new emerging economic and societal constraints require a more rational design and alternative methods for polymer synthesis, formulation and shaping, to meet the needs of greater sustainability and more virtuous end-of-life management, while maintaining optimal performance in application. Polymer materials of the future will be one of the pillars of the circular economy. Thus, the discovery of new polymers will lead to a paradigm shift and to new methods for their design, processing, and assessment of their properties at all stages of analysis. The recent development of high-throughput processes (HTP) and artificial intelligence (AI) provides enormous opportunities to meet these challenges. Although such methods are emerging in the field of chemistry, they have yet to be implemented in France in Polymer Sciences. Thereby, the AMETHIST demonstrator project proposes, as proof of concept, a combined use of HTP and AI methods to handle three distinct case studies in the field of polymers. The issues addressed were selected for their relevance in addressing pressing scientific and societal challenges.

- Case study No.1 - Design of polymeric materials with programmable degradability,
- Case study No.2 - Organic-inorganic polymer, nano-composite and composite-based materials,
- Case study No.3 – Bio-sourced polymeric materials.

In each case study, for each type of material, the HTP synthesis and characterisation method will be implemented at molecular, macromolecular and material scale. The data stemming from the HTP analysis will be used to feed machine learning approaches to determine the best combination with multiple targeted properties. Optimised materials designed by AI will be manufactured and assessed.

DIAMS: Design by artificial intelligence and high-throughput data of advanced alloys and innovative metallurgic concepts for structural application

Summary: The targeted DIAMS project aims to set up infrastructures to accelerate the design of metal alloys for structural applications, to develop a methodology to help implement these platforms for the entire French metallurgy community, and to demonstrate its capabilities through three demonstration projects conducted in partnership with the stakeholders involved in the project.

The accelerated synthesis of metal alloys will be implemented through high-throughput alloy screening platforms. This screening can be done with platforms for additive manufacturing with powder mixture / wire made available and developed, within the framework of this project, at CEA, IJL and SIMAP, and through manufacturing of compositionally graded alloys. A high-throughput characterisation platform capable of conducting an *in situ* structural and microstructural study during thermomechanical processing representative of industrial development processes, will be deployed on a set of high-energy lines of the European ESRF synchrotron. This tool allows the creation of unique metallurgy databases on the alloys developed as part of the project. This platform will be supported on other synchrotron lines dedicated to the DIADEME programme, and particularly the DIAMS project, with the resources of SOLEIL's MARS beamline. In addition to manufacturing alloys and acquiring data, artificial intelligence, combined with physical modelling, will be implemented at all levels of the process, from the proposal of alloy compositions to supporting the high-throughput characterisation and modelling of microstructural evolutions and the optimisation of alloys.

The three demonstration projects covered by the targeted DIAMS project will each involve working in collaboration with several stakeholders of the project, each with their own platforms or skills in the approach:

- The first project will implement an advanced methodology for the design of high-entropy alloys and complex concentrated alloys, to be applied in extreme environments (irradiation / corrosion). It will follow a proposal on alloys by calculations of an AI, followed by screening and high-throughput of the microstructure, and then high-throughput characterisation of the behaviour in extreme environments (in partnership with the targeted A-DREAM project).
- The second project will manufacture compositionally graded alloys to assess alloying effects on the design of 3rd generation high strength steels (medium manganese), and their high-throughput characterisation combined with AI modelling through a thermomechanical platform on a high energy synchrotron beamline.
- The third project will implement the design of light alloys based on specific aluminium for additive manufacturing, through the project's powder mixing platforms. The alloys screened with these synthesis methods can also be characterised at high-throughput, and the data generated can be included in an AI-based alloy design approach.

FastNano: Nanomaterials

Summary: The French strengths in low-dimensional materials were structured, from 2011, around several Labex involving hundreds of researchers. This community can manufacture a wide range of high-quality nanomaterials. However, France has yet to be involved in Artificial Intelligence (AI)-assisted synthesis, even though Machine Learning is currently used to improve characterisation and performance assessment, and may guide towards optimal synthesis parameters. Therefore, we aim to move beyond existing methods, by improving our synthesis capabilities towards high-throughput manufacturing, coupled with online Ai-assisted assessment, to accelerate progress towards new 0D, 1D and 2D nanomaterials. FastNano will thus build four

generic synthesis reactors, including online dedicated characterisation tools to develop AI-assisted data processing and feedback loops on synthesis or assembly processes, in order to achieve, as soon as possible, the most appropriate properties on targeted low-dimensional materials, and optimal deposition protocols for new low-dimensional materials. The reactors will target nanoparticles synthesised from liquid and gas phases, and corresponding nanocomposite films, ultrathin films deposited one layer at a time through quick combinatorial ALD and two-dimensional heterostructures prepared for 2D nanomaterials automated assembly, in order to cover the widest possible range of potential new materials and applications. The reactors will also rely on external characterisation (synchrotrons, TEM, etc.) and modelling resources to develop AI-based data processing and improve synthesis conditions through feedback loops. The full development will take 4 years, with deliverables provided as open operational tools after 2 years. Once they are approved on known and new nanomaterials, these reactors will become open synthesis platforms available for the community through open calls with DIADEME, as direct deliverables of FastNano (from T0+2 years to T0+8 years).

2FAST : Autonomous fluidic labs to speed up synthesis processes for materials with controlled properties.

Summary: The implementation of chemical synthesis in continuous and miniaturised conditions (microfluid, flow chemistry, etc.) is the key to intensifying processes and the promise of exceptional control over operational conditions. Combined with controlled environments that can be perfectly emulated and provided by miniaturised fluidic tools, the research and discovery in Materials Chemistry can now substantially benefit from recent digital developments. Optimising the best route of synthesis may be based on databases or *in situ* or online measurements which, in turn, develop the databases. However, unlike chemical composition measurement, the methods and instruments required to conduct a full nano/micro-materials characterisation are expensive and tedious to implement, which restricts them to only a few research laboratories. Furthermore, there is no universal way to develop a continuous chemical process. Research and development are often expensive, solvents and materials are not always environmentally friendly. Therefore, agility and frugality are essential.

In this project, we will use digitization to its full potential in so-called orchestrated microfluidic laboratories.

By uniting major stakeholders in miniaturised fluidics, who have a great level of expertise in i) the design and manufacturing of chips, ii) their operation in extreme conditions, iii) the implementation of analytical techniques; and through recent progress in machine learning methods for Materials Science, we will co-develop and assemble interoperable microfluidic chips for the synthesis of materials with controlled properties. We will demonstrate how these automated platforms are relevant, using the synthesis of 0D metal materials (with rapid chemistry), 2D mineral materials (synthesised at high pressure and temperature) and, eventually, hybrid materials such as MOFs, from environmental to solvo/hydrothermal conditions, with live monitoring and smart feedback.

In addition, the project will generate high-quality data which are required to model the properties of these materials and to provide an understanding of the role played by the chemical environment, and to research optimal synthesis conditions.

Hiway-2-Mat: Autonomous and combinatorial high-throughput exploration methods in solid-state chemistry

Summary: In recent years, innovative approaches were developed to accelerate the discovery of novel materials: the combinational approach and autonomous research approach The combinational approach allows the production of materials libraries that formally include several hundreds, even thousands, of compositions. Autonomous research implies the deployment of materials which include synthesis and characterisation modules for automated structural and functional properties, and using AI models to select the areas to be explored. Such a combination allows the exploration of complex multidimensional areas to optimise the composition of materials without human action. Europe is lagging behind the United States and China in this research area. Under this targeted project, our objective is both to use high-throughput combinatorial approaches and to develop autonomous configurations to explore material composition spaces for low-energy applications. In practical terms, we will apply the approaches proposed to accelerate the discovery of oxide materials for smart windows, smart sensors, low-consumption lighting and electronic systems. The parallel combinatorial approach will be implemented and completed with AI models. Interactions with other targeted projects will help extend this oxide strategy to other types of materials. Finally, in addition to automating the discovery of novel materials, this strategy should help researchers gain statistically sound knowledge and an understanding of the composition-(micro)structure-property relationship.

MOFLearning: Accelerating MOF design through a combinatorial machine learning approach

Summary: Hybrid porous crystalline solids, such as Metal Organic Frameworks (MOFs) can be of interest for a wide range of applications (separation, catalysis, detection, biomedicine, etc.). However, most often their synthesis is not monitored, which makes it difficult to make them 'on demand', according to the target property. The state of the art is based on ‘big data' with few guarantees that the materials selected may be synthesized. As a result, there were several successes in predicting structural-activity correlations at large scale, but for a very limited number of properties (e.g., adsorption). Furthermore, the high-throughput characterisation of physical or chemical properties (at classical or quantum level) is not an established methodology and would require other developments to support the expansion of databases as learning tools for AI-type approaches. This demonstration project aims to establish, for the 1st time in MOFs, a methodological approach supported by synthesis and high-throughput characterisation methods. We will call on a set of existing MOFs with adequate structural and chemical diversity and the systematic assessment of their adsorption/separation properties of gas

molecule models (C02, CH4, N2, rare gases, etc.), essentially polycarboxylates or metal phosphonates with high oxidation, functionalized by polar or apolar groups, which can be easily made and activated on a few grams scale. This experimental effort will be complemented by a high-throughput prediction of their chemical and physical properties to create enriched databases, with indicators as learning tools for statistical algorithms to identify key descriptors, coupled with generative algorithms to explore the space of new phases and guide future discoveries. In a second phase, based on a new high-throughput synthesis and characterisation platform and new predictive models, for 1 or 2 applications of interest, we will identify and synthesise new high-performance MOFs.

RUBIS: Data-driven development and manufacturing of thermo-structural ceramics and composites: Research platforms on Factories of the future, Big Data, Artificial Intelligence and associated Information Systems

Summary: RUBIS focuses on ceramics and thermo-structural composites that are resistant in extreme environments. Indeed, the need for such high-temperature materials is urgent in several fields: energy, transport, defence, etc. Their toughness/refractory nature allows them to be used in aviation, space and nuclear applications, for instance. The science of these modern materials and associated manufacturing processes requires considering a multidisciplinary approach that includes chemistry, physics and engineering, closely linked to the exploitation of data science via artificial intelligence (AI) to accelerate the entire manufacturing value chain.

RUBIS covers all materials design and processing issues: shaping through additive manufacturing, post consolidation processing (e.g., drying, debinding/pyrolysis, sintering). The RUBIS project aims to transform a set of design and manufacturing tools into an “integrated smart factory” to improve productivity and quality control by providing traceability for all manufactured parts. With the complete digitisation of all stages, RUBIS also intends to optimise the performance of the manufactured parts, reduce their costs, energy consumption and environmental impact, and increase the degree of flexibility in production, allowing the delivery of fully customisable and high-quality products.

2 platforms, in year 5, will be delivered as part of RUBIS: a CAD software to design optimised ceramic and composite structures and a fully digitised manufacturing platform integrating stages of additive manufacturing shaping and thermal post-consolidation, with Machine Learning (ML) capabilities for each of these manufacturing stages. The two milestones associated are planned for year 3 and meet the specifications for the platforms. The materials under study will be both oxidic and non-oxide materials that are adapted to the extreme environments explored. In the special case of the manufacturing process, oxides such as alumina with well-documented behaviour laws will be used to initiate developments.

MicroElec: High-throughput development and characterisation of heterostructures for microelectronic applications

Summary: Innovation in functional materials is key to increasing the competitiveness of a sustainable and more efficient microelectronics European industry. In recent years, a new approach aiming to accelerate the discovery of novel materials has been imagined with the development and high-throughput characterisation of material libraries. We propose to extend this combinatorial high-throughput approach to multi-tier microelectronic devices whose functional properties depend both on the nature of each of their constituent layers and their interactions. Improving their performance means optimising the overall layer staking. Understanding and optimising such complexity, using AI-based high throughput synthesis, characterisation and analysis processes for heterostructures with systematic and simultaneous variation of its key parameters would accelerate the development of efficient devices and massively supply material databases. In order to approve this AI-based high-throughput approach for microelectronic applications, existing combinatorial synthesis and characterisation platforms will be strengthened and extended, and then used to define the most suitable unleaded compound/heterostructure for their inclusion in into piezoelectric micrometre actuators and non-volatile nano-scale ferroelectric memories.

ARTEMIS: Accelerated development and discovery of smart materials and active structures through 4D printing

Summary: Introduced in 2013 by the Massachusetts Institute of Technology and the University of Colorado (USA), 4D printing combines additive manufacturing and active materials to build physical objects that can change shape and/or properties in response to an energy boost. By including the time parameter in 3D space, the relationship between the requirements of the applications and the technological means to meet them becomes more complicated, even complex. In this project, the national consortium will address various research areas, including digital technology (knowledge base and machine learning for materials and structures), materials and processes, long-term anticipative actions (e.g., by connecting 4D printing and biomimicry as a thread and/or on material intelligence). Meeting the needs expressed in this "technological leap" should [finally] help switch 4D printing from an academic role to industrial applications.

ATHERM_COAT: Accelerated thermodynamics and high-throughput data to optimise component coatings for the energy transition

Summary: The main objective of the ATHERM_COAT project is to implement a tool to capture thermodynamic data on metalorganic precursors and their disintegration products to accelerate the development of CVD and ALD-based coating solutions, and to strengthen our scientific and technological sovereignty in this field, particularly for applications on energy and digital transitions. This tool will strengthen a state-of-the-art national mass spectrometry platform that is strategic to generate thermodynamic data for Materials Science and

Engineering.

An important objective of experimental thermochemistry is to generate sufficient thermodynamic data to calculate heat and chemical reaction-free energy to develop materials, coatings and perform calculations or simulations on service behaviour (e.g., corrosion behaviour).

In the case of Chemical Vapor Deposition (CVD) and Atomic Layer Deposition (ALD) coating manufacture, one of the first stages in controlling the deposits is choosing the precursors (molecules which, when being transported in the gaseous state towards the substrate surface to be coated, lead to the formation of a deposit). Vapor pressure and evaporating, transport and deposition temperature stability are decisive properties in order to select a molecular precursor that is suitable for the desired conditions and properties of thin film. Knowledge of the gaseous phase, during the thermal cracking of the precursor, is also required to analyse the possible mechanisms leading to the formation of a deposit. Because the identification of the molecules playing a role in the deposition and set up of a thermodynamic database are also prerequisites to simulate the deposition process.

The case for application and methodological demonstration selected in the ATHERM_COAT project is the development of coatings that are resistant to high-temperature oxidation, using DLI MOCVD (Direct Liquid Injection Metal Organic Chemical Vapor Deposition) and ALD (Atomic Layer Deposition) technologies. The applications targeted for these coatings include materials for high-temperature water electrolysis intended for hydrogen production and materials for nuclear fuel cladding.
In addition, once these coatings have been developed, they can also be optimised with regard to their in-service performance and with a view to eco-design by minimising the critical and/or toxic elements therein. Thermodynamics (determining stable and metastable phase diagrams in new systems) coupled with artificial intelligence can guide this kind of option, to some extent, and accelerate solution optimisation.

The generic methodological approach developed within the framework of the targeted ATHERM_COAT project may then be generalised to solve numerous cases requiring the development of innovative coatings for energy and digital transitions.

APPENDIX 3 – PROGRAMME CO-DIRECTORS

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GOUVERNEMENT

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Information about the administrative process (compiling the application, online procedures, aid rate) may be obtained from the ANR at: PEPR-DIADEM@anr.fr