PEPR DIADEM: Priority Equipment and Research Program on the development of innovative materials using artificial intelligence

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To foster the rapid research and market entry of more efficient, sustainable materials derived from non-critical and non-toxic resources is a major challenge. To this aim, a nationwide program has been launched in France in 2021. This exploratory Priority Equipment and Research Program (PEPR) DIADEM is focussed on the Development of Innovative Materials Using Artificial Intelligence). Through the orchestrated synergy of scientific endeavours powered by artificial intelligence (AI), PEPR DIADEM aims to speed up the innovation chain "from concept to fruition," thereby fundamentally reshaping the approach to Materials Science in a sustainable manner. This global approach is similar to some undergoing projects, worldwide.

Addressing contemporary and future societal challenges across energy, transportation, digitalization, and healthcare necessitates the rapid discovery of novel materials, spanning from metallic alloys to functional nanostructures. Given the pressing timelines outlined in the Green Deal framework, there is an urgent call for accelerated development in this domain. Fortunately, the requisite technologies, including rapid synthesis and characterization tools, automation, digital simulations, data management capabilities, AI, additive manufacturing, and thin films engineering, are readily available to meet these challenges head-on.

Led by the CNRS and the CEA in collaboration with seven academic partners, PEPR DIADEM aims to expedite the discovery and integration of materials while addressing environmental and societal concerns. Endowed by France 2030 with a budget of €85M, the program seeks to facilitate the design and market entry of superior and sustainable materials, with a strong emphasis on leveraging AI. This funding is initially allocated to establish a network of four cutting-edge platforms across France, strategically distributed and meticulously coordinated under the banner of the DIADEM DISCOVERY HUB. These platforms integrate high throughput synthesis, combinatorial formulation, automatized shaping, broadband characterization, and digital tools for multi-scale modelling, data mining, supervised learning, and AI adaptation.

Seventeen targeted projects aim to establish this unique network and demonstrate its effectiveness in accelerating the discovery of innovative materials. Additionally, three calls for projects, open to the extensive French materials community comprising approximately 4000 researchers and engineers, have been launched from 2023 and

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extended up to 2025. Interaction with existing infrastructures and research networks is a key criterion for project selection and co-funding by companies and international partners is strongly encouraged. The openness of the DIADEM DISCOVERY hub to various partners will be a key indicator of its global success, with approximately 30 projects set to be selected through an international panel across the three rounds of calls.

A dedicated program for the training of scientists, both novice and experienced, complements this framework, with international cooperation, such as co-supervision of PhDs, playing a crucial role. PEPR DIADEM leverages existing infrastructure such as the SOLEIL and ESRF synchrotron facilities and collaborates with the recently established "AI for sciences and sciences for AI" centre by CNRS. International cooperation is central to DIADEM's mission, both in research and development and in training. At the European level, DIADEM aligns with initiatives such as IAM4EU and AMI2030.

The DIADEM DISCOVERY HUB project builds upon platforms initially dedicated to key material classes, crucial for accelerating the materials identification cycle from two decades to a range of four to ten years. These platforms ideally encompass:

1. Combinatorial and/or high-throughput synthesis and shaping of materials: Leveraging various robotized synthesis and additive manufacturing techniques to swiftly develop novel material compositions, including metallic, inorganic, and potentially bio-sourced polymer matrices. Thin film engineering plays a significant role in achieving desired performance outcomes, with special emphasis on synthesizing new architectured materials, composites, hybrids, and bio-inspired constructs.
2. High-throughput chemical and structural characterization: Utilizing cutting-edge facilities such as the SOLEIL and ESRF synchrotrons, advanced TEM, and fast chemical mapping methods such as LIBS, to assess usage properties; in situ and operando characterizations are crucial for broadening and expediting data acquisition, particularly under extreme conditions.
3. Digital simulation of materials and processes: Employing multiscale simulation tools, including AI approaches, seamlessly integrated into workflows to enable automated and high-throughput calculations.
4. Databases for storage, management, and AI-driven exploitation: Structuring resulting data into databases and developing AI tools to enhance data exploitation, crucial for facilitating a productive dialogue between data and material sciences. The digital platform DIAMOND is the green part of figure 1, binding the entire experiment-oriented platform. This raises the challenge that all similar projects are facing, which is the necessary dialog between data and material sciences.

The interplay among these platforms holds the potential to revolutionize innovation in materials science, driving sustainable solutions to address global challenges.

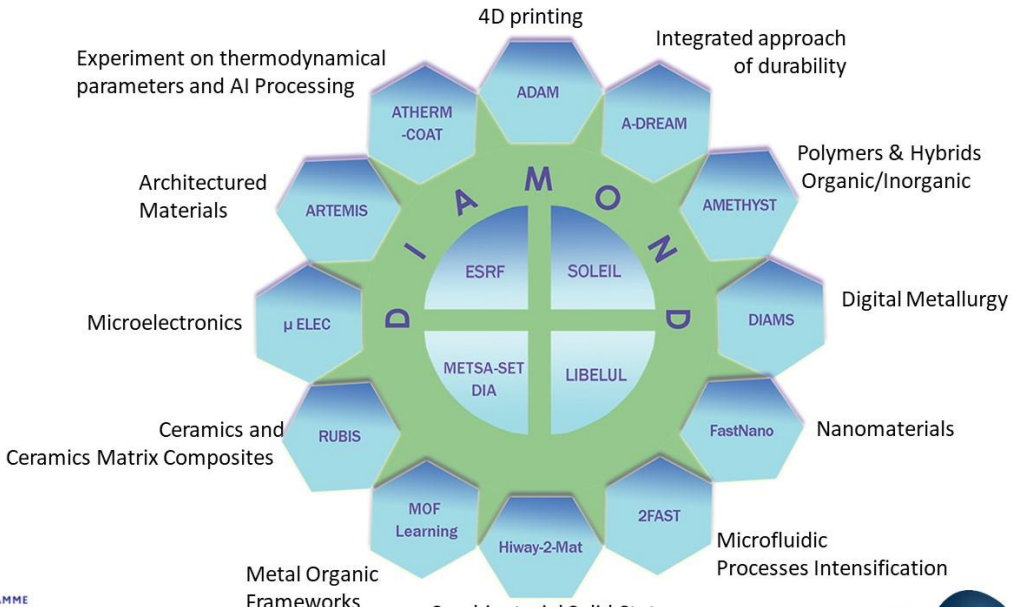

Figure 1: Actual seventeen targeted projects of PEPR DIADEM more details at https://www.pepr-diadem.fr/en/