THE SIGNIFICANCE OF ACCELERATED DISCOVERY OF ADVANCED MATERIALS TO ADDRESS SOCIETAL CHALLENGES

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Preface

Societal Challenges demand for Advanced Materials, which in turn promise economical potential. Material Acceleration Platforms (MAPs) will decrease their development time and cost. We comment on implications for science, industry and policy concluding with necessary steps towards establishment of MAPs.

Abstract

Climate Change and **Materials Criticality** challenges are driving **urgent responses** from global governments. These global responses drive policy to achieve **sustainable, resilient, clean solutions** with **Advanced Materials (AdMats)** for industrial supply chains and economic prosperity.

The **research landscape comprising industry**, academe and government identified a critical path to **accelerate the Green Transition** far beyond slow conventional research through Digital Technologies that harness Artificial Intelligence, Smart Automation and High Performance Computing through **Materials Acceleration Platforms, MAPs** (c. p. Fig. 1).

It is recommended that international, national and regional institutions **collectively support** accelerated materials discovery and development as a foundational element in climate mitigation and resource sustainability through **Materials Acceleration Platform** technology.

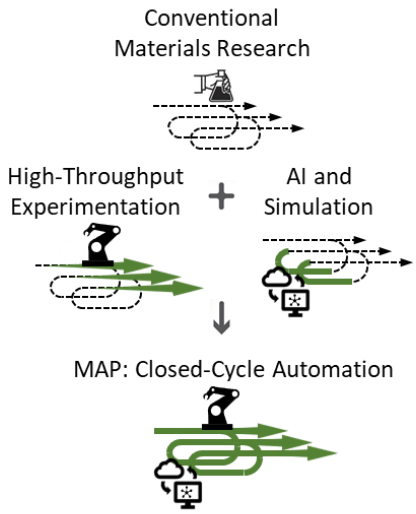

Fig. 1: The concept of Materials Acceleration Platforms (MAP)

Background

Advanced Materials (AdMats) play a critical role in society today, whether in **health, energy or industrial** processing, just to name a few. AdMats are enablers of new medical methods and devices, improved energy production and use, and contribute to the decarbonization of age-old industrial processes like chemicals and steel production. The urgency to decarbonize society is clearly understood and the energy transition is ongoing. However, **new challenges** such as **resource availability, supply chain security** as emphasized by recent pandemics and geopolitical crisis**, and sustainability** have constrained our regional ability and capacity to rapidly find new materials solutions. The likelihood of achieving a comprehensive and rapid **conversion from a fossil-fuel-driven society to renewables, green and circular technologies** depends significantly on our collective **ability to develop a wide spectrum of novel materials** and devices.

Given the need for a rapid transition to a **low carbon economy** under the **European Green Deal** and the **UN Framework Convention on Climate Change** (UN FCCC)[1], as well as the need to make our resources and industrial complex **resilient and sustainable** in alignment with the UN Sustainable Development Goals[2], **novel AdMats must be discovered and developed** at an unprecedented rate. This is only possible through a concerted green and digital transformation in accordance with the European **Twin Transition**. Consequently, the **AMI2030 Strategic Agenda**[3] calls for "delivering on the opportunities of combining digital and physical technologies, like automation, robotics and AI to accelerate materials discovery via autonomous experimentation or dedicated demonstrators and pilot lines, integrating materials development/testing, production and processing (including end of use)." Building on sophisticated **robotic automation, high performance computing** for advanced multiscale simulation and modeling, and the **revolution in artificial intelligence** and digital technology, **a novel approach** to fulfil this demand was conceived, known as **Materials Acceleration Platforms, MAPs**.

About MAPs

The MAP concept **couples robotically executed high-throughput** materials synthesis and characterization in a **closed loop** that is **accelerated by AI**-driven experimental planning, data analytics, and advanced simulation techniques to realize materials and device development at **least 10 times faster**[4] than conventional science methods and at a fraction of the cost. The ability to rapidly find **AdMat solutions tailored to geopolitical and regional supply chain** constraints directly supports technical and economic sovereignty**.**

In materials science, this automation of closed-looped research has only recently begun to accelerate discoveries. Nevertheless, there are **already several success stories** of individual projects that apply MAP concepts consistently, particularly in the research of new **batteries** (BIG-MAP[5]), **photovoltaics** (AMANDA[6]) and **bio-materials** (Tissue MAP[7]). As an example, AMANDA, an automated photovoltaic cell production and testing line, can now **produce hundreds of samples per day** adapting the mixture of ingredients and process parameters in each run. It has led to **extraordinary discoveries in organic photovoltaics** and AMANDA is already being repurposed to accelerate development of solar PV perovskites.

Building Blocks

A MAP is a **holistic and integrated approach** consisting **of interoperable hardware and software** that connects a **community of researchers**. The hardware components of a MAP enable highly integrated **automation of laboratory experiments**. The software of a MAP enables its operation by interfacing with instruments; connecting experiments, simulation, and hardware; providing data storage and analysis tools; and **controlling and orchestrating** the various MAP components. Finally, but most importantly, the ecosystem of a MAP depends on a **research community and its domain knowledge** that nurtures and steers the MAP, provides feedback, and **leverages the knowledge** generated at an **accelerated rate**.

As an **entire ecosystem, a MAPs goes far beyond its technical components** and represents a novel meta-method of scientific research.

Impact

A society that **succeeds first in fully implementing** the vision of a **MAP** will be able to **stand out** significantly **in international competition**.

The MAP robotic system makes research results particularly **reliable, reproducible and transferable**, so that research communities can easily **collaborate to address problems of a global scale**. From the industry perspective, the MAP approach makes it possible to **synchronize material innovation and end-product development** by enabling the industry to respond much faster and more flexibly to application requirements. Instead of focusing only on materials properties in early-stage development, strategic considerations such as techno-economics, sustainability and manufacturing are already taken into account. By **focusing on device manufacturability** instead of pure material synthesizability, MAPs will **reduce CapEx, time-to-market, and commercialization risk** for new materials. Finally, MAPs **transform open innovation into societal impact** by serving as a central platform that **brings together economic, regulatory, social, and political aspects** in a community enabling the successful rollout of **disruptive and sustainable innovation** in materials and devices.

Gaps and Recommendations

While the initial implementations of MAPs **clearly demonstrate the potential**, they also reveal the hurdles that still prevent **widespread establishment across the research community** and the steps that need to be taken to overcome them, both on the political/organizational and technical level.

Time is overdue for a revolutionary **shift in Materials Science** from the conventional trial-and-error, bench-top approach on very specific problems with many separate and manual processes to facilities with **automation** and **shared data spaces** that couple the physical hardware **to close the loop on accelerated materials discovery**. In order for MAPs to be quickly **adapted, implemented, and used by industry**, **long-term funding concepts** should be developed so that digital methods for materials research can be standardized and further developed at the same time as **providing value-added, materials solutions to industry**. In addition, this new methodology must be **incorporated into the training concepts of scientists**.

Funding should also **de-risk infrastructure access** for industry, especially SMEs and startups to enable the **transfer of the technology concepts** of the MAP community **into industry** in order to achieve a broad and fast-track adoption.

The community behind this call is working on a **policy paper** that elaborates on the framework for implementation, as well as **detailed technical guidance** for actual deployment through existing and future research initiatives.

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