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Materials Acceleration Platforms (MAPs): Accelerating Materials Research and Development to Meet Urgent Societal Challenges

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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. In this perspective, following the short paper, a broad overview about the challenges addressed, existing projects and building blocks of MAPs will be provided while concluding with a review of the remaining gaps and measures to overcome them.

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1. Motivation and Background

1.1. A Global Challenge

Globally, governments have embraced an indisputable fact: society will face significant impact from climate change and our growing demand for natural resources. This will inevitably call for new policies and technologies to improve quality of life and mitigate negative impacts globally and locally.[1] In the broadest sense, governments are addressing these challenges through key initiatives under the United Nations, specifically the UN Framework Convention on Climate Change[2] and the 2030 Strategic Agenda for Sustainable Development[3] with its 17 sustainable development goals[4] (SDGs).

Meanwhile, global energy consumption continues to rise, and recent gas shortages in Europe have led to an increase in coal usage in 2022 (IEA press release[5]). This highlights the urgent need to address SDG 7 (clean and affordable energy) by developing sustainable and abundant materials for energy generation and storage. This will not only help combat the enhanced greenhouse effect and the strong climate changes (SDG 13) but also affects drinking water safety (as highlighted by the IPCC report[6]) and support efforts to achieve SDG 6 (clean water and sanitation). In a broader perspective, it is necessary that we learn how to more efficiently produce, recycle and reuse materials to make the best use of our limited resources on earth. This requires concerted efforts and partnerships across government, industry, and academia to drive innovation, and ensure sustainable development for the future generations.

These global actions drive regional and national government policy in both developed and developing nations that must focus on clean and green, as well as sustainability and resilience. These policies co-exist in a framework of an industrial complex and its associated economic prosperity leading to societal challenges such as sustainable land use, efficient mobility and livable cities.

1.2. Importance of Advanced Materials

It is known that climate change impact mitigation strategies, energy resilience and economic prosperity hinge significantly on Advanced Materials (AdMats). With 20% of the industrial base and 70% of technical innovations relying on AdMats,[7] close attention to materials supply chains and accelerated materials discovery and development is needed. Further, as the percentage of the cost of materials technologies, particularly renewables, in new devices and systems increases, intense efforts are needed to find a lower cost, less toxic, environmentally friendly and more earth-abundant AdMat solutions. AdMats, alongside the pressing demand for accelerated advancements in discovery, development, and commercialization of novel processes, devices, and systems, are intricately intertwined with the environmental, energy, and resource imperatives set forth by governments worldwide.

Aligned with the industrial landscape, they aim to foster sustainable practices, facilit ating the judicious utilization of raw materials, ensuring a resilient energy infrastructure, fostering the development of eco-friendly chemical materials, and enhancing healthcare solutions for all. Their importance is not based solely on the value added by the industries directly involved in materials production, but rather on their significance as a cross-sectional technology. Materials research can have a significant and decisive impact on raw material sovereignty if we accelerate the development and scaling up of technologies that require fewer

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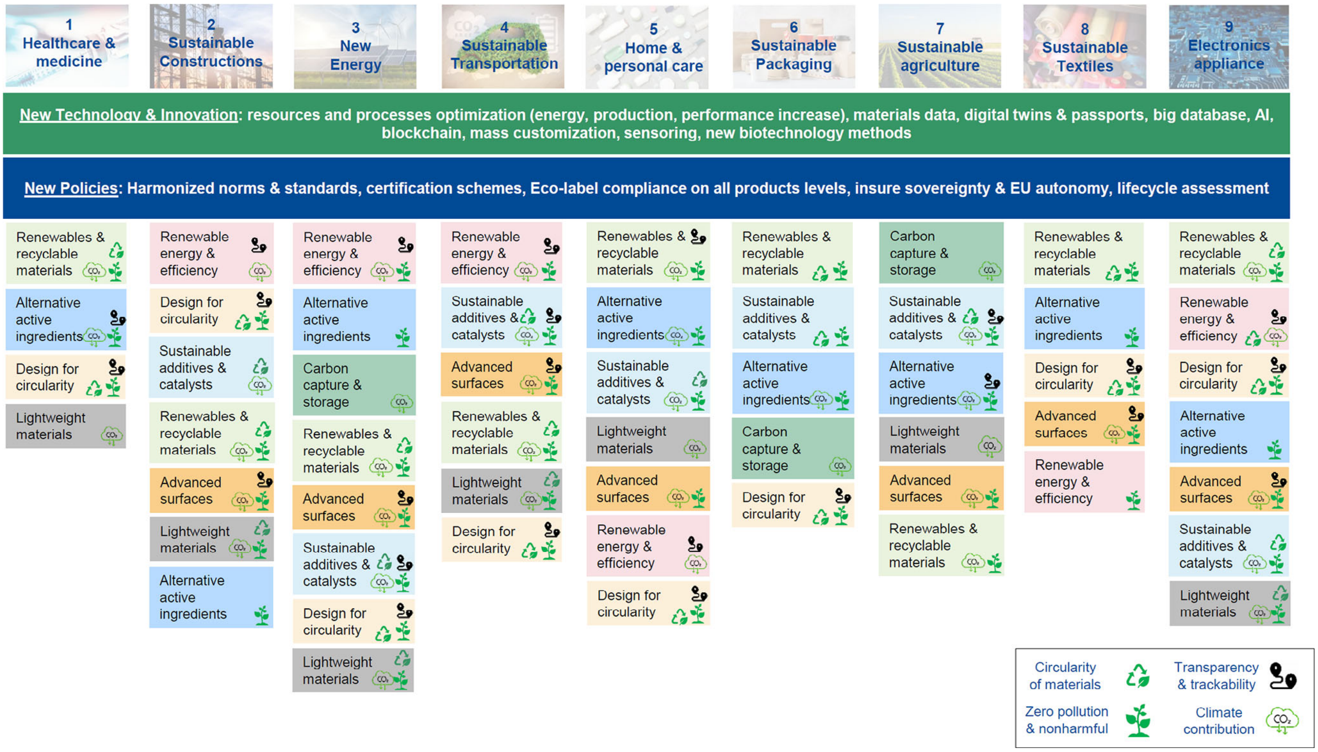

Figure 1. Nine innovation markets identified by the Materials 2030 Manifesto for which the development of advanced materials is critical. Reproduced with permission.[13] Copyright 2022, AMI2030.

(elimination) critical raw materials (CRMs) or those that already exist on territory (replacement). New materials are also needed for new device design for a circular economy and life cycle management that minimizes CRM usage (e.g., longer product life span, reuse, remanufacture, dematerialization, from products to services). Material research can also support the extraction of CRMs from old excavation ore materials or mine waste using, for example, floatation methods with more specific chemicals.

European Strategy: In Europe, the Green Deal Industrial Plan,[8] supports the transition to climate neutrality by enhancing the competitiveness of Europe's net-zero industry. Bolstered by the Digital Transition[9], the Green Deal played a major role in setting the 2020 Industrial Strategy.[10–12] This strategy is built upon the strength of a single EU market as its most important asset that offers resilience through certainty, scale and global access for European companies.

The Materials 2030 Manifesto: Most recently, the critical underpinning of advanced materials on a green transformation, and economic security and prosperity was articulated in the Advanced Materials 2030 Manifesto.[13] It calls upon systemic collaboration horizontally across sectors and vertically within the sector supply chains. The systemic collaborative approach will offer faster, scalable and efficient responses to advanced materials challenges to create opportunities for the European society. The Manifesto identified nine innovation markets (see **Figure 1**) and example applications critical within the European context. The need and actions necessary to achieve such a systemic approach under the Manifesto were elaborated in the Materials 2030 Roadmap,[14] and established a draft set of actions needed for the realization of the Materials 2030 initiative.[15] A crucial factor in this initiative is that it is founded on a public-private partnership model where a competitive advanced materials sector could lead globally by identifying 1) low-hanging fruit; 2) long-term game changers accelerated by efficient materials research (technology push); and 3) the requirements of the markets for new solutions or products (market pull). This is where the convergence of digital technologies, advanced computation, and automated experimental synthesis and characterization moves high-throughput experimentation, processing and analytics to a new level - one seeking to span the materials value chain and accelerate the discovery, development and commercialization of new advanced materials, devices and systems. The degree and nature of acceleration will vary but recent examples (see Section 2.3) have confirmed that advanced materials development cycles could be reduced from tens of years to years, with a commensurate reduction in the development cycle costs. These will be explored further in this article.

1.3. The History of Accelerated Advanced Materials Research

High-Throughput History: First, AdMats screening using high-throughput theoretical and computational predictive approaches is an effective initial step in the acceleration of the R&D process.[16] There is in fact a rich history in acceleration of research through accessible high-throughput research strategies pioneered in Germany in the 1950s.[17] With the push for automation at the turn of the century in Asia and the USA, pioneers deployed automation through the paradigm of combinatorial materials science to accelerate research. The realization by the USA government that AdMats play a critical role in global competitiveness then led to the USA's Materials Genome Initiative in the early 2010s.[18,19] The idea of inverse design within this initiative was driven through theoretical predictions that identify attractive candidate materials for experimental validation.

High-Throughput state of the Art: Next, automated, combinatorial and/or high-throughput experiments aim at rapidly and systematically screening large library of materials. While automatic synthesis of organic molecules has become a standard in pharmaceutical R&D and synthetic and industrial chemistry,[20,21] accelerating experimental exploration of AdMats in other fields such as inorganic battery materials remain challenging because of the complexity of automating some of the synthetic routes employed for the preparation of these materials. However, by building on high-throughput experimentation, automated systems can significantly reduce the quantity, and therefore the cost of pricy input materials and improve statistical significance, allowing for a larger number of highly efficient experiments under comparable budgets. As a result, the costs associated with materials discovery and development can be significantly reduced, paving the way for transformative breakthroughs in various fields of research.

Combination of High-Throughput with AI: Further, the generalization and systematization of digitalization as well as the recent and rapid advances in Artificial Intelligence (AI) offer a unique opportunity to transform the R&D culture and accelerate the development of AdMats. AI has already demonstrated its ability to speed up individual research tasks, such as planning experimental campaigns in a high-dimensional materials development workspace, processing large amounts of data (Big Data); and accelerating simulation and modeling methods. However, AI research can go beyond these tasks to include the rigorous organization and standardization of R&D data, such as creating ontologies and enabling semantic querying to interlink data repositories with data production and processing pipelines. Overall, AI can significantly enhance the AdMats development process by enabling more efficient and effective R&D practices.

From High-Throughput and AI to MAPs: By gathering and articulating high-throughput computational and experimental approaches together with digitalization and AI, so-called Material Acceleration Platforms (MAPs) represent a disruptive, cross-sectional technology across materials science disciplines that will enable faster and more cost-effective R&D as outlined in the presented paper. Given the significant dependence of society on advanced materials, and the revolution occurring in AI methods and advanced automation technologies, there is no surprise that MAPs will play a major role in what Mario Molina, Nobel Laureate, considers the "second revolution in science."[22]

2. About MAPs

2.1. The Idea of a MAP

The concept of a MAP is to use methods of automation and digitalization in material research to accelerate innovation (c.f. **Figure 2**) by orders of magnitudes in order to tackle specific present and future challenges of mankind.

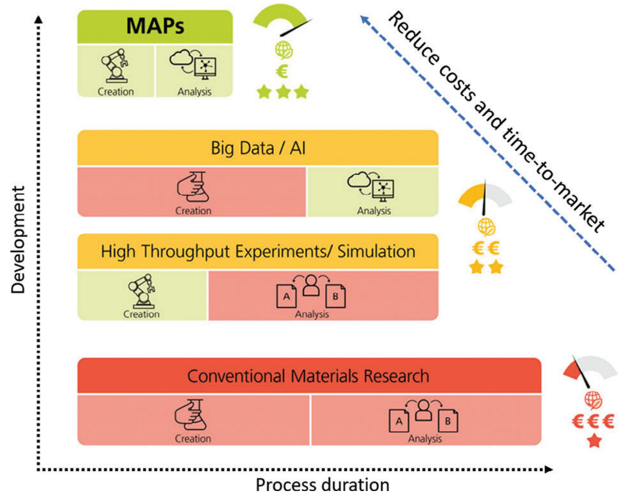

Figure 2. Automation in production and research. Automation in production has accelerated the manufacturing of goods and resulted in a massive increase in materialistic wealth. Conventional materials research is dominated by human-centric processes. High-throughput methods and AI data analytics accelerate parts of the scientific workflow but leave scientists intuition as the origin of materials discovery and further bottlenecks in the workflow where manual experimentation is still needed. The synergistic combination of both key elements results in the idea of a MAP which aims to accelerate the entire research cycle to yield advanced materials for solving problems and tackling challenges of society.

MAPs[22] provide a general framework to jointly work on faster, more efficient development and production of new advanced materials for specific applications and targets, with energy materials being a focal area of acceleration today.[23] MAPs are collaborative infrastructures integrating automation and digitalization to accelerate the innovation and development of AdMats. They complement and enhance the productivity of a research team by replacing labor-intensive experimentation and processing with automated high-throughput laboratory techniques and AI-supported data analysis, simulation/modeling and experimental planning. This closes the optimization loops and allows scientists to focus on rapidly accessed, high-fidelity data. Further, with the world population rapidly aging, MAPs can also help increase productivity to counterbalance the shrinking active research workforce. Thus, they will enable more rapid adaptation to ongoing changes in the environment, geopolitical issues, and regulation, and in particular they will help the development of new materials using, and reusing, locally abundant resources.

The MAP concept (c.f. **Figure 3**) follows the vision of a human-supervised, self-learning autonomous lab which automates the production and evaluation (synthesis and characterization) of a material or a device in an environment supported by AI-informed experimental planning and data processing, computation and simulation that can also be accelerated by AI, and is built on a framework of mechatronics to handle materials processing and analysis.

This enables MAPs to provide the following capabilities:

1. MAPs automate mundane and repetitive tasks, allowing researchers to focus on the underlying scientific questions.

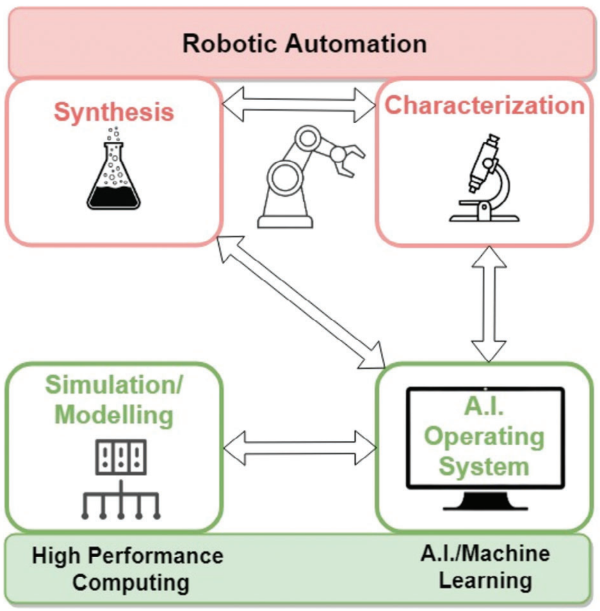

Figure 3. The MAP concept, integrating automated synthesis, manufacturing, and characterization with high-performance computing and AI/Machine Learning. Reproduced with permission. Copyright 2024, Mark Kozdras.

2. MAPs are end-to-end workflows that supersede manual and stepwise approaches.
3. MAPs can target (not optimize in a narrow range) materials and devices in a much larger experimental space that has yet to be imagined.
4. MAPs solve multi-dimensional and multi-level problems that conventional methods cannot handle.
5. MAPs are predestined for inverse design and thus, ideal tools for application-oriented material development.
6. MAPs can be used in a shared way by individuals, educators, trainers, and organizations to streamline their learning and development initiatives.

2.2. Why Will it Be Superior?

Closed Loop: Through the use of advanced computational approaches guiding experiments for new materials and devices, which in turn provide feedback in a continuous improvement loop, MAPs target the whole addressable parameter space.[24] For instance, a battery MAP simultaneously optimizes the materials (electrodes, electrolytes) and the whole battery itself, on a set of defined properties for the end use (e.g., charging and discharge times under a set of conditions, capacity and safety amongst others).

FAIR: MAPs will revolutionize data-driven experimentation producing complete, fully documented, meta-data rich and structured data sets. They are FAIR by design as they will include sufficient information about the process or material they encompass. FAIR is an acronym for Findability, Accessibility, Interoperability, and Reuse and refers to the guiding principles for scientific data management and stewardship.[25,26] The FAIR data principles focus on machine-readable and processable metadata on scientific data to enable the use of computational tools to support humans processing data with increasing volume, complexity, and creation speed. Findable implies that data should be easy to find for humans and computers, which requires a dataset to have a globally unique identifier and to be described by rich metadata, that allows to filter and distinguish datasets. Accessible means that (meta)data are retrievable by their identifier from a publicly accessible source, with optional authentication and authorization, over a standardized communication protocol. FAIR (meta)data need to use a formal, accessible, shared and broadly applicable language for knowledge representations. It is thereby Interoperable. The reuse of data is the ultimate goal of FAIR. This last principle requires the scope and limitations of the data to be described, which is achieved by including all information needed to reproduce, reevaluate and repurpose (meta)data in a particular context. In the first instance, MAPs will satisfy the internal integrity of the digital process/material and in the second they will provide a sufficient level of autogenerated description - metadata, semantics and ontology to comply with minimum FAIR standards (e.g., OntoCommons,[27] DOME 4.0,[28,29] FAIR4RS[30]).

Holistic: MAPs provide a holistic approach to developing and producing new materials for optimum impact. They can accelerate materials development across a myriad of industrial sectors, including chemicals, electronics, pharmaceuticals, and energy. MAPs go beyond a single material, optimizing the whole device for the intended application. MAPs provide a means to simultaneously develop and test materials and processes all the way to devices and systems.

Collaborative and Cross-Domain: MAPs enable unprecedented connectivity of material data across multiple industry sectors, leveraging AI-driven transfer learning from energy to pharmaceuticals and biomaterials. In addition, designed to facilitate extensive collaboration, both virtually and physically, MAPs empower researchers and stakeholders alike. Overall, this will foster new collaborative approaches exploiting synergies previously undiscovered, while advocating for "Safe and Sustainable by Design" approaches. By engaging basic researchers, translators from different disciplines, and industry RD&I, MAPs seamlessly traverse Technology-Readiness Level scales, mitigating the "valley of death" and bridge knowledge gaps between industries.

Decentralized and Modular: MAPs can be implemented in one location, or they can integrate decentralized pieces of equipment in different geographic locations through a centralized data repository, experimental analysis and orchestration. They can be remotely controlled providing access for researchers from all over the globe that can utilize the data and submit experimental designs and questions. As such they make it possible to utilize intellectual capacities in countries where experimental infrastructure may not meet high standards, offering "experiments as a service" to researchers in these regions.

2.3. Research Projects and Initiatives

There is already consensus about the opportunities. While the broad application of MAPs is still outstanding there are already a number of platforms that are beyond the concept phase and demonstrate the potential of these approaches. There has been a growing number of programs and initiatives seek to accelerate

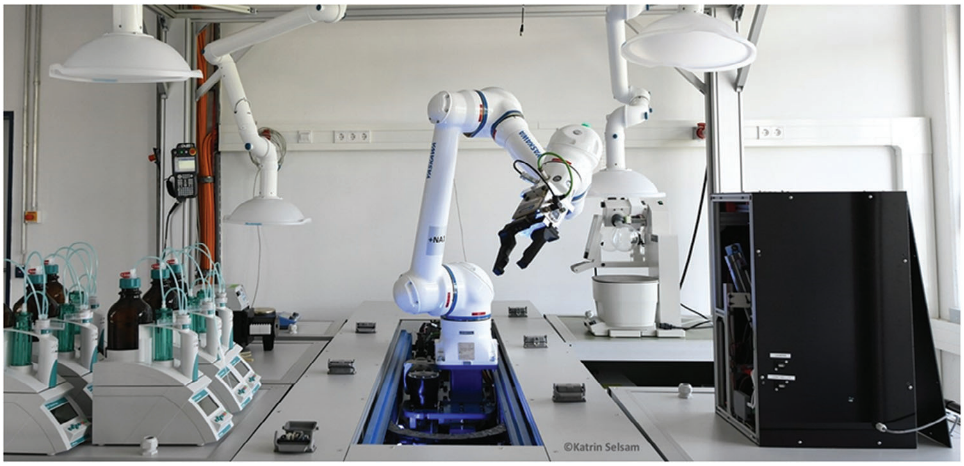

Figure 4. One of the robotic platforms (located at Fraunhofer ISC) developed in BIG-MAP utilizing a pluggable module system where each module is dedicated to a specific task like dosing, mixing, heating, evaporation and phase separation. A six-axis robot in the center of the platform integrates the modules and handles the material and container transport between them. (Reproduced with permission. Copyright 2024, Fraunhofer ISC.).

materials development and technology transition through automated closed-loop discovery systems that blend robotic platforms together with high-throughput screening (HTS), all orchestrated by AI-based data analytics and computing.[31,32] They have been deployed in areas such as peptide synthesis,[33] the pharmaceutical industry,[34,35] and the development of high-efficiency solar cells.[36] More recently, semi- and fully automated platforms have started to target chemical synthesis and fuel production (from atmospheric feedstocks).[37,38] Furthermore, there are several projects preparing the background infrastructure that will be necessary to exploit the full potential of these platforms and their output for the broader research community and society:

BIG-MAP[39]: The Battery Interface Genome - Materials Acceleration Platform (BIG-MAP) project is part of the large-scale and long-term European research initiative BATTERY 2030+.[40] It proposes a radical paradigm shift in battery innovation, which will lead to a dramatic speed-up in the battery discovery and innovation time; reaching a 5–10-fold increase relative to the current rate of discovery within the next 5–10 years. BIG-MAP relies on the development of a unique R&D infrastructure and accelerated methodology that unites and integrates insights from leading experts, competencies and data across the entire battery (discovery) value chain with AI,[41] High Performance Computing (HPC), large-scale and high-throughput characterization, and autonomous synthesis robotics.

In short, BIG-MAP aims to reinvent the way we invent batteries and to develop core modules and Key Demonstrators of a MAP specifically designed for accelerated discovery of battery materials and interfaces.

MAPs@Fraunhofer ISC: In addition to research on battery materials (see BIG-MAP), the Fraunhofer Institute for Silicate Research (ISC) is also active in many other fields such as glass, ceramics, polymers, particles and biomaterials, where it is increasingly adopting the MAP concept (c.f. **Figure 4**).[42] Particularly in the field of biological tissues engineering,[43] significant increases in quality and throughput have been achieved through laboratory automation (c.f. **Figure 5**) while human effort for nanoparticle synthesis could be reduced by ≈44 %.[44] Overall, the focus at Fraunhofer ISC lies strongly on modular concepts, both in hardware and software, so that individual modules can be easily transferred between the different specialized departments.

VIPERLAB[45] *and AutoPeroSol*[46,47]: The EU-funded project VIPERLAB is offering access to a distributed virtual laboratory for Perovskite solar cells. While VIPERLAB is not a MAP, it has a strong focus on data curation and databases for perovskite solar cell data that will create an important data repository that future MAPs can utilize. The AutoPeroSol project funded by the German Helmholtz Association has a similar focus on data sharing between Helmholtz Centers. A strong collaboration between the projects has evolved targeting a comprehensive ontology for perovskite solar cells which could form an important basis of semantic learning for MAPs.

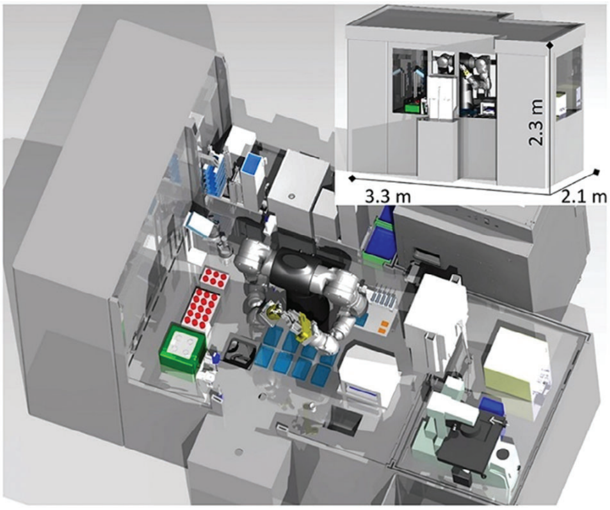

Figure 5. Robotic cell for tissue engineering utilizing a two-arm robot and conventional lab equipment. (Reproduced under the terms of the CC-BY license.[43] Copyright 2021, Haeusner et al.).

Figure 6. Line1 is a functional MAP for the development of organic solar cells at the Helmholtz Institute Erlangen–Nuremberg. Reproduced with permission. Copyright 2023, HI ERN/Kurt Fuchs.

AMANDA/Line1[48]: One of the most complex and advanced MAPs currently operating. AMANDA is the orchestration and data management interface that is able to manage multiple MAPs at the same time. Line1 is an automated processing line for the manufacturing and characterization of full organic solar cells (c.f. **Figure 6**). Line1 is capable of formulating inks, depositing thin functional films, characterization of films (imaging + spectral characterization), evaporating electrodes, performing jV-characterization under illumination, and light aging of full organic photovoltaic (OPV) devices to determine stability. AMANDA integrates Bayesian Optimization and Gaussian Process regression to perform fast optimization of devices (c. f. **Figure 7**). AMANDA and Line1 were built with funding by the DFG and the project ELF-PV by the state of Bavaria in cooperation between the Friedrich–Alexander–University Erlangen–Nuremberg and the Helmholtz Institute Erlangen–Nuremberg for Renewable energies (HI ERN). Over time, AMANDA has, with reference to edisonian high-throughput experimentation, achieved an acceleration starting at 30-fold[49] reaching recently over 100-fold.[50,51] Among others this has led to the identification of ultrastable perovskite compositions in the multi-dimensional parameter space.[52]

MAPz@BAM: Federal Institute for Materials Research and Testing (BAM) started the module development for MAPs in 2020 for three application areas: Nano and advanced materials, structural materials for green energy transition and sustainable construction materials (c.f. **Figure 8**). In different MAPs along these priority topics, the generated data is used for experiment planning through sequential learning and artificial intelligence. BAM MAPs follow a circular and multi-stage approach by integrating up-scaling, process development and stability through proxy experiments and workflows. Through collaborations with national initiatives MaterialDigital and MatWerk/FAIRMat, concepts for data and metadata structures as well as data sharing workflows are established. Different modules from different branches of BAM are currently being merged in MAPz@BAM

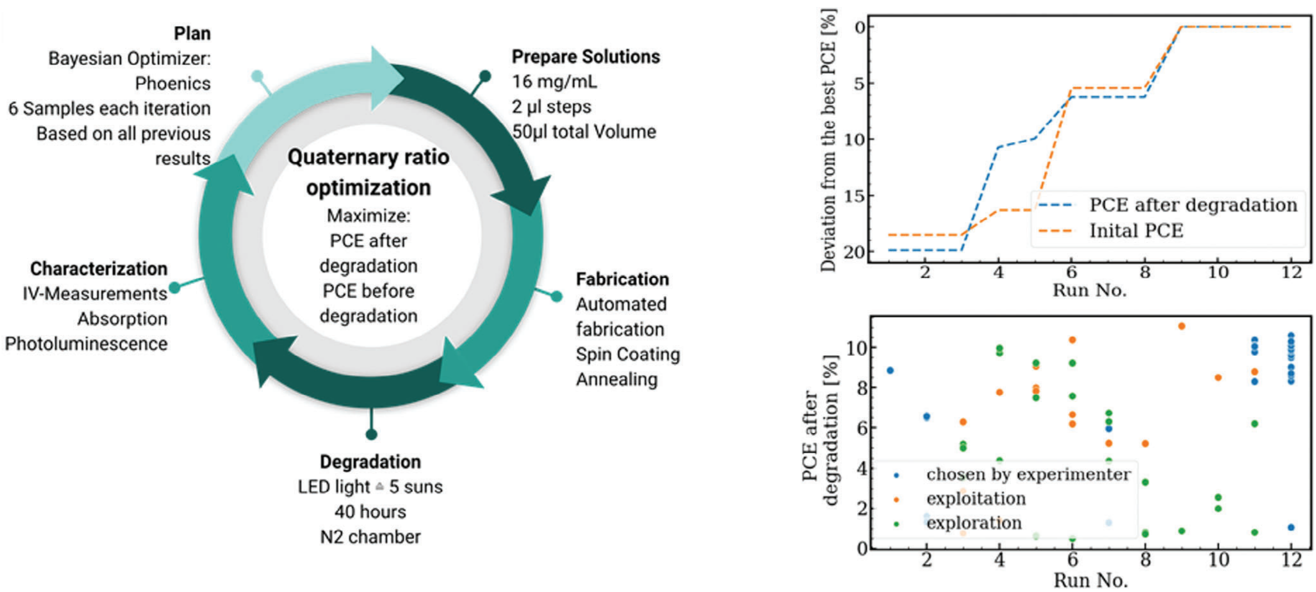

Figure 7. Example of an autonomous optimization of a quaternary OPV-mixture performed on AMANDA/Line1. The Bayesian optimizer Phoenics was used to optimize two objectives (initial efficiency and efficiency after aging test) in a 3D-process parameter space. Six samples were investigated in each iteration, the optimum was found after nine iterations. (Reproduced with permission.[53] Copyright 2021, Tobias Osterrieder.).

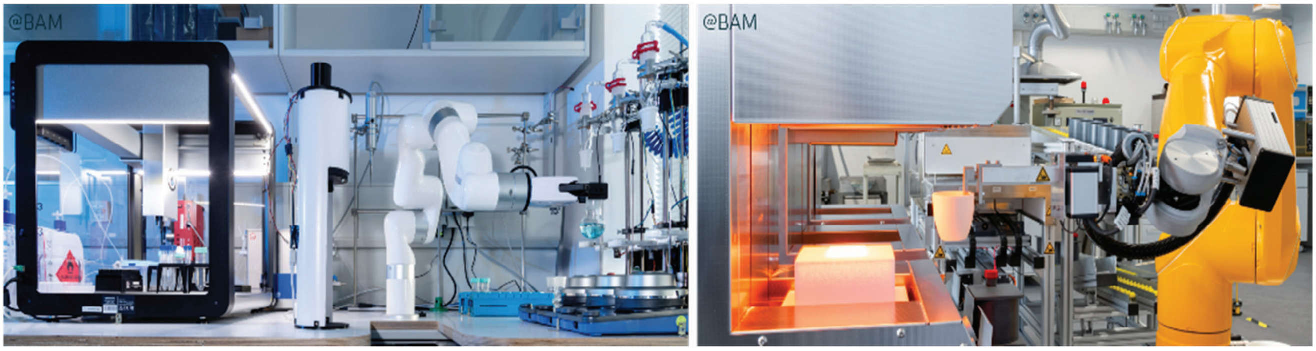

Figure 8. Nano and advanced materials and glass modules (built in cooperation with Fraunhofer ISC) of MAPz@BAM (Reproduced with permission. Copyright 2024, BAM).

(MAP-Zentrum of BAM) that will be operational in the Summer of 2025 in the Adlershof Campus as a core facility for transfer projects.

ION-SELF: A Spanish project initiated in 2019 for the development of an autonomous experimental MAP, capable of making effective predictions and self-driving high-throughput syntheses and characterizations of battery materials.[54] This innovative autonomous lab, which is continuously upgraded, has already permitted to successfully explore new families of electrode materials in collaboration with several European battery industrial partners.

Synbio-MAP: An effort in Finland by VTT to develop a biotechnology-based MAP linking synthetic biology to high throughput screening and testing of materials and precursors to physics-driven modeling and AI for structure and functionality prediction and design.[55] The initial focal areas are protein-based materials and bioplastic, especially polyesters.

AMDEE[56]: The AI-Driven Integrated and Automated Materials Design for Extreme Environments (AMDEE) project in the United States linking robotic, high-throughput characterization, a centralized automation control data hub, and streaming scientific data focused on development of refractory multi-principal-element alloys (RMPEAs), light alloys, and ceramics with dynamic and high-temperature properties needed for impact resistance and hypersonic performance (c.f. **Figure 9**). AMDEE laboratories utilize streaming, event-driven integration of data infrastructure integrates design, decision, and control loops for orchestrated deployment of AI/ML decisions.

BasCat/FHI: The Fritz Haber Institute - UniCat BASF JointLab[57] aims to develop accelerated or self-driving laboratories for heterogeneous catalysis (often also referred to as digital catalysis, c.f. **Figure 10**). In recent research[58] an active learning loop was established, in which an adaptive design of the experiment algorithm queried batches of experimental data. The catalysts were synthesized and tested, and on the basis of the gained performance data, a model for the explored design space was established. The design space consisted of promoter species and their concentrations to enhance a specific reaction (conversion of propane to propylene). Within less than 100 catalysts thus created and tested (requiring less than 3 months), a new promoter combination was found that is competitive to the one presently used by BASF in their commercial Oleflex process.

MARK@KIST: The Korea Institute of Science and Technology (KIST) launched the MARK (Materials Acceleration Research K-lab) project in 2022. This initiative aims to accelerate the discovery of nano-materials for electrochemical water-splitting

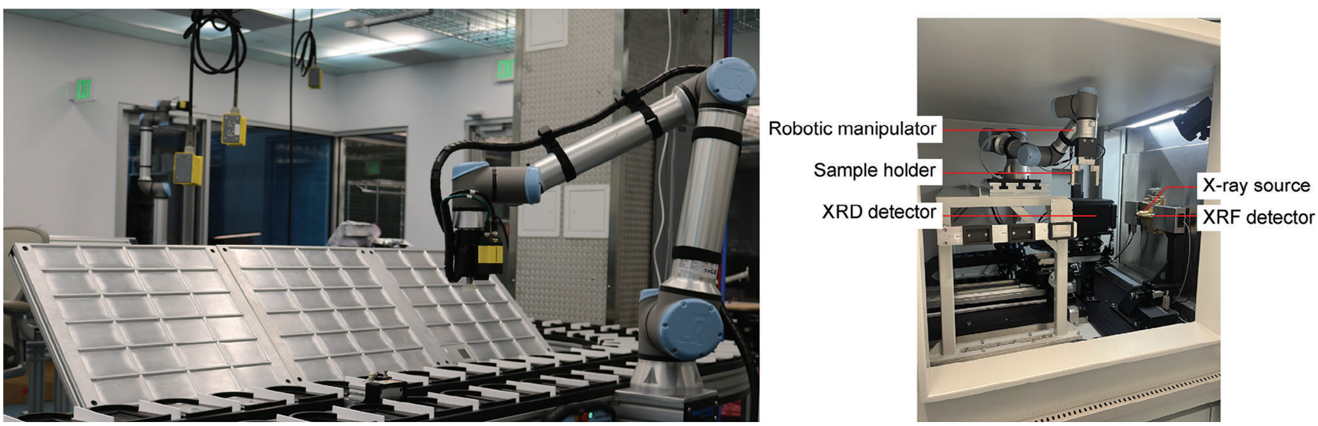

Figure 9. Left: UR10e robot hovering above the bi-directional conveyance system that delivers samples in the AMDEE project. Six such robots are equipped with vacuum grippers to deliver samples to testing and characterization stations around the laboratory. Right: A smaller, UR3e robot within the MAXIMA high-transmission XRD and XRF system receives samples from the conveyance-line robot to complete fully automated sample loading and X-ray characterization. Reproduced with permission. Copyright 2024, David Elbert.

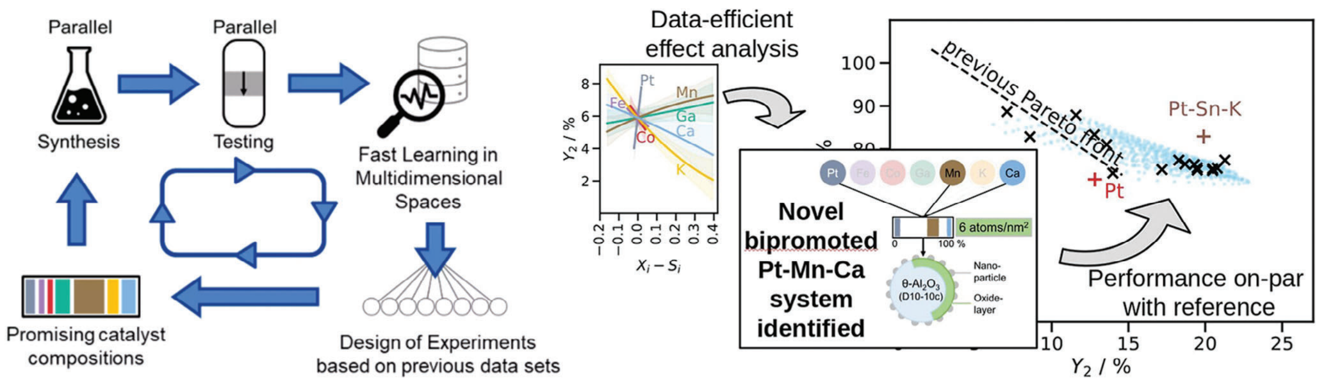

Figure 10. Concept of accelerated catalysts laboratories at BasCat (left, reproduced with permission.[57] Copyright 2024, Frederik Rüther) and identified promotor system (right, reproduced under the terms of the CC-BY 4.0 license.[58] Copyright 2024, Kunkel et al.).

catalysts and display quantum dots (see **Figure 11**). The project emphasizes full lab automation, the development of AI models for experimental planning, the creation of an operating system (OS) for orchestration, data generation including negative materials data, and data mining from literature using natural language processing. Recently, KIST emphasized the value of autonomous laboratories, which offer twofold benefits of enhancing material developmental efficiency and elucidating novel chemical knowledge by analyzing the datasets accumulated form the operations of AI robotic platforms.[59] Moreover, the OS for MAP will streamline the management of diverse experiments conducted by multiple users, thereby enhancing the scalability of MAP in materials discovery.[60]

2.4. Academic and Industrial Research Frameworks

Besides focused research projects there are numerous research frameworks with a broader view on digital materials research. They aim to join efforts on common cross-domain requirements and demand from industry (e.g., research infrastructure and standards).

MaterialDigital: This platform is an initiative funded by the German federal government to coordinate the activities of a program to develop and demonstrate tools to enable the seamless decentralized exchange of materials data between various stakeholders based on a semantic data exchange.[61] Academic and industrial partners collaborate in the development of a platform for decentralized data exchange that accommodates both the needs of industry for data provenance, as well as the established FAIR principles in academics. Besides data exchange, this also includes the establishment of decentralized workflow environments for data processing, modeling, and simulations.

FAIRmat: The FAIRmat project[62] aims to create a federated FAIR data infrastructure for materials data with a central hub, the FAIRmat Portal. FAIRmat aims to advance and develop metadata schemas and ontologies and enables the efficient exchange of FAIR research data, ensuring that the FAIRmat data infrastructure will advance basic science of condensed-matter and materials physics by supporting active researchers, and also be of great value for engineering. It tries to convince scientists to also share data they consider useless for their present purpose-oriented research, and reaches out within and beyond the community providing advice, training, and user support. FAIRmat is funded

Figure 11. Overview of the MARK project by KIST. The KIST team has recently developed an autonomous experimental platform system, featuring a mobile robot and three fully automated modules: a batch-type nanoparticle synthesis module with UV–vis measurement, a washing process module, and electrochemical half-cell testing module (RDE). (reproduced with permission. Copyright 2024, KIST).

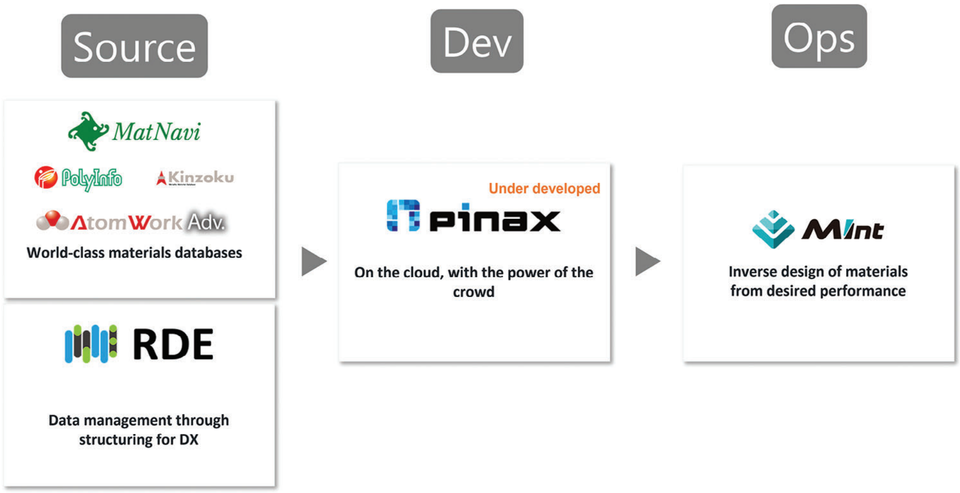

Figure 12. Digital services provided by Materials Data Platform (MDPF) in NIMS, Japan (reproduced with permission. Copyright 2024, NIMS).

under the scheme of the German National Research Data Initiative (NFDI).

DIADEM: In 2022, the French government has funded € 85M an 8-years project for accelerating materials discovery.[63] The goal is to set a nation-wide hub of platforms including high-throughput synthesis, shaping, and characterization of materials and establishing strong links with a digital platform for materials and processes design, databases, deep learning, and AI.

PSDI: In 2021 the UK government agency Engineering and Physical Sciences Research Council (EPSRC) funded the Physical Sciences Data Infrastructure project (PSDI).[64] The aim of PSDI is to enable researchers in the physical sciences to handle data more easily by connecting the different data infrastructures they use by improving finding, accessing and combining reference quality data from different commercial and open sources, using AI to explore data and enabling sharing of data, software, and models according to FAIR principles.

CAPeX: In 2023, five Danish foundations and the Ministry of Higher Education and Science funded a 45M€ and 13-year "Pioneer Center for Accelerating P2X Materials Discovery."[65] CAPeX is hosted at the Technical University of Denmark (DTU) and Aalborg University and unites five Danish universities with international consortia like the Acceleration Consortium at the University of Toronto, the SUNCAT Center at Stanford University, and the European SUNERGY initiative at Utrecht University in a trans-disciplinary research center focused on accelerating the discovery of sustainable and scalable materials and electrocatalysts for Power-to-X, through the development of an AI-orchestrated Decentralized and AsynchroNous Materials Acceleration Platform (DANMAP).

NIMS-MPDF: The National Institute for Materials Science (NIMS) Japan has established the Materials Data Platform (MDPF) to provide digital services that accelerate materials research and development. As illustrated in **Figure 12**, MDPF's services are comprised of materials data resources (Source), a materials model development environment (Dev), and a materials model operation environment (Ops).[66]

The materials data resources include MatNavi, one of the world's largest materials databases. For example, AtomWork-Adv., the inorganic materials database, contains 379 736 existing inorganic crystal structures collected from academic papers along with phase diagrams and properties (as of March 2024).[67,68] PoLyInfo, a polymer database, includes data on 32 924 unique polymers, detailing their repeated structures, monomers, and properties (as of March 2024).[69,70] In addition to the databases curated from academic papers, NIMS publishes databases derived from standardized tests conducted by the institute over many years, covering mechanical performances such as creep, fatigue, and corrosion.[71–73] Other noteworthy databases include the Diffusion Database (Kakusan),[74] the Computational Phase Diagram Database (CPDDB),[75] and the Thermophysical Property Database.[76] The Research Data Environment (RDE) is a system developed to digitize all research workflows and capture the research data produced. It was launched in January 2023.[77] By using templates composed of Python codes for the automatic extraction of measurement conditions from instrument data files and customized forms for entering sample information, research work data can be structured and recorded in a reusable format. As of August 1, 2024, there are more than 1000 active templates, 3447 users, and 1 158 615 data files.

As for the Dev environment, a new AI platform called pinax is under development and is expected to become operational by the end of 2025. The Ops environment, known as MInt, is a scientific workflow system capable of linking processing, structure, property, and performance on a computer.[78–81] Numerous modules (or models), primarily focused on structural materials, have already been registered and are being utilized by an industry-academia consortium operated by NIMS. MInt is contributing to solving the inverse problem of designing materials and processes from performance.[82]

The MDPF, in collaboration with the Advanced Research Infrastructure for Materials and Nanotechnology (ARIM) and the Data Creation and Utilization Type Material Research and Development Project (DxMT), forms the core of the Materials DX Platform initiatives funded by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. Furthermore, the MDPF services are planned for use in various national projects.

MGI: The U.S. Materials Genome Initiative (MGI), launched in 2011, is a multi-agency effort aimed at accelerating the discovery, development, and deployment of advanced materials. The initiative seeks to transform the materials science field by integrating computational tools, experimental methods, and digital data management, thereby reducing the time and cost associated with material innovation. By fostering collaboration between government, industry, and academia, MGI enables the rapid screening of material properties and the optimization of material performance for various applications, including energy, transport, and manufacturing. Key federal agencies involved include the Department of Energy, the National Science Foundation, and the National Institute of Standards and Technology (NIST).[19,83]

Acceleration Consortium: The Canadian Acceleration Consortium is a initiative designed to speed up the discovery, development, and commercialization of advanced materials in Canada. Launched with a focus on using artificial intelligence (AI), robotics, and high-throughput experimentation, the consortium aims to bridge the gap between academic research and industrial application. By fostering collaboration between universities, research institutions, and industry partners, the Acceleration Consortium supports the rapid prototyping and scaling of new materials, particularly in areas like clean energy, pharmaceuticals, and advanced manufacturing.[84]

European Materials Modeling Council (EMMC) and European Materials Characterization Council (EMCC): EMMC[85] was created in 2014 and aims to combine materials modeling and digitalization to accelerate and maintain the development of novel materials. They recommend improving communication and collaboration among stakeholders, identifying hurdles and providing solutions, facilitating integrated modeling and digitalization, connecting academic research with industrial exploitation, sustaining material modeling digitalization in Europe, informing industrial awareness, and supporting the software industry. An important asset governed by the EMMC is the Elementary Multiperspective Material Ontology (EMMO)[86] building the foundation of interoperable materials research. EMCC[87] was established in 2016 with objectives including involving stakeholders in developing characterization tools, identifying requirements, organizing R&I initiatives, creating a nano-characterization framework, and linking nanometrology with industry. Both councils play crucial roles in advancing materials science and technology in Europe. Important results of the EMCC are efforts the standardize characterization (CHADA) and model data (MODA) initiatives.[88]

Energy Materials Industrial Research Initiative (EMIRI): EMIRI[89] is an organization that focuses on accelerating the development and deployment of advanced materials for clean energy technologies. EMIRI brings together industry, research institutes, and other stakeholders to collaborate on innovative solutions for energy transition. Their primary goal is to support the commercialization of energy materials by fostering research and development, knowledge sharing, and market uptake. EMIRI plays a vital role in advancing the transition toward a sustainable and low-carbon energy system by promoting the use of advanced materials in areas such as renewable energy, energy storage, and energy efficiency. EMIRI provides strong support of the MAP approach and regularly hosts workshops to bring the community together.

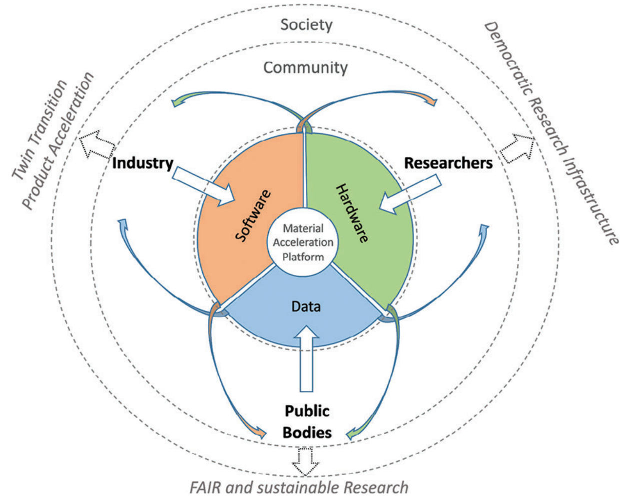

Figure 13. Layers of a MAP: Core components Hardware, Software, and Data in the center surrounded by a community driving the MAPs with strong embedding the scientific domains, industry applications, and public funding.

3. Building Blocks

Here we provide the technical context regarding the necessary building blocks of MAPs to illustrate why they fall outside traditional funding and governance schemas and require an interdisciplinary, coordinated effort. As displayed in **Figure 13**, MAPs are more than just technology—they are community-driven ecosystems that combine multiple components in a working system.

In essence, MAPs are a new concept or meta-method that will fundamentally change how we conduct and record the process of materials research and transformation. They are transiting from traditional costly analog trial-and-error approaches to more agile digital research powered by automation and AI-enhanced decision-making. Being disruptive by nature, MAPs do not exist in isolation. Instead, they reside in a research community with democratized access to lab-of-the-future infrastructure and public bodies to govern FAIR and sustainable science.

MAPs come in different shapes and forms such as locally and fully integrated to run specific materials development programs, distributed between different facilities or even highly decentralized entities. The latter are cloud labs that provide democratized access to MAPs and serve a broader academic and industrial community. Regardless of their specific implementation, the same key components are always involved:

A MAP is an ecosystem that goes far beyond its technical components. Those technical components can be divided into two groups, hardware and software, while the third non-technical component is the research community providing the MAP's context and area of impact.

The **hardware components** of a MAP provide a highly integrated automation of laboratory experiments. A suitable setup is designed and maintained by dedicated mechatronic teams. The setup consists of synthesis equipment to produce materials and devices, characterization equipment to analyze the experimental output, and robots to automate and accelerate sample handling between the two. Peripheral components include safety and resource infrastructure.

The **software components** are the backbone of the MAP that enables its operation by interfacing instrumentation, controls, simulation and hardware, providing data storage and analytical tools as well as orchestrating the components of the MAP. Important tasks of the software include the data management and analyses (involving the development of new analytical tools for automated high-throughput analyses), and then AI-driven experimental planning, employing digital twins of R&D workflows and experiments by multi-scale modeling (electronic, atomistic, mesoscopic, continuum, and macro-scale modeling).[90]

Finally, the ecosystem of a MAP depends on a **research community** that nourishes and guides the MAP, provides feedback and leverages the knowledge generated. To date, the feedback alone is not enough to operate a MAP. Even more, the input provided by human creativity - which machines do not possess - is indispensable and creates the area of impact for a MAP in the first place.

3.1. Hardware

Materials synthesis and analysis require a wide range of often highly specialized laboratory equipment, encompassing processing tools like solid and liquid dispensers, mixers, coaters and ovens, as well as characterization instruments such as microbalances and thermocouples to sophisticated spectrometers. Hardware requirements, particularly for synthesis, vary widely and can be highly dependent on the scope of application, ranging from additive manufacturing solutions for structural and functional materials to high-throughput bioreactors. This high level of specialization of the equipment has led to a fragmented market, characterized by numerous small-scale specialized equipment manufacturers. Even within a modestly sized MAP, integration of equipment from a variety of manufacturers is necessary to address the multifaceted processes inherent in typical materials science challenges. A common problem when integrating these systems into a MAP is the fact that they are often designed as standalone pieces of equipment meant to be operated by humans, the lack of comprehensive standards (unlike in industrial automation) and the frequent lack of documentation for digital interfaces that may exist. Consequently, the interconnection of this equipment is commonly an initial obstacle in the establishment of a MAP.

In MAPs, automated laboratories are typically constituted of different modules or stations, each of them dedicated to a specific task or subtask (e.g., materials synthesis, materials characterizations, materials handling and materials processing). The diversity of synthesis routes, characterization techniques and materials processing approaches represent a large variety of technical solutions to be designed and implemented in MAPs. These tasks can be carried out in high-throughput or inline manner, in sequence or in parallel, rather than in small batches in traditional labs operated by humans. Though commercial solutions are available for high-throughput lab experimentations, but can be very specifically designed, with limited flexibility for customizations or upgrades as well as with limited options for a facile integration in a larger interconnected system such as a MAP. For these reasons, MAPs often require custom design and in-house built modules and stations, which enable greater flexibility in the design, integration and possible future upgrades. Robots and automation are of particular importance as an integrative element of a MAP in order to manipulate and transport samples and consumables required to carry out the experiments. In particular, multi-axis systems can flexibly transport materials and samples between different stations/modules of the MAP or, conversely, guide tools and measuring instruments over the materials. Unlike humans, robots do not suffer from the monotonous repetitive activity and perform it with constant high speed and precision. In addition to work ethics aspects, this also has a direct positive influence on the reproducibility and data quality of the results.

However, the use of robots may require substantial initial investments as well as specialized personnel for designing, maintaining and integrating automated laboratories, as the automation of trivial manual motion sequences is often associated with considerable complexity. Automation of laboratory hardware is thus a main enabling technology for MAPs. In recent years the cost of automation has decreased significantly and the range of small- to midscale robots which are available for the integration in a laboratory environment has increased significantly.

Nevertheless, automation in a laboratory environment is still different from automation in an industrial production environment. In industry robots are made to repetitively perform a single task over and over. They must be robust as the failure of a robot can stop a production line. They also often need to operate under the control of a factory worker, which requires very robust and easy-to-use human-machine interfaces. In industry, there are often highly trained teams of software engineers performing the system integration of industrial robots into large production lines, utilizing large-scale virtual environments or digital twins.

In research laboratory environments, the requirements differ significantly. Robots intended for scientific applications must be seamlessly integrable, user-friendly, and readily upgradable. They should offer swift reconfigurability to adapt experiments quickly and carry out complex designs of experiment. In these environments, robots are often operated by highly trained scientists and technicians, possessing some programming proficiency. However, such profiles are not widespread, as programming remains a rare inclusion in educational training programs for materials science and engineering. Consequently, these experts frequently need to change setups and reconfigure systems to integrate newly developed information. Indeed, MAPs evolve and improve constantly as technology advances and learning in the particular area of application takes place. In addition, robotic equipment in MAPs will need to be interfaced with highly specialized analytical equipment performing measurements and generating the data that needs to be integrated into an adaptive AI-driven optimization workflow. As such MAPs are expected to be constantly evolving in order to perform the required tasks better and better over time.

In MAPs, the integrated equipment platform provides an interface of the software and data infrastructure in the background to the physical system. Robots and automation must handle and manipulate materials, samples, and consumables. Each of these tasks is usually very application-specific and, therefore, must be reasonably easy to reconfigure. MAPs will also integrate standard lab equipment designed for scientific tasks like scales, spin-coaters, or spectrometers. Their integration is often a particular challenge and sometimes the robot in a MAP needs to precisely mimic a human operator to execute a task like loading and unloading a piece of equipment.

Safety requirements in laboratories are also quite different from industry. Robots in MAPs are usually smaller and do not pose as much threat to the physical safety of the operator. Therefore, truly collaborative robots are not necessarily a requirement, although the collaborative feature may be of benefit for making the robots more flexible in application. On the other hand, other safety issues prevail in materials science laboratories. The MAPs may handle hazardous substances, or materials that are inherently sensitive to oxygen or water. As such the required equipment will have to be designed to operate in protected atmospheres and in glove boxes. They may be exposed to vapors from solvents, other chemicals, high temperatures, intense light, or even radiation in operation. This poses new challenges, which need to be kept in mind when selecting or developing such equipment. But it should be remembered that this approach removes the potential for human exposure to chemicals.

Many of these challenges faced by hardware in MAPs are highly domain-specific. In addition to that, it is difficult to foresee all the future requirements in highly dynamic research areas. To overcome this problem, MAPs generally need to be flexible and easy to use, offering remote-controlled interfaces and be easily reconfigurable, while remaining resilient to environmental factors. Through well-documented interfaces and user-friendly libraries, they should be programmable by scientists to further evolve in their application. Additionally, they should support many protocols and interfaces to efficiently deliver data and receive commands from the control software environment.

3.2. Communication Protocols and Interfaces

Interfaces connect the hardware components of a MAP to each other and to the superordinate IT infrastructure. Protocols implemented on top of the interfaces enable communication between the hardware controllers and to the common software overlay to control and reconfigure laboratory instruments while performing optimization loops.

To make this possible, peripheral devices and laboratory equipment that can be remotely controlled are required. This is far from being an established standard as of today. Many lab devices come with proprietary interfaces which are particularly difficult to automate and specialized software to control the device. These interfaces are often undocumented or suppliers are unwilling to provide the command sets required for automation. This will remain a challenge in coming years, however, providers with a flexible approach may benefit considerably.

To successfully foster the development of MAPs scientific equipment well documented APIs are needed. In general, Ethernet should be used as the interface and IP-based protocols as far as possible. This constellation is extremely widely adopted and represents the basis for the Internet of Things (IoT) with its flexibility, expandability, throughput and stability. Where robustness/safety, real-time capability and industrial transfer is important, industrial ethernet/field buses like EtherCAT and ProfiNET should be used.

When integrating legacy systems, it may be necessary to wrap outdated and proprietary protocols and interfaces into a standardized and self-describing version before integrating them into modern systems. OPC-UA,[91] an upcoming industry standard, is an excellent option for this purpose as it provides a semantic, self-standardized communication protocol which is supported by a growing number of device manufacturers.

For simple setups, OpenAPI[92] conform HTTP REST[93] protocols are another option. While not designed for secured high-performance asynchronous communications like OPC-UA they are very easy to learn and provide a low-barrier entry.

3.3. Software Infrastructure

Software infrastructure refers to the underlying technical systems that provide the development, deployment, and operation of software applications. These include hardware systems, network infrastructure, cloud platforms, databases, operating systems, development tools, and other components that form the backbone of a software system. The goal of software infrastructure is to create a stable, secure and scalable environment for the development and deployment of software.

Materials discovery programs are a rather complex interplay of experimental design, digital experiments, lab experiments, and insights from existing data. This complexity poses multiple technical design principles on the software architecture.

1. *Compatibility*: Support multiple hardware systems, network infrastructure, cloud platforms, databases, operating systems, development tools, and other components required to run materials discovery programs.
2. *Agility*: Provide the flexibility to add, substitute or change individual components to address the fact that scientific workflows are constantly adjusted and differ from program to program. Further, lab equipment, simulation, and AI technology are continuously evolving. MAPs need to be able to adapt and add functionality.
3. *Accessibility*: Provide multi-user access via web interfaces to set up, run, and monitor materials discovery programs.
4. *Security*: Besides data and software hosting in secure on-premises or cloud environments, security extends to safety standards in running (automated) lab experiments.
5. *Operational Stability*: It is necessary to go beyond just open-source software on GitHub and establish governing processes to maintain the software, release regular updates, ensure quality standards, and invest in training and education.

The above-listed criteria are best met by microservice-based architectures that offer modern approaches for workflow orchestration and automation of software infrastructures. Applications and software modules are encapsulated in containerized services[94] as decomposable units to execute them independently of each other. In this way, not only data but also complex software configurations can be persisted, versioned and reproduced. This enables programmers to develop systems independently yet ensure interoperability between the components via suitable Application Programming Interfaces (APIs) like REST, defined data schemas, and standards. The emergence of decoupled streaming architectures provides a natural backbone for microservices as well as seamless connection of data producers, consumers, and processors. Streaming infrastructures provide decoupled automation of data curation, reduction, and analysis; real-time experiment monitoring and control; and flexible deployment of AI/ML to guide autonomous research.[95]

To process computing workloads, particularly those relying on massive quantities of data, high-performance computing (HPC) makes use of large-scale computing resources. Such clusters offer a way to manage the demanding computational requirements for technologies such as machine learning (ML), AI, and the Internet of Things (IoT). Common HPC applications typically involve simulation and emulation tasks for a wide range of engineering and scientific challenges.

3.4. Software

R&D applications differ significantly in scope, such as the considered materials classes and intended functionality. This diversity results in specific implementations and uses of application software, distinguishing this layer from the backend software infrastructure. Nonetheless, the fundamental concept of a MAP stays the same, regardless of whether the scientific research pertains to next-generation battery materials, polymers, or flexible electronic devices. Nevertheless, the best combination of individual components may vary depending on the particular application of the MAP.

In general, on top of the software infrastructure, application software modules of a MAP need to cover multiple aspects along the life cycle or continuum of experimental data, ranging from abstract modeling to result sharing (c.f. **Figure 14**). Along this cycle, a larger community should be involved, at least through sharing of (intermediate) results through a larger knowledge graph built on the FAIR principles or even across the cycling through distributed MAPs with shared infrastructure.

Application software modules can be implemented as fully supported commercial packages, open-source algorithms for predicting material properties (such as physical, optical, electronic, and mechanical), or customized implementations that cater to the specific needs of a material discovery program. The latter includes digital twins for application testing or project-specific data analytics and should support the MAP philosophy to move from a linear design-make-test approach to a closed feedback loop with fast iteration cycles accelerated by AI and automation. At the end of each cycle, the generated data trains the predictive materials modeling modules allowing the AI to trigger a more informed subsequent cycle. In this way, materials discovery programs converge quickly towards the desired target property profile.

Each cycle comprises several stages, starting with identifying the necessary properties and defining the design space for the material. This is followed by predictive materials modeling, planning, and executing experiments, capturing data, analyzing data, and sharing knowledge. The key software components involved in this process are:

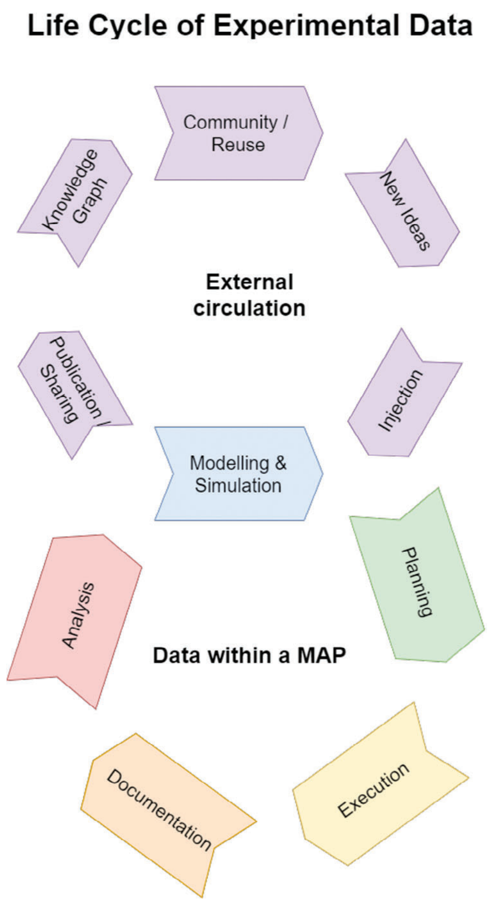

Figure 14. Life Cycle of Experimental Data: Steps in the closed-loop materials discovery.

1. *Planning and Optimization*: In the R&D workflow, finding the optimal design in a high dimensional design space is a common challenge that occurs at multiple stages. This includes identifying the optimal material composition, process parameters for synthesis and manufacturing, and or device engineering. Human experimental planning is performed by defining a simple matrix of experiments intended to scan the parameter space. The experiments are executed according to the plan and the limited results are often evaluated after all experiments have been completed. The MAP concept replaces the static and linear experiment planning by an iterative and adaptive, AI-driven research process. The AI-driven research planner starts with a few data points to create an initial crude model. The model is used to propose the next generation of experiments, which are used to improve the model. This procedure is iterated in order to explore the relevant regions of the parameter space and to find an optimum. This iterative process ensures that experimental resources are spent efficiently and exploiting existing knowledge and data in the best way possible. Algorithmic implementations rely on Bayesian optimization, active learning, reinforcement learning, and related methods. This technique methodically explores and exploits, as appropriate, with fewer constraints than conventional experimental methods. A major responsibility lies in the hand

of scientists, who need to closely monitor the progress of the MAP to ensure that the model evolves in a physically sound way.

2. *Experimental Execution*: Application software modules act as an interface and driver between the planning and optimization modules, the laboratory equipment and backend orchestration system to automate the execution of experiments and results acquisition. This ensures proper data handling, data quality, lab safety, and secure connections to the hosting cloud or on-premises system within an Internet of Labs (IoL) concept. However, the scientists need to oversee the experimental execution with graphical user interface to prevent that the AI-driven research planning is driving the search into directions inaccessible for the experimental setup.
3. *Predictive Material Modeling and Digital Twins*: Lab experiments may be complemented by digital experiments, which are executed virtually/in silico. Physics-based simulations can contribute additional information or act as virtual twins to deliver properties with sufficient accuracy in less resource-consuming ways. This can take place at multiple levels; for example, on the molecular level (chemical, ab-initio), on single parts (multi-physics), or for full systems (device modeling). Simulations and inverse-design approaches can be used for virtual materials screening to identify the most promising candidates. Data-driven ML models can be trained with physics-based simulation data to provide surrogate models for faster exploration or to bridging all length scales, from microscopic behavior to macroscopic impact on engineering. It is important that scientists critically evaluate the prediction of data-driven models to determine their accuracy, generalizability, and thus application range. Therefore, models should be built as self-contained containers with proper documentation and associated runtime requirements. As for research data, metadata standards based specific ontologies[96,97] should also apply to those artefacts.
4. *Documentation*: Data management and documentation of experimental procedures are critical aspects in R&D labs. Electronic lab notebooks (ELNs) and lab informatics systems (LIMS) are widely used by scientists to document their work. However, the data acquisition and storage need to be standardized and put into an ontology to make it useful for an AI-enabled MAP. The challenge is consistently handling both the raw data together with the context and metadata, which is critical for ML across all methods used and partners participating in the MAP. This is especially critical in an R&D environment where experimental setups constantly adapt to the latest insights. Frameworks like OpenSemanticLab[98] represent first approaches for an integrated MAP ELN/LIMS providing a holistic perspective including both human and machine agents.
5. *Data Analytics and Insights*: Data analytics is not a post-processing activity, as commonplace in conventional research projects, but a central component of a MAP. Data generated in each generation must be analyzed and integrated into the next generation of the model in a continuous manner to progress the MAP-based research. Insight into the problem can be gained both from the evolution of the experimentally based model and from refined simulation models. Nevertheless, vivid statistical visualizations must be provided to the human operator to improve data understanding and to integrate abstraction capabilities.
6. *Data and Knowledge Sharing*: Data, data sets and databases are assets that may be used to answer various questions. The data set from a MAP-based research project may act as the starting point for another MAP addressing another research question. This requires that databases and software modules use standards for easy ingestion and queries of data repositories and ontologies. Besides the software, governance is necessary to ensure data quality and support. Suitable technical implementations include data lakes and data warehouses with enterprise-level quality and intuitive access through graphical interfaces. Application-dependent modules for knowledge sharing are tightly integrated within the orchestration system of the backend software infrastructure. In general, MAPs should create linked and semantically enriched data aligned to common standards (JSON-LD[99]/RDF[100]) directly at the source through documentation with general and domain-specific ontologies that allow FAIR data exchange via Data Spaces or Data Repositories without any further manual steps.
7. *Intuitive software through GUIs*: Democratizing access to a MAP requires guaranteeing that the R&D community can readily interact with its software infrastructure. Thus, a MAP must provide intuitive graphical user interfaces (GUIs) that ensure the diverse range of skill sets of a multidisciplinary R&D community, which may lack in knowledge in software development or scripting, are not a burden to its safe and efficient use. Thereby, GUIs can be managed and maintained as commercial packages or as free and open-source software embedded in a community of developers.

In recent years, significant progress has been made in advancing each individual software component, and breakthrough technologies are expected to continue. For instance, neural networks offer enormous potential to speed up computationally intensive materials simulation and enable more accurate simulations of larger systems. Probabilistic ML and Bayesian Neural Networks provide uncertainty estimates that allow researchers to evaluate the trustworthiness of predictions, which is particularly important for exploring novel material ideas outside of the training data. However, further research is needed to make ML more reliable and interpretable and automate its integration within the research cycle, running in parallel with physical experiments. Another important point is to gain more understanding of which components, such as AI-driven optimizer, experimental methods, and simulations, should be harmoniously combined to create a MAP tailored to address specific problems.

Due to safety and economic reasons, requirements of software development for large-scale software products directly transfer to MAPs. The code steering a multi-million-dollar machine and evaluating the generated data needs to be of high quality, applying strict coding standards, and employing automated testing before roll-out to the physical system ("code in production" in terms of software development) in a mode known as Continuous Integration/Continuous Delivery (CI/CD).

3.5. Community

Only a strong and interdisciplinary community is able to build and successfully use a MAP, and subsequently, MAPs offer a joint platform for collaboration to solve social challenges.

While operating traditional labs in smaller and often single-disciplinary teams has been a long-standing integral part of chemistry and material science, MAPs represent a new concept in academia and industrial research. Therefore, an interdisciplinary ecosystem that creates the necessary skill set and supportive environment to develop, maintain, and conduct research on MAPs becomes mandatory. Such a community needs to rest on the following pillars:

1. *Governance*: A community that provides all aspects to sustainably operate MAPs, including establishing standards, integrating new modules, managing automated labs, and ensuring quality control for closed and open-source hardware and software (c.p. Free/Libre Open Source Software, FLOSS).
2. *Training and Education*: MAPs represent a fundamentally new approach to R&D and are more than just a replacement for traditional tools. As such, the research community needs to get trained on how to adapt R&D programs to take advantage of MAPs while also providing education for developers in the MAP community to ensure the high quality, scalability, and reusability of new software and automation modules.
3. *Create Awareness*: Dissemination of knowledge and success stories is essential to generate awareness and momentum for widespread technology adoption.
4. *Technology Transfer*: Establishing an ecosystem encompassing startups and corporations is crucial for the smooth transition of technology into the industrial sector for broader adoption. This is when the Twin Digital & Green Transition will materialize, leading to a significant economic and societal impact.

Such ecosystems are routed in an organizational structure that coordinates the activities around each MAP. Depending on the size and scope of the project, governing entities are established at the project level, at the scientific level, or as part of international government-led initiatives.

In recent years, communities in each category have been formed (see also Section 2.4). For instance, BIG-MAP (Battery Interface Genome – Materials Acceleration Platform) is part of the Battery2030+ initiative, which includes various renowned experts and institutes, and maintains close connections with a diverse set of key industrial stakeholders in battery research and production. Meanwhile, the French initiative DIADEM aims to create synergies between material sciences and data sciences. The UK initiative, PSDI (Physical Sciences Data Infrastructure), focuses on integrating experiments and material simulation to establish a data-centric framework for materials. The German-Canadian Materials Acceleration Center (GC-MAC)[101] is a binational approach to aligning methodologies. The European Materials Acceleration Center for Energy (EU-MACE)[102] aims to build a community of MAPs across Europe. Complementing this, the European Materials Informatics Network (EuMINe)[103] focuses on method development and application in the area of materials informatics. On the international level, the Materials for Energy Innovation (M4E) initiative is arguably the most prominent community dedicated to providing education, shared infrastructure, and strong networks around MAPs. This initiative is part of Mission Innovation (MI), a global effort to accelerate progress toward the Paris Agreement goals and pathways to net zero.

To build on the early successes and encourage wider adoption, we need to continue strengthening connections among stakeholders from academia, industry, and the public sector. Ecosystems that focus on professional training and serve as breeding grounds for startups and technology pioneers are necessary. The logical next step for MAPs is to bring the new concepts into industrial R&D operations and thus increase the velocity and agility of materials innovation.

4. Impact

Current societal challenges (see also Section 1.1) imply an increasing complexity of AdMats innovation, while at the same time require drastically accelerating the R&D & innovation process. New regulatory frameworks (including initiatives like the Green Deal) could present a risk to industries ability to meet market demands due to increased development time and costs. Traditional R&D approaches are often slow, expensive, and labor-intensive. However, with the proliferation of computing resources and advancements in data analytics, AI, and lab automation, we have the opportunity to revolutionize materials R&D. MAPs are expected to considerably reduce resources needed for materials development as compared to traditional R&D approaches by: 1) optimizing the number of experiments through predictive screenings to identify the most promising materials, 2) significantly reducing the materials resources needed for individual experimental trials, 3) automating repetitive and low-value-added tasks to enhance experimental reproducibility and liberating researchers for more impactful work, and 4) accelerating the overall process, directly reducing costs. Hence, MAPs will result in managing and exploiting knowledge, data, and resources in a more efficient way and a society that succeeds first in fully implementing the vision of a MAP will be able to stand out clearly in international competition.

With all the tools available to de-risk and accelerate disruptive materials innovation, we propose the following threefold strategic goals to be achieved with MAPs:

1. *Synchronize material innovation and end-product development*: Today's long cycle time for novel materials does not match the cycle time of engineering. By accelerating materials discovery, MAPs enable the industry to respond with greater agility to the application requirements of multi-material devices.
2. *Enable innovation that maximizes the use of existing assets*: Today, early-stage discovery focuses primarily on getting material properties right. Techno-economic and production considerations are taken into account only at later stages. By focusing on manufacturability instead of just synthesizability, MAPs will reduce the capex, time, and risk of commercialization of new materials and devices by enabling simultaneous development and verification of novel process or manufacturing methods.
3. *Turn open innovation into societal impact*: Today, material innovation is at the beginning of the value chain and too often remains isolated from relevant downstream stakeholders

limiting its actual implementation in the real world. By serving as an ecosystem, MAPs will bring together technical, economic, regulatory, social, and policy as a community to enable the successful rollout of disruptive and sustainable innovation in materials.

The aforementioned aspects have immediate implications for governments and their strategies:

1. Reduced dependency on raw materials: Better utilization of materials, e.g., by reducing the use of rare metals by 20%, would have a significant impact on raw materials sourcing for consumer electronics, electric vehicles, solar cells, etc.
2. Technology Sovereignty: Winning the race of artificial intelligence and accelerated materials innovation is crucial to sustaining or expanding economic leadership positions.
3. The Twin Transition (EU Term for green and digital transition): Materials acceleration platforms are a blueprint for how fast transitioning to AI, modern digital R&D process and materials innovation can fuel each other to reach NetZero, thus synergistically combining digital transformation and sustainability.

4.1. Technological Scope

Synthesis: High-throughput synthesis of materials requires a small amount of matter at each processing step when screening complex compositional and structural phase spaces. Thin films with in-plane composition or structural gradients are a way to achieve this requirement. Micro or mili-fluidic tools are another way to achieve the same goal for powders. Pixelized annealing/sintering of 2D or 3D materials may provide libraries of different structures starting from a monolithic bulk sample. Structural, morphological and functional characterization are then to be involved for the accelerated processing loop to be efficient.

Catalysis: Catalysis is involved in the manufacturing of the majority of our products.[104] By lowering the activation barrier, it can produce new materials at lower energy costs and/or generate less wasteful byproducts. MAPs can target better catalytic materials and processes, which will lower energy consumption and can lead to better-performing materials. First impact on catalyst discovery have already been demonstrated.[105]

Biotechnology: Synthetic biology provides the industry with the ability to develop products and processes that are sustainable in terms of our use of natural resources. Integration of biology, digitalization and automation for the respective technologies to become mainstream and adoptable as an enabling field of technology.[106] MAPs are expected to increase the speed and efficiency of strain engineering 20-fold to speed up biotechnological applications largely due to enabling high throughput while minimizing trial-and-error. Current applications exist in chemicals and pharmaceuticals, while the scope of applications essentially covers the structural and functional field as a whole and is rapidly expanding toward topics necessitating sustainable materials and solutions.

Bio-Sourced Polymers Hybrids and Composites: Molecular chemistry is already using high-throughput platforms to produce building blocks for polymers materials.[143,144] The next step using MAPs will be to achieve polymers of advanced functionalities either intrinsically or through the inclusion of inorganic particles. Additive manufacturing is a route toward accurate control of the microstructure in such composites. MAPS are of interest for the acceleration of monomer discovery (including bio-sourced ones) and for the full automatization of the processing of hybrids. Designing process twins, manufacturing optimization and functional testing all require AI-based tools. Such advanced polymers can also be produced in view of easier recycling at end of life.

Health, Pharma and Bio-Medicine: Drug discovery and development is thus a long, costly, and high-risk process with excessive failure rates (>90%), especially in the final stages. The adoption of MAPs in the pharmaceutical industry can offer huge productivity gains by completing the already well established high-throughput approaches with AI-based data analytics and experimental planning. MAPs result in higher throughput and greater efficiency, while maintaining strict performance criteria, enabling multisite and cross-department collaboration through access to real-time data.

Energy Materials: The demand for sustainable energy production and storage solutions is exponentially increasing. Energy has been identified as a strategic sector by the EU.[107] Developing novel, innovative solutions for sustainable energy production and storage requires developing new materials. Facing the current challenges requires that research and development of new energy materials should be drastically accelerated. Several regional, national and international initiatives have been initiated to create MAPs dedicated to the development of new materials for batteries, photovoltaics, and more.

Photovoltaics: Photovoltaic technologies play a crucial role in advancing renewable energy technologies and addressing climate change. Acceleration in this field is necessary to further improve the efficiency and cost-effectiveness of solar panels, develop new materials with enhanced properties, and optimize the integration of photovoltaic devices. By applying MAPs approaches, especially multi-target optimizations like high efficiency in combination with flexibility or absence of critical raw materials, can be addressed.

Metamaterials: Metamaterials derive their properties from their artificially designed structure rather than from their chemical composition and naturally occurring atomistic structures. Because of the large investigation space which comprises also mesoscopic and macroscopic structuring in addition to chemical and atomistic structure, it is necessary to accelerate the design and fabrication of metamaterials through MAPs. MAPs can not only speed-up the discovery but also open up new fields for the use of metamaterials, where their properties change during operational conditions. Possible applications are electrochemistry, membranes, catalysis, and in addition more conventional use-cases such as structural, acoustic and photonic materials.

High Entropy Alloys and Oxides: In some cases, like corrosion resistance or substitution of critical raw metals, high entropy alloys resulting from the mixing of more than five individual metals are among the solutions. Screening the whole phase diagram in such complex cases is out of reach using the standard approach. Automatized thermodynamic modeling (e.g., CALPHAD), robotized casting, additive manufacturing and high-throughput structural and functional probing are then used. This is to be extended to non-metallic inorganic materials in which more than four chemical elements are mixed over the full compositional space. MAPs would be a way to bridge the gap between different material classes opening the way to advanced functionalities (electromechanical, optoelectronic, multiferroic, etc.)

Materials for Additive Manufacturing and the Relation to Digital Twins: Additive manufacturing largely emerged in the processing of powder metal parts with geometries impossible to fabricate by conventional manufacturing methods. It is now extending to diverse materials classes: inorganic glasses, polymers, hybrids made of inorganic inclusions in a polymer matrix. Novel materials require additional control of thermodynamical and thermochemical parameters. Such additional parameters have to be included in the digital twins of the targeted materials and of the manufacturing processes. Microstructure modeling, in situ monitoring of the processing parameters and post-processing functional checks will produce a very large amount of data, the handling of which will require MAPs tools. Beyond the real space control of the 3D architectures, additive manufacturing can add a fourth dimension which is the well anticipated reaction to a given stress (mechanical, electrical, magnetic, optical). Scanning such 4D spaces makes the use of MAPs even more relevant.

Per- and Polyfluoroalkyl Substances (PFAS): Due to health and environmental implications, the use of per- and polyfluoroalkyl substances (PFAS) in various industry sectors like aerospace, automotive and consumer products is subject to regulations that aim to limit or prohibit its use. This confronts affected companies with the challenge of quickly finding alternatives for the comprehensive property profile (thermal and chemical resistance, lubricity and processability) of PFAS. Of particular significance is the relevance to the battery and H_2/CO_2 electrolyzers using PFAS membranes as well as consumer goods such as cooking utensils. MAPs can provide decisive support here by optimizing suitable replacement candidates in the relevant property profiles and testing of results directly at the device level.

Recycling Processes (Polymers, Precious Metals): In order to promote a circular economy where materials are efficiently reused, thereby reducing the reliance on virgin resources and minimizing waste generation, MAPs can support a process for both maximizing recycled material use while keeping the required product properties. MAPs can further target the recycling (detection, sorting, extraction, and refining) process itself to tolerate a broader input material stream and to provide higher grades on the output side.

4.2. Use of MAPs in Industry

The 150-year-old materials industry faces radical upheavals from multiple directions. There is an increasing urge for breakthrough innovation to solve sustainability needs. Faster product development is needed to respond to ever-accelerating market trends. Supply chain challenges and scientific complexity are adding additional pressure on the industry.

All taken together, the margins in the industry are decreasing[108,109] due to increased supply chain and production costs which diminishes the resources available for research and development. When the industry favors incremental development of existing products with a predictable outcome rather than development of next-generation products that require innovative and disruptive technologies, technological and economic progress are stifled.

The introduction of MAPs in industrial research and development is a very promising strategic response to promote and accelerate innovation. Almost all major global players have already developed AI strategies to increase their organizational agility, so they should also consider to make use of the full MAP approach.

The major impact of introducing MAPs for industrial research lies in the reduction of resource consumption, shortening of the development cycles and cost, potentially more optimized materials for the target application and most importantly a more predictable outcome of the research process. The reduction in resource consumption is achieved by using the adaptive design of experiments, which systematically use the most relevant points in a large parameter space. This reduces the number of experiments and the amount of materials used. This also reduces the time needed for the research campaign, which shortens the time to market. The systematic and adaptive search of the parameter space also has the advantage to be more likely to really find the optimal material combination in the search space, which is superior. This makes the MAP approach more predictable and reliable to find a solution to the problem compared to the traditional Edisonian trial-and-error approach. Another advantage of the MAP approach lies in the fact that the AI model can be directly used or easily converted into a digital twin of the product. This digital twin can be used both in the upscaling toward production and for the tracking of the product during its lifetime. Having a record of the history of the product from production and usage is simplifying the recycling of the product. The lifetime information of the digital twin is invaluable in ultimately being used in the development of the next generation of products.

This makes the MAP approach very appealing to the industry and they have been quick to embrace this methodology. Collaboration across companies may be less attractive due to IP issues, but large corporations have R&D centers distributed across the globe. Connecting these R&D centers into a common, internal R&D MAP is providing a significant opportunity. The companies participating in the Workshop "Re-inventing Materials Research Workshop" organized by EMIRI[110] and the Accelerate Conference series[111] presented various versions of how they are using MAPs in their research and development. These insights and cooperation announcements[112] in the field indicate that the MAP concept is neither science fiction nor science only, and it has already gained attention and traction in commercial applications.

Multiple proof points have demonstrated that digital technology, artificial intelligence, and closed-loop self-learning systems will fundamentally change chemical R&D. For instance, recently published success stories claim a reduction of experimental workloads in general by up to 90%[113] and an acceleration of the development of new rare earth-free permanent magnets by a factor of 200[114] The natural next step is to support the industry to move toward larger adoption to make the concept of MAPs the new standard in a modernized R&D process.

The MAP concept may also open up space for new business models. The main application in industry will be the internal MAP, but there are also possibilities to extend the offering of research services between companies and universities. Outsourcing research to Contract Research Organizations (CROs) has been done for a long time, in particular in the pharmaceutical industry, but it is much more complicated to establish a connection between universities, research institutes and companies. There are usually hurdles to be overcome in terms of how the information exchange between the service provider and the buyer is done and the IP rights. Making the lab "MAP ready," establishing the MAP communication protocols and establishing a market place for research services will decrease this barrier to entry into the services market and helps to align to common initiatives like Dataspaces and Marketplaces.

Besides the chemical industry,[32,115,116] the most prominent example for which we see signals for an emerging adoption is the pharmaceutical industry[117] where drug discovery is finding solutions amid strict requirements, harsh regulations, and high costs.[118] Cumulative investments in AI companies for drug development surpassed $60B at the beginning of 2023.[119]

The benefits of MAPs in the industry can be summarized as:

1. R&D resources are used more effectively due to accelerated developmental cycles (from set-up to development and production).
2. More predictable outcome of research projects.
3. Higher Internal Rate of Return (IRR) of innovation.
4. Creation of virtual twins of the products.
5. Products are simultaneously developed to optimize capital expenditure (CAPEX) and operational expenditure (OPEX) in manufacturing.
6. New business models, e.g. (cloud) lab as a service.
7. Shorter time to market including production and testing lead times.

5. Gaps

While initial implementations of MAPs clearly demonstrate their 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. In general, challenges are beyond the individual researcher, individual lab, individual country and need coordinated regional, national and international research strategy.

Despite the first successes of such platforms, there are still gaps in the realization of their utility and maturity for acceleration and efficiency gains in the process from materials discovery to device integration.[105,120] A major bottleneck is still their limitation in technological scope. There is limited interconnectivity with modeling, computational, or experimental modules beyond those readily integrated into the "closed-loop" hardware platform. Therefore, the "closed-loop" future labs concept has found modest traction in the field of electrochemical energy conversion and storage, encompassing hydrogen fuel cells and electrolysis cells.

5.1. Compatible Infrastructure, Data Structures and Data Sharing

While the "open" idea is already widely established in software, this is not the case to the same extent in hardware. However, OpenHardware[121] is a prerequisite for assembling, optimizing and maintaining complex MAPs from different hardware modules. This includes not only construction and circuit diagrams but also device drivers and communication protocols. With OPC-UA LADS,[122] the OPC foundation has been laid for at least the latter, which must now be implemented in the field.

Nevertheless, a robust cloud-native software infrastructure including cloud management and CI/CD pipelines to deploy apps and models must be set up on the basis of an open hardware platform to enable secure access to the system components and data. Up to now, this has mainly been implemented by the need for local access to the relevant terminals or, more indirectly, through shared data repositories. However, in order to realize shared and distributed MAPs, it is essential to also implement web-based access which, depending on the user role, enables, for example, the sending of synthesis requests, the viewing of log data and the retrieval of analysis results, for example.

Within this scope, data sharing has its own shortcomings and arising opportunities. Storage and retrieval of the integrated data from various sources, enable an effective development of self-serve online analytical tools for automated data analysis, improving the ability to connect to the analytical tools and the responsiveness to semantic and integrated queries, and the data access performance, all features that lie beyond the capabilities of current disjoint, heterogenous and often transaction-oriented databases and data infrastructures in the materials domain. Robust data governance and data management protocols in an interoperable ecosystem - including the management of data quality, data lineage and tracking, and data security - involve data standardization and metadata management at its core to provide context to the data and thus enable materials scientists to locate the data they need most efficiently.

To accelerate research, production and innovation, we therefore need to semanticise these domains (Industry Commons[123]) with common data schemas and vocabulary (ontologies) and create documentation and metadata standards in the huge effort of knowledge digitalization. The semantization and standardization will offer a pathway to interoperability across domains, while documenting and standardizing will offer a pathway to validation across complex workflows from raw materials to advanced materials solutions.

While general ontologies for the material domain (e.g., EMMO,[86] MSEO[124] and the PMD ontologies[125]) as fundamental basis for FAIR data management are established, gaps still exist in standardization and development of domain-specific ontologies, guiding meta-data management and harmonizing approaches across different self-driving labs. Applying FAIR guidelines to material R&D and manufacturing[126] is challenging due to the complex and highly dimensional parameter space and the lack of standardization in fabrication and characterization techniques.[127] To enforce FAIRness, ontologies provide semantic context to data and make the interpretations unambiguous but it is essential to build in intuitive software tools that are useable by any researcher. This will, in addition to ontologies, require annotated data schemas[128] to provide dedicated shapes for the common patterns in research data. Finally, this will enable not only sharing data, but generating knowledge within and across the domain communities.

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5.2. International, Decentralized and Asynchronous MAP Structures

Given the scale and complexity of the challenges ahead, we cannot achieve these goals in isolation. International partnerships and collaborations are essential to accelerating materials discovery and promoting economic prosperity. By joining forces with like-minded partners around the globe, we can strengthen our research capabilities, share expertise and resources, and achieve our common goals more effectively. Therefore, we must prioritize building strong, collaborative relationships across borders and work together toward a more sustainable and prosperous future for all.

There is a great need to orchestrate research campaigns beyond a single lab, research organization and across the globe with dozens of partners complementing and replicating capabilities to build truly global platforms. However, there are additional challenges to create a distributed and asynchronous MAP. The requirements for standardization of communication protocols and ontologies become crucial for distributed MAPs, which include multiple labs and may stretch across borders and time zones. The data and methodologies from different partners need to be integrated together. The standardization initiatives mentioned above are vital and the next step is to implement these standards into broadly accepted orchestrator and tenant software.

5.2.1. Standardized Software for Distributed MAPs

The research group building the MAP will need to set up an orchestrator server as described in Section 3.3. Writing an orchestrator software from scratch is a large task, in particular if it needs to handle multiple tenants, integrate various types of data from different methods and adhere to defined ontologies. An additional challenge for the orchestrator for a distributed MAP is to handle the waiting time for tenants operated in the asynchronous mode. Creating such an orchestrator for a distributed MAP is a significant hurdle to set up the MAP. While there are many generic workflow environments and orchestrators[129] there are a few attempts to create or adapt such orchestrator software specifically for MAPs. On the pure data side, the globus project[130] is pushing to enable semantic data transfer at great speeds whereas software like FINALES,[131,132] and OpenSemantiLab-MAP[133] which were developed and demonstrated withing the BIG-MAP project, emphasizes flexibility and ontology linkage.

There are similar requirements for standardized software agents, which can easily connect lab equipment or simulation software to the MAP. These agents should be able to receive requests for measurements, to translate the meta data into parameters for the setup of the experiment, execute measurements, gather data and finally report result data back to the orchestrator according to the communication protocol and ontology of the MAP. Open-source software is flexible and may easily be adopted to the specific problem to be solved by the MAP. Commercial software solutions may provide more reliability, which is required in industrial MAP applications.

5.2.2. Make existing labs "MAP ready"

Integrating standardized software agents in existing labs to connect to the local infrastructure and automate the task execution will decrease the effort to connect the lab to a MAP. The connection to a MAP would then be limited to configuring the tenant software according to the problem addressed by the MAP. It would in particular make sense to install agent software at large-scale facilities to make them "MAP ready" as they may serve many MAP initiatives.

5.3. Education and Training

The MAP approach, which is still evolving, is multidisciplinary and collaborative. A full understanding of its impact by the community is yet to come. As such, increased awareness, training and implementation is needed to build a critical mass to achieve acceleration toward new materials and devices. It integrates multiple domains together with their knowledge, tools and workflows to a holistic system.

As a cross domain approach, MAPs require a unique skillset not present in conventional research institutions. This includes IT experts in the area of core software and engineers in the area of automation, but specific domain knowledge is also required in almost all places. Therefore, also due to the tense labor market situation, a continuous (re)training of domain researchers toward digitization and automation competencies is necessary.

By implementing modular MAPs with encapsulated building blocks, the need to understand the overall system can be eliminated and specialization can take place instead. Best practices can be adopted from bioinformatics, where such a transformation has already taken place. Possible methodologies include an international Open MAP Academy construct, supporting the development of trans-disciplinary competencies, e.g. machine learning, autonomous robotics, orchestration, FAIR data and the continuous improvement/evolution to build the bridges between domains of Materials Science, Informatics and Processing/engineering. Other possibilities include the establishment of international postgraduate degree programmes (MSci, binational/cotutelle PhDs) or an international school, dedicated to students and experienced scientists including lectures and several weeks long stay at MAP platforms for training. A model for that could be the successful HERCULES school[134] dedicated to training at large-scale neutrons and synchrotron facilities and the Summer School for MAPs for energy materials[135] hosted by the German-Canadian Materials Acceleration Center (GC-MAC).[101]

5.4. IP, Ownership

Similar to large software projects and AI-generated results, the issue of intellectual property is complex for MAPs. Assuming the final result is an AI model trained with the data generated by various actors at a MAP, its intellectual ownership cannot be determined in a lump sum. Not only the model developer, but also the system developer, the operator and the data generators are candidates for (partial) ownership. The research questions posed to a MAP and its associated community may also be subject to confidentiality, especially if they originate in industry. In addition, the cross-border movement of data, information and goods is the rule in distributed, multinational MAPs, requiring compliance with a wide range of export control regulations.

MAPs would therefore need to be established not only as physical facilities and software services, but also as a legal framework defining access and usage rights. This legal framework should precisely define the conditions under which the MAP can be used and who is entitled to the rights to the result. Resulting open data must be free to use, but this does not mean that it must be free to access since there are costs to creating, maintaining the necessary infrastructure. A hybrid model is conceivable, as is already established for many software systems: If the user agrees to the disclosure (e.g., CC BY) or only partial ownership of his results, he can benefit from favorable conditions that are possibly compensated by public funding. If the user wants to place the results under a proprietary license, this is also possible, although without preferential conditions (e.g., higher price). This provides the opportunity to link MAP with the digital contract and data management of Data Space initiatives (e.g., IDS[136]) and offer both open and proprietary data in common marketplace, as well as the experimental and software service of MAPs themselves. MAP providers that can guarantee confidential handling of sensitive data, for example through a sealed-off environment, can in turn be attractive service providers for industry.

5.5. Research Strategy

Current Funding: The current funding landscape in materials science focuses primarily on specific materials (such as hydrogen) or industrial applications. The methodology and specifically the meta-method of the research infrastructure (hardware and software), is insufficiently taken into account making sustainable investments in MAPs that can be applied to whole classes of materials difficult. With a few exceptions (BIG-MAP) no specific funding/call for funding to build full MAPs are available, therefore, MAPs are usually built from parts of budgets of a project focused on a particular application or AdvMat. In addition, there's no funding to maintain a MAP (pay dedicated engineers, technicians) beyond the duration of the creating project.

Necessary Funding: Funding programs are needed that explicitly address the meta-method level in a pan-European scope. Emphasis should be placed on FAIR and, where practical, OPEN research results that provide the greatest openness of the research results of public funding, not only with regard to OpenData and OpenSoftware, but also to OpenHardware in order to maximize the flexibility of the emerging MAP and the innovation speed of its components. In parallel, support should be provided to commercial enterprises, especially startups, that develop innovative building blocks for MAPs in compliance with open standards.

In this regard MAPs are shared infrastructure with contributions from various members of a community. Established examples of such an infrastructure are synchrotrons like CERN where investments are in the order of billions of Euros. Their main purpose is to understand the structure of materials, which could be important to improve materials modeling. Building MAPs accounts for only a few percent of synchrotron investment, but they are accelerating the discovery of many new, more powerful materials by understanding the behavior of materials in a device or a system resulting from complex processing. MAPs and their AI system rely on good materials modeling, so the synchrotron and MAP system complement each other.

AI starts with quality data, thus, a major initial effort needs to focus on AI-aware (data) governance measures. This means improving secured cloud AI/data infrastructures, new harmonization activities, including ontologized data infrastructures and common data management frameworks. The inclusion of promising MAPs and self-driving labs in general needs to be continuously supported by high-quality, AI-ready data from conventional labs. Connection to conventional labs could guarantee the long-term availability of MAPs and complement conventional labs, with decentralized data hubs aligned with national and European activities such as PMD,[61] NFDI,[62] DIADEM,[63] EUDAT[145] and EOSC.[139]

European and National Funding Strategies: Funding should be carried out strategically and take place at different levels.

The first goal should be to create a long-term European ecosystem of RTOs, universities and industry that supports the general development, takes care of standardization issues, and exchanges information. This ecosystem should also organize the different research infrastructures and take care of training. Projects should be announced for lower technology readiness level (TRL) to improve the infrastructures and to develop new standards, also including software and ontologized data infrastructure. Supporting actions would be making MAP building part of postdoctoral assistants/young excellent scientists funding programs like ERC[137] grants would shape a new generation of experts dedicated to the challenges in this field. Pushing promising MAPs to the European Strategic Forum on Research Infrastructure (ESFRI[138,139]) Roadmap could ensure their long-term availability and complement to conventional labs that should become MAP-ready and virtually connected to a decentralized MAP.

Other projects with higher TRL should have the goal of integrating new materials into applications as quickly as possible, in particular sectors where new materials are urgently needed (e.g., hydrogen catalysis, batteries, and more, c.f. Section 4.1) to fulfill the second goal of the funding: The transfer of knowledge to industry and the use of MAPs by industry. To achieve this, we need infrastructures focused on specific application areas, data management systems, and we need to train enough experts in modeling, robotics, materials science, and industrial automation to accelerate the innovation chain.

Efforts in the EU and other regions should be flanked by an acceleration consortium similar to the already established Canadian initiative[84] receiving long-term funding from the Canada First Research Excellence Fund (CFREF). Those consortia should aim to link projects that want to make use of the MAP methodology, with national initiatives, academia, industry and political stakeholders. A European acceleration consortium could take the SET Plan[107] and its implementation groups as a blueprint and be composed of experts from academia (RTOs and universities), industry, member states, and European Commission representatives supporting material research projects, e.g., shaped by the upcoming Innovative Advanced Materials for Europe (IAM4EU) Partnership,[140] with a strong connection to the Technology Council for advanced materials that the European Commission will set up in the frame of the policy communication on Advanced Materials for Industrial Leadership.[141,142]

At the outset, funding schemas, data and AI infrastructures need to be developed and established with clear differentiations, cohesiveness, and complementarity to other similar activities in Canada, the US and the UK. This ecosystem should develop and organize access to the various research infrastructures and ensure continuous expansion.

6. Conclusion

The advanced materials sector, particularly in the field of emerging energy technologies, is facing a major challenge: the pace of development is trailing behind commercialization targets and urgent societal needs. The main cause of this situation is that stakeholders with complementary capabilities still operate largely in isolation, with a lack of coordination between their efforts. This situation has given rise to a new breed of future labs: material-acceleration platforms (MAPs) that combine artificial intelligence (AI) with automated experimental hardware to drive the autonomous discovery and development of new materials. Worldwide, a number of multidisciplinary MAP initiatives involving governments, academia and industry have recently emerged.

MAPs have emerged as indispensable tools for expediting materials and manufacturing process development. By leveraging advanced technologies and automation, MAPs offer immense potential to revolutionize various industries. One of their most significant advantages is the reduction of research and development (R&D) time, enabling faster innovation and quicker time-to-market for new materials.

An important consideration in the MAP landscape is the distinction between open and closed MAPs, the first being focussed on shared access, the latter on protected intellectual property with the primary aim of financial profit. With firstly MAPs of both kinds growing, we are at a pivotal moment that will shape the future of MAPs. Open MAPs promote collaboration, knowledge sharing, and collective growth, fostering a collaborative ecosystem that benefits all participants. Conversely, closed IP protected MAPs limit access to valuable information and hinder the progress of the industry as a whole.

In order to unleash the full potential of MAPs, key initiatives need to be launched to overcome the remaining obstacles and spread skills and know-how that will promote game-changing technology that benefits all of society.

To shape funding opportunities and pave the way for MAP development, several key aspects must be addressed. First, governments should focus on supporting the development of self-driving lab platforms that facilitate methodology development rather than solely focusing on materials solutions. This approach encourages a foundation of technological advancement that can benefit a wide range of industries.

Furthermore, governments should incentivize industry and academia to develop internal MAP systems through both technical and financial support. By fostering partnerships and providing resources, governments can accelerate the adoption and implementation of MAPs in various sectors, driving innovation and economic growth.

Lastly, it is crucial to establish education programs that bridge the gap between data and materials science. The interface between these two fields presents unique challenges and opportunities. By nurturing a skilled workforce with expertise in both areas, we can fully exploit the potential of MAPs and maximize their impact on materials development and manufacturing.

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[1] S. Stier, C. Kreisbeck, H. Ihssen, M. A. Popp, J. Hauch, K. Malek, M. Reynaud, J. Carlsson, L. Gold, F. Goumans, I. Todorov, A. Räder, S. T. Bandesha, W. Wenzel, P. Jacques, O. Arcelus, F. Garcia-Moreno, P. Friederich, M. Maglione, S. Clark, A. Laukkanen, M. C. Cabanas, J. Carrasco, I. E. Castelli, H. S. Stein, T. Vegge, S. Nakamae, M. Fabrizio, M. Kozdras, *Zenodo* **2023**, https://doi.org/10.5281/zenodo.8012140.

[2] United Nations Framework Convention on Climate Change, *UNFCCC*, https://unfccc.int/ (accessed: July 2024).

[3] United Nations, *Transforming our world: the 2030 Agenda for Sustainable Development*, https://sdgs.un.org/2030agenda (accessed: July 2024).

[4] United Nations, *Sustainable Development - THE 17 GOALS*, https://sdgs.un.org/goals (accessed: July 2024).

[5] IEA, *Global electricity demand growth is slowing, weighed down by economic weakness and high prices - News - IEA*, **2022**, https://www.iea.org/news/global-electricity-demand-growth-is-slowing-weighed-down-by-economic-weakness-and-high-prices (accessed: July 2024).

[6] H. Lee, K. Calvin, D. Dasgupta, G. Krinner, A. Mukherji, P. W. Thorne, C. Trisos, J. Romero, P. Aldunce, K. Barrett, G. Blanco, W. W. Cheung, S. Connors, F. Denton, A. Diongue-Niang, D. Dodman, M. Garschagen, O. Geden, B. Hayward, C. Jones, F. Jotzo, T. Krug, R. Lasco, Y.-Y. Lee, V. Masson-Delmotte, M. Meinshausen, K. Mintenbeck, A. Mokssit, F. E. Otto, M. Pathak, et al., *IPCC, 2023: Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team, H. Lee and J. Romero (eds.)]. IPCC, Geneva, Switzerland*, https://doi.org/10.59327/IPCC/AR6-9789291691647.001.

[7] Joint Research Centre European Commission, *Materials for Energy, SETIS magazine* **2015**, https://op.europa.eu/s/zMVE (accessed: July 2024).

[8] Secretariat-General European Commission, *The European Green Deal*, **2019**, https://eur-lex.europa.eu/legalcontent/EN/ALL/?uri=COM:2019:640:FIN (accessed: July 2024).
[9] European Commission, *A Europe fit for the digital age*, **2024**, https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/europe-fit-digital-age_en (accessed: July 2024).
[10] Secretariat-General European Commission, *A New Industrial Strategy for Europe*, **2020**, https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:52020DC0102 (accessed: July 2024).
[11] Secretariat-General European Commission, *Updating the 2020 New Industrial Strategy: Building a stronger Single Market for Europe's recovery*, **2021**, https://commission.europa.eu/document/download/9ab0244c-6ca3-4b11-bef9-422c7eb34f39en?filename=communication-industrial-strategy-update-2020_en.pdf (accessed: July 2024).
[12] Secretariat-General European Commission, *European industrial strategy*, https://single-market-economy.ec.europa.eu/industry/strategy_en (accessed: July 2024).
[13] AMi2030, *MATERIALS 2030 MANIFESTO: Systemic Approach of Advanced Materials for Prosperity – A 2030 Perspective*, **2022**, https://research-and-innovation.ec.europa.eu/system/files/2022-02/advanced-materials-2030-manifesto.pdf (accessed: July 2024).
[14] AMi2030, *The Materials 2030 roadmap*, https://www.ami2030.eu/roadmap/ (accessed: July 2024).
[15] AMi2030, *Advanced Materials 2030 Initiative*, https://www.ami2030.eu/ (accessed: July 2024).
[16] A. Benayad, D. Diddens, A. Heuer, A. N. Krishnamoorthy, M. Maiti, F. Le Cras, M. Legallais, F. Rahmanian, Y. Shin, H. Stein, M. Winter, C. Wölke, P. Yan, I. Cekic-Laskovic, *Adv. Energy Mater.* **2022**, *12*, 17.
[17] R. Thun, *Rev. Sci. Instrum.* **1959**, *30*, 399.
[18] NSTC Subcommittee on the Materials Genome Initiative, *Materials Genome Initiative Strategic Plan*, **2021**, https://www.mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf (accessed: July 2024).
[19] MGI, *Materials Genome Initiative*, https://www.mgi.gov/ (accessed: July 2024).
[20] hte, *the high throughput experimentation company*, https://www.hte-company.com/en/ (accessed: July 2024).
[21] Wildcat Discovery Technologies, *US-made Cathodes High-Performance Producer*, https://www.wildcatdiscovery.com/ (accessed: July 2024).
[22] A. Aspuru-Guzik, K. Persson, *Materials Acceleration Platform: Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods and Artificial Intelligence. Mission Innovation: Innovation Challenge 6*, **2018**, https://dash.harvard.edu/handle/1/35164974 (accessed: July 2024).
[23] G. A. Ozin, J. Y. Y. Loh, *Energy Materials Discovery: Enabling a Sustainable Future*, Royal Society of Chemistry, Cambridge, **2022**, https://doi.org/10.1039/9781839163838.
[24] S. Divilov, H. Eckert, D. Hicks, C. Oses, C. Toher, R. Friedrich, M. Esters, M. J. Mehl, A. C. Zettel, Y. Lederer, E. Zurek, J.-P. Maria, D. W. Brenner, X. Campilongo, S. Filipović, W. G. Fahrenholtz, C. J. Ryan, C. M. DeSalle, R. J. Crealese, D. E. Wolfe, A. Calzolari, S. Curtarolo, *Nature* **2024**, *625*, 66.
[25] GO FAIR, *FAIR Principles*, https://www.go-fair.org/fair-principles/ (accessed: July 2024).
[26] M. D. Wilkinson, M. Dumontier, I. J. J. Aalbersberg, G. Appleton, M. Axton, A. Baak, N. Blomberg, J.-W. Boiten, L. B. da Silva Santos, P. E. Bourne, J. Bouwman, A. J. Brookes, T. Clark, M. Crosas, I. Dillo, O. Dumon, S. Edmunds, C. T. Evelo, R. Finkers, A. Gonzalez-Beltran, A. J. G. Gray, P. Groth, C. Goble, J. S. Grethe, J. Heringa, P. A. C. 't Hoen, R. Hooft, T. Kuhn, R. Kok, J. Kok, et al., *Scientific Data* **2016**, *3*, 160018.
[27] G. Goldbeck, A. Simperler, N. Adamovic, S.-E. Björling, V. Cantrill, S. Chiacchiera, T. Exner, I. Furxhi, D. Gao, M. Karray, D. Kiritsis, J. Lomax, I. Lynch, N. Matentzoglu, M. Noeske, F. Piroi, M. Poveda-Villalón, A. Sarkar, K. Vladislavleva, *Zenodo* **2023**, https://doi.org/10.5281/zenodo.10057816.
[28] E. Ghedini, A. Hashibon, J. Friis, *DOME 4.0: Deliverable D3.1 - "Semantic data exchange ontology"*, **2022**, https://dome40.eu/sites/default/files/DOME%204.0%20D3.1%20Semantic%20data%20exchange%20ontology%202022.02.28%20PU.pdf (accessed: July 2024).
[29] GitHub Contributors, *DOME-4-0/data-set-ontology: DOME EMMO compliant Dataset Ontology*, https://github.com/DOME-4-0/data-set-ontology (accessed: July 2024).
[30] M. Barker, N. P. Chue Hong, D. S. Katz, A.-L. Lamprecht, C. Martinez-Ortiz, F. Psomopoulos, J. Harrow, L. J. Castro, M. Gruenpeter, P. A. Martinez, T. Honeyman, *Scientific Data* **2022**, *9*, 622.
[31] D. P. Tabor, L. M. Roch, S. K. Saikin, C. Kreisbeck, D. Sheberla, J. H. Montoya, S. Dwaraknath, M. Aykol, C. Ortiz, H. Tribukait, C. Amador-Bedolla, C. J. Brabec, B. Maruyama, K. A. Persson, A. Aspuru-Guzik, *Nat. Rev. Mater.* **2018**, *3*, 5.
[32] R. Mullin, *The lab of the future is now: Recent demonstrations of AI-directed automation may herald a new world for drug and materials discovery*, **2021**, https://cen.acs.org/business/informatics/lab-future-ai-automated-synthesis/99/i11 (accessed: July 2024).
[33] R. B. Merrifield, J. M. Stewart, N. Jernberg, *Anal. Chem.* **1966**, *38*, 1905.
[34] H. Winicov, J. Schainbaum, J. Buckley, G. Longino, J. Hill, C. E. Berkoff, *Anal. Chim. Acta* **1978**, *103*, 469.
[35] J. S. Lindsey, *Chemom. Intell. Lab. Syst.* **1992**, *17*, 15.
[36] Fraunhofer ISE, *Center for High Efficiency Solar Cells*, https://www.ise.fraunhofer.de/en/rd-infrastructure/center/center-for-high-efficiency-solar-cells.html (accessed: July 2024).
[37] S. Back, A. Aspuru-Guzik, M. Ceriotti, G. Gryn'ova, B. Grzybowski, G. H. Gu, J. Hein, K. Hippalgaonkar, R. Hormázabal, Y. Jung, S. Kim, W. Y. Kim, S. M. Moosavi, J. Noh, C. Park, J. Schrier, P. Schwaller, K. Tsuda, T. Vegge, O. A. von Lilienfeld, A. Walsh, *Digital Discov.* **2024**, *3*, 23.
[38] M. S. Strano, S. M. Walsh, *Robotic Systems and Autonomous Platforms: Advances in Materials and Manufacturing*, Woodhead Publishing in materials. Woodhead Publishing an imprint of Elsevier, Duxford, United Kingdom, **2019**, https://doi.org/10.1016/C2016-0-01129-4.
[39] BIG-MAP, *Battery Interface Genome - Materials Acceleration Platform*, https://www.big-map.eu/ (accessed: July 2024).
[40] Battery 2030+, *Sustainable batteries of the future*, https://battery2030.eu/ (accessed: July 2024).
[41] A. Bhowmik, M. Berecibar, M. Casas-Cabanas, G. Csanyi, R. Dominko, K. Hermansson, M. R. Palacin, H. S. Stein, T. Vegge, *Adv. Energy Mater.* **2022**, *12*, 17.
[42] Fraunhofer ISC, *Materials Acceleration Platforms (MAPs)*, https://www.isc.fraunhofer.de/en/fields-of-activity/applications/digital-transformation/maps-materials-acceleration-platforms.html (accessed: July 2024).
[43] S. Haeusner, L. Herbst, P. Bittorf, T. Schwarz, C. Henze, M. Mauermann, J. Ochs, R. Schmitt, U. Blache, A. Wixmerten, S. Miot, I. Martin, O. Pullig, *Front. Med.* **2021**, *8*, 712917.
[44] S. Dembski, T. Schwarz, M. Oppmann, S. T. Bandesha, J. Schmid, S. Wenderoth, K. Mandel, J. Hansmann, *Sci. Rep.* **2023**, *13*, 11440.
[45] Viperlab, *Fully connected virtual and physical perovskite photovoltaics lab*, https://www.viperlab.eu/ (accessed: July 2024).
[46] HMC, *AutoPeroSol: Towards automatic data management and a common ontology for perovskite solar cell device data*, https://helmholtz-metadaten.de/en/inf-projects/autoperosol-

towards-automatic-data-management-and-a-common-ontology-for-perovskite-solar-cell-device-data (accessed: July 2024).
[47] T. Unold, *Faraday Discuss.* **2022**, *239*, 235.
[48] J. Wagner, C. G. Berger, X. Du, T. Stubhan, J. A. Hauch, C. J. Brabec, *J. Mater. Sci.* **2021**, *56*, 16422.
[49] S. Langner, F. Häse, J. D. Perea, T. Stubhan, J. Hauch, L. M. Roch, T. Heumueller, A. Aspuru-Guzik, C. J. Brabec, *Adv. Mater. (Deerfield Beach, Fla.)* **2020**, *32*, e1907801.
[50] T. Osterrieder, F. Schmitt, L. Lüer, J. Wagner, T. Heumüller, J. Hauch, C. J. Brabec, *Energy Environ. Sci.* **2023**, *16*, 3984.
[51] J. Zhang, B. Liu, Z. Liu, J. Wu, S. Arnold, H. Shi, T. Osterrieder, J. A. Hauch, Z. Wu, J. Luo, J. Wagner, C. G. Berger, T. Stubhan, F. Schmitt, K. Zhang, M. Sytnyk, T. Heumueller, C. M. Sutter-Fella, I. M. Peters, Y. Zhao, C. J. Brabec, *Adv. Energy Mater.* **2023**, *13*, 48.
[52] Y. Zhao, T. Heumueller, J. Zhang, J. Luo, O. Kasian, S. Langner, C. Kupfer, B. Liu, Y. Zhong, J. Elia, A. Osvet, J. Wu, C. Liu, Z. Wan, C. Jia, N. Li, J. Hauch, C. J. Brabec, *Nat. Energy* **2022**, *7*, 144.
[53] T. Osterrieder, *Investigation and Optimization of quaternary Organic Solar Cells utilizing HTE and Bayesian Optimizer in a semiautonomous laboratory approach [Unpublished master's thesis]*, Ph.D. Thesis, FAU Erlangen, **2021**.
[54] J. Carrasco, O. Lakuntza, *Artificial intelligence for automated and autonomous discovery of better battery materials*, **2021**, https://cicenergigune.com/en/blog/artificial-intelligence-discovery-battery-materials (accessed: July 2024).
[55] SynBio Powerhouse, *Synthetic Biology Ecosystem*, https://www.synbio.fi/ (accessed: July 2024).
[56] CAIMEE, *AI-Driven Integrated and Automated Materials Design for Extreme Environments (AMDEE)*, https://hemi.jhu.edu/caimee/research/ai-driven-integrated-and-automated-materials-design-for-extreme-environments-amdee/ (accessed: July 2024).
[57] TU Berlin, *BasCat - UniCat BASF JointLab*, https://www.tu.berlin/en/bascat (accessed: July 2024).
[58] C. Kunkel, F. Rüther, F. Felsen, C. W. P. Pare, A. Terzi, R. Baumgarten, E. Gioria, R. Naumann d'Alnoncourt, C. Scheurer, F. Rosowski, K. Reuter, *ACS Catal.* **2024**, *14*, 9008.
[59] H. J. Yoo, N. Kim, H. Lee, D. Kim, L. T. C. Ow, H. Nam, C. Kim, S. Y. Lee, K.-Y. Lee, D. Kim, S. S. Han, *Adv. Funct. Mater.* **2024**, *34*, 27.
[60] S. S. Han, H. J. Yoo, K.-Y. Lee, D. Kim, *OCTOPUS: Operation Control System for Task Optimization and Job Parallelization via a User-Optimal Scheduler*, **2024**, https://doi.org/10.21203/rs.3.rs-4254570/v1.
[61] MaterialDigital, *The Material Digitalization Platform*, https://www.materialdigital.de/ (accessed: July 2024).
[62] FAIRmat, *FAIRmat: is building a FAIR data infrastructure for condensed-matter physics and the chemical physics of solids*, https://www.fairmat-nfdi.eu/fairmat (accessed: July 2024).
[63] ,*DIADEM: an exploratory Priority Research Programme and Infrastructure linking materials and AI*, https://www.pepr-diadem.fr/en/ (accessed: August 2024).
[64] EPSRC, *Physical Sciences Data Infrastructure (PSDI) Phase 1 Pilot*, https://gow.epsrc.ukri.org/NGBOViewGrant.aspx?GrantRef=EP/W032252/1 (accessed: July 2024).
[65] CAPeX, **08.08.2024**, https://capex.dtu.dk/.
[66] *NIMS-MDPF: Materials Data Platform in National Institute for Materials Science*, **07.08.2024**, https://dice.nims.go.jp/.
[67] Y. Xu, M. Yamazaki, P. Villars, *Jpn. J. Appl. Phys.* **2011**, *50*, 11RH02.
[68] *Atomwork-adv: Inorganic materials database*, **07.08.2024**, https://atomwork-adv.nims.go.jp/.
[69] M. Ishii, T. Ito, H. Sado, I. Kuwajima, *Sci. Technol. Adv. Mater.: Meth.* **2024**, *4*, 1.
[70] *PoLyInfo: Polymer database*, **08.08.2024**, https://polymer.nims.go.jp/.
[71] K. Sawada, K. Kimura, F. Abe, Y. Taniuchi, K. Sekido, T. Nojima, T. Ohba, H. Kushima, H. Miyazaki, H. Hongo, T. Watanabe, *Sci. Technol. Adv. Mater.* **2019**, *20*, 1131.
[72] Y. Furuya, H. Nishikawa, H. Hirukawa, N. Nagashima, E. Takeuchi, *Sci. Technol. Adv. Mater.* **2019**, *20*, 1055.
[73] *Kinzoku: Metallic material database*, **08.08.2024**, https://metallicmaterials.nims.go.jp/.
[74] *Kakusan: Diffusion database*, **08.08.2024**, https://diffusion.nims.go.jp/.
[75] *CPDDB: Computational Phase Diagram Database*, **08.08.2024**, https://cpddb.nims.go.jp/.
[76] *Thermophysical: Thermophysical property database*, **08.08.2024**, https://thermophys.nims.go.jp/.
[77] *RDE: Research Data Express*, **08.08.2024**, https://rde.nims.go.jp/.
[78] M. Demura, T. Koseki, *Mater. Trans.* **2020**, *61*, 2041.
[79] S. Minamoto, T. Kadohira, K. Ito, M. Watanabe, *Mater. Trans.* **2020**, *61*, 2067.
[80] M. Demura, *ISIJ International* **2024**, *64*, 503.
[81] *Mint: Materials integration by network technology*, **08.08.2024**, https://www.mintsys.jp/.
[82] V. Nandal, S. Dieb, D. S. Bulgarevich, T. Osada, T. Koyama, S. Minamoto, M. Demura, *Sci. Rep.* **2023**, *13*, 12660.
[83] *MGI: Materials Genome Initiative*, https://www.nist.gov/mgi (accessed: July 2024).
[84] University of Toronto and Acceleration Consortium, *Accelerating the discovery of materials and molecules needed for a sustainable future*, https://acceleration.utoronto.ca/ (accessed: July 2024).
[85] EMMC ASBL, *The European Materials Modelling Council*, https://emmc.eu/ (accessed: July 2024).
[86] GitHub Contributors - emmo-repo/EMMO, *Elementary Multiperspective Material Ontology (EMMO)*, https://github.com/emmo-repo/EMMO (accessed: July 2024).
[87] EMCC, *The European Materials Characterisation Council*, http://characterisation.eu/ (accessed: July 2024).
[88] M. T. Horsch, B. Schembera, H. A. Preisig, in *2023 3rd International Conference on Applied Artificial Intelligence (ICAPAI)*, IEEE, **2023**, pp. 1–6, https://doi.org/10.1109/ICAPAI58366.2023.10193944.
[89] EMIRI, *The Energy Materials Industrial Research Initiative*, https://emiri.eu/ (accessed: July 2024).
[90] European Commission, Directorate-General for Research, Innovation and A. Baas, *What makes a material function? – Let me compute the ways – Modelling in H2020 LEIT-NMBP programme materials and nanotechnology projects – Sixth version*, Publications Office of the European Union, **2017**, https://doi.org/10.2777/417118.
[91] OPC Foundation, *Unified Architecture*, https://opcfoundation.org/about/opc-technologies/opc-ua/ (accessed: July 2024).
[92] OpenAPI Initiative, *The world's most widely used API description standard*, https://www.openapis.org/ (accessed: July 2024).
[93] R. T. Fielding, *Architectural Styles and the Design of Network-based Software Architectures*, Dissertation, University of California, Irvine, **2000**, https://ics.uci.edu/⟨fielding/pubs/dissertation/fielding_dissertation.pdf (accessed: July 2024).
[94] C. Pahl, *IEEE Cloud Comput.* **2015**, *2*, 24.
[95] M. Eminizer, S. Tabrisky, A. Sharifzadeh, C. DiMarco, J. M. Diamond, K. T. Ramesh, T. C. Hufnagel, T. M. McQueen, D. Elbert, *J. Open Source Softw.* **2023**, *8*, 4896.
[96] M. Dreger, M. J. Eslamibidgoli, M. H. Eikerling, K. Malek, *J. Mater. Inform.* **2023**, *3*, 1.
[97] S. Clark, F. L. Bleken, S. Stier, E. Flores, C. W. Andersen, M. Marcinek, A. Szczesna-Chrzan, M. Gaberscek, M. R. Palacin, M. Uhrin, J. Friis, *Adv. Energy Mater.* **2022**, *12*, 2102702.
[98] GitHub Contributors - OpenSemanticLab, *Web-based semantic data platform and workflow environment*, https://github.com/OpenSemanticLab (accessed: July 2024).

[99] W3C, *JSON-LD 1.1*, **2020**, https://www.w3.org/TR/2020/REC-json-ld11-20200716/ (accessed: July 2024).
[100] W3C, *RDF 1.1 Concepts and Abstract Syntax*, **2014**, https://www.w3.org/TR/2014/REC-rdf11-concepts-20140225/ (accessed: July 2024).
[101] GCMAC, *Knowledge & Infrastructure to Accelerate Energy Materials Pipeline*, https://gcmac.ca/ (accessed: July 2024).
[102] COST Association, *CA22123 - European Materials Acceleration Center for Energy (EU-MACE)*, https://www.cost.eu/actions/CA22123/ (accessed: July 2024).
[103] COST Association, *CA22143 - European Materials Informatics Network (EuMINe)*, https://www.cost.eu/actions/CA22143/ (accessed: July 2024).
[104] C. R. Catlow, M. Davidson, C. Hardacre, G. J. Hutchings, *Philos. Trans. Ser. A, Math., Phys., Eng. Sci.* **2016**, *374*, 2061.
[105] B. Burger, P. M. Maffettone, V. V. Gusev, C. M. Aitchison, Y. Bai, X. Wang, X. Li, B. M. Alston, B. Li, R. Clowes, N. Rankin, B. Harris, R. S. Sprick, A. I. Cooper, *Nature* **2020**, *583*, 237.
[106] J. Sarkar, A. Kumar, *Biotechnol. J.* **2021**, *16*, 2000288.
[107] European Commission, Directorate-General for Research and Innovation, *Strategic Energy Technology (SET) Plan*, **2023**, https://eur-lex.europa.eu/legal-content/EN/ALL/?uri=CELEX:52023DC0634 (accessed: July 2024).
[108] A. Gocke, A. Rothman, F. Flock, H. Schönberger, A. Gandhi, J. Hu, *Facing Unprecedented Pressures*, **2023**, https://www.bcg.com/publications/2023/resilience-chemicals-industry (accessed: July 2024).
[109] I. Herrmann, P. Suresh, S. Struwe, *The Chemical Industry Outlook For 2023 And Beyond*, **2023**, https://www.oliverwyman.com/our-expertise/insights/2023/jan/chemical-industry-outlook-for-2023-and-beyond.html (accessed: July 2024).
[110] EMIRI, *Re-inventing materials research: Towards accelerated development by closely orchestrating ai, data, robotics, and high-performance computing*, **2023**, https://emiri.eu/2022/07/04/digital-revolution-in-materials-discovery/ (accessed: July 2024).
[111] *Accelerate conference*, **08.08.2024**, https://www.accelerate24.ca/.
[112] *Hitachi high-tech and hitachi have started collaborating on digital transformation of materials development with itri, contributing to improvements of taiwan's industrial standards*, **08.08.2024**, https://www.hitachi-hightech.com/global/en/news/nr20240520.html.
[113] Cambridge Enterprise, *Intellegens – cambridge enterprise*, **09.07.2023**, https://www.enterprise.cam.ac.uk/portfolio-companies/intellegensaml/.
[114] Materials Nexus, *Uses AI-Based Materials Discovery Platform to Create MagNex, a Novel Rare Earth-Free Permanent Magnet, Materials Nexus* **11.06.2024**.
[115] A. D. Little, M. Samoylova, S. Wilmet, D. Witthaut, M. Kolk, *Digital technologies for sustainability in the European chemical industry*, **2023**, https://www.adlittle.com/en/insights/report/digitaltechnologies-sustainability-european-chemical-industry (accessed: July 2024).
[116] Cefic, *New Report Offers a Blueprint for Overcoming Bottlenecks and Unlocking the Full Potential of Digitalisation in the Chemical Industry*, **2023**, https://cefic.org/media-corner/newsroom/new-report-offers-a-blueprint-for-overcoming-bottlenecks-and-unlocking-the-full-potential-of-digitalisation-in-the-chemical-industry/ (accessed: July 2024).
[117] Analytics Insight, *How Robots And Robotics are Powering the Drug Discovery Processes?*, **2020**, https://www.analyticsinsight.net/cryptocurrency-analytics-insight/crypto-gurus-have-their-eyes-on-memecoins-this-q3-200x-is-only-the-start (accessed: July 2024).
[118] O. J. Wouters, M. McKee, J. Luyten, *JAMA* **2020**, *323*, 844.
[119] Deep Pharma Intelligence, *AI for Drug Discovery Q1 2023*, **2023**, https://www.deep-pharma.tech/ai-in-dd-q1-2023-subscribe (accessed: July 2024).
[120] X. Li, P. M. Maffettone, Y. Che, T. Liu, L. Chen, A. I. Cooper, *Chem. Sci.* **2021**, *12*, 10742.
[121] OSHWA, *Open Source Hardware Definition (English)*, **2012**, https://www.oshwa.org/definition/ (accessed: July 2024).
[122] OPC Foundation, *LADS - Laboratory and Analytical Device Standard*, https://opcfoundation.org/markets-collaboration/lads/ (accessed: July 2024).
[123] Industry Commons, *Building Systems for Industry Collaborations*, https://industrycommons.net/ (accessed: July 2024).
[124] GitHub Contributors - Mat-O-Lab/MSEO, *Repository of Material Science and Engineering Ontology MSEO*, https://github.com/Mat-O-Lab/MSEO (accessed: July 2024).
[125] GitHub Contributors - materialdigital/core-ontology, *The PMD Core Ontology (PMDco) official release repository*, https://github.com/materialdigital/core-ontology (accessed: July 2024).
[126] S. P. Stier, X. Xu, L. Gold, M. Möckel, *Energy Technology* **2024**, https://doi.org/10.1002/ente.202301305.
[127] J. Francisco Morgado, S. Chiacchiera, Y. Le Franc, M. Poveda-Villalón, H. Karray, M. Gall, Y. Nahshon, D. Helm, A. Simperler, G. Goldbeck, *Zenodo* **2023**, https://doi.org/10.5281/zenodo.10402214.
[128] Simon Stier, *Zenodo*, **2024**, https://doi.org/10.5281/ZENODO.11401726.
[129] GitHub Contributors - meirwah/awesome-workflow-engines, *A curated list of awesome open source workflow engines*, https://github.com/meirwah/awesome-workflow-engines (accessed: July 2024).
[130] The University of Chicago, *Globus: Research IT. Reimagined*, https://www.globus.org/ (accessed: July 2024).
[131] M. Vogler, J. Busk, H. Hajiyani, P. B. Jørgensen, N. Safaei, I. E. Castelli, F. F. Ramirez, J. Carlsson, G. Pizzi, S. Clark, F. Hanke, A. Bhowmik, H. S. Stein, *Matter* **2023**, *6*, 2647.
[132] M. Vogler, S. Steensen, F. Ramirez, L. Merker, J. Busk, J. M. Carlsson, L. Rieger, B. Zhang, F. Liot, G. Pizzi, F. Hanke, E. Flores, H. Hajiyani, S. Fuchs, A. Sanin, M. Gaberscek, I. Castelli, S. Clark, T. Vegge, A. Bhowmik, H. S. Stein, *ChemRxiv* **2024**, https://doi.org/10.26434/chemrxiv-2024-vfq1n.
[133] S. P. Stier, M. A. Popp, *Zenodo* **2024**, https://doi.org/10.5281/zenodo.11653807.
[134] HERCULES - LPSC, *Hercules School*, https://hercules-school.eu/ (accessed: July 2024).
[135] GCMAC, *GCMAC Summer School 2023*, **2023**, https://gcmac.de/event/summer-school-2023/ (accessed: July 2024).
[136] International Data Spaces, *The future of the data economy is here*, https://internationaldataspaces.org/ (accessed: July 2024).
[137] ERC, *European Research Council: Apply for a grant*, https://erc.europa.eu/apply-grant (accessed: July 2024).
[138] ESFRI, *European Strategy Forum on Research Infrastructures*, https://www.esfri.eu/ (accessed: July 2024).
[139] ESFRI-EOSC Task Force, G. Rossi, *Zenodo* **2024**, https://doi.org/10.5281/zenodo.10980285.
[140] Cefic, *IAM4EU in the spotlight: Pioneering Advanced Materials for Europe's Future*, https://cefic.org/media-corner/newsroom/iam4eu-in-the-spotlight-pioneering-advanced-materials-for-europes-future/ (accessed: July 2024).
[141] European Commission, Directorate-General for Research, and Innovation, *Advanced Materials for Industrial Leadership*, https://research-and-innovation.ec.europa.eu/document/download/0fcf06ea-c242-44a6-b2cb-daed39584996_en?filename=com_2024_98_1_en_act_part1.pdf (accessed: July 2024).

[142] European Commission, Directorate-General for Research, and Innovation, *Communication on advanced materials for industrial leadership*, Publications Office of the European Union, **2024**, https://doi.org/10.2777/401624.

[143] F. Strieth-Kalthoff, H. Hao, V. Rathore, J. Derasp, T. Gaudin, N. H. Angello, M. Seifrid, E. Trushina, M. Guy, J. Liu, X. Tang, M. Mamada, W. Wang, T. Tsagaantsooj, C. Lavigne, R. Pollice, T. C. Wu, K. Hotta, L. Bodo, ... A. Aspuru-Guzik, *Science* **2024**, 384, https://doi.org/10.1126/science.adk9227.

[144] T. Chen, Z. Pang, S. He, Y. Li, S. Shrestha, J. M. Little, H. Yang, T.-C. Chung, J. Sun, H. C. Whitley, I.-C. Lee, T. J. Woehl, T. Li, L. Hu, P.-Y. Chen, *Nature Nanotechnol*. **2024**, *19*, 782.

[145] EUDAT, *The EUDAT Collaborative Data Infrastructure*, (accessed: September 2024), https://www.eudat.eu/.