Brussels, 12 May 2023

COST 033/23

DECISION

Subject:	Memorandum of Understanding for the implementation of the COST Action "European Materials Acceleration Center for Energy" (EU-MACE) CA22123

The COST Member Countries will find attached the Memorandum of Understanding for the COST Action European Materials Acceleration Center for Energy approved by the Committee of Senior Officials through written procedure on 12 May 2023.

MEMORANDUM OF UNDERSTANDING

For the implementation of a COST Action designated as

COST Action CA22123
EUROPEAN MATERIALS ACCELERATION CENTER FOR ENERGY (EU-MACE)

The COST Members through the present Memorandum of Understanding (MoU) wish to undertake joint activities of mutual interest and declare their common intention to participate in the COST Action, referred to above and described in the Technical Annex of this MoU.

The Action will be carried out in accordance with the set of COST Implementation Rules approved by the Committee of Senior Officials (CSO), or any document amending or replacing them.

The main aim and objective of the Action is to create a new form of alliance across the entire innovation value chain of materials for clean energy applications by overcoming the fragmentation of materials research and technology development and via supporting informed decisions by diverse stakeholders. This will be achieved through the specific objectives detailed in the Technical Annex.

The present MoU enters into force on the date of the approval of the COST Action by the CSO.

TECHNICAL ANNEX

OVERVIEW

Summary

Materials have played a decisive role in nearly all rupture technologies in the industrial history of our society. Faced with the current climate, geopolitical and humanitarian crisis, many international and regional entities (political, industrial and scientific alike) recognize the importance of a strong materials innovation ecosystem for driving the clean energy transition. In response, self-driving laboratories (SDL) (a.k.a. MAPs - materials acceleration platforms) are created at institutional, regional and international levels. SDLs integrate combinatorial synthesis, high-throughput characterization, automated analysis and machine learning for fast-track discovery and optimization of advanced materials. While these platforms are proving their effectiveness in producing advanced materials with targeted functionalities and physical properties, a large margin of improvement still exists. Streamlining materials integration into components and to safe and sustainable products is one example challenge in order to enable rupture technology. Another challenge is that of geographical concentration of MAPs that practically excludes a substantial fraction of research labs and tech-companies in Europe from contributing and benefiting from such platforms. Finally, next generation material science researchers need to develop new skills to be able to integrate such systemic and automated approach into their future R&D framework. To this end, EU-MACE will become an ecosystem for accelerated materials development at the user end, gathering researchers and stakeholders with state-of-the-art digital and material competences combined with the market/social pull. Our inclusive & systemic approach will lay the foundation for a future centre of excellence for advanced functional materials to assist transition toward a united and stronger EU.

Areas of Expertise Relevant for the Action	Keywords
● Materials engineering: New materials: oxides, alloys, composite, organic-inorganic hybrid ● Materials engineering: Sustainable engineering ● Environmental engineering: Sustainable engineering ● Materials engineering: Characterization methods of materials for material engineering applications	● advanced energy materials ● materials acceleration platform ● safe and sustainable by design ● clean energy transition

Specific Objectives

To achieve the main objective described in this MoU, the following specific objectives shall be accomplished:

Research Coordination

● To coordinate human resources, knowledge exchange and existing infrastructure among the Action participants to facilitate collaborations and to foster inclusiveness within Europe via a platform sharing agenda with a specific time allocation for scientists from Inclusiveness Target Countries.
● To create a collaborative knowledge platform accessible to the public beyond the Action duration.
● To provide an example R&D roadmap for accelerated material integration built upon a truly systemic approach to become a future EU centre of excellence for advanced materials.
● To coordinate strategic dissemination of activities and results targeting not only research communities, but also companies, policymakers, certification bodies and citizens.

Capacity Building

● To create inclusive and interdisciplinary knowledge-sharing space for investigators from all innovation value chains, naturally promoting new collaborations from several communities and countries to “close the loop” between the R&D and innovation cycle while keeping focus on societal challenges.

● To ensure the generation and the gender balance, and thus minimize the prejudice in the decision making processes when seeking future application and market opportunities for newly developed advanced materials.
● To increase the preparedness of ECI and PhD students for leading the future ‘systemic approach’ pursued by the Action via Fostering innovation and entrepreneurship.
● To foster continued growth (further education) among senior investigators for adapting the digital-driven and holistic research approach, which will ultimately increase the acceptance-rate of ‘new’ methodologies and collaboration schemes, and speed up the implementation of SDL/MAP-like platforms across Europe.
● To incubate trans-national education programmes for generating a pool of young scientists whose academic knowledge spans all facets of advanced materials development prior to settling their PhD research agenda.
● To increase awareness about the potential and challenges of materials research among private and public decision makers in order for them to take informed decisions, and among a wider public in order to feed an informed public discussion.

TECHNICAL ANNEX

1. S&T EXCELLENCE

1.1. SOUNDNESS OF THE CHALLENGE

1.1.1. DESCRIPTION OF THE STATE OF THE ART

Materials have played a decisive role in nearly all rupture technologies in the industrial history of our society. In the current climate, geopolitical and humanitarian crisis, rapid material breakthroughs are needed more than ever for enabling innovation in the clean energy technology sector. However, the traditionally pursued sequential, largely empirical, and non-automated process of materials discovery and development is fragmented, inefficient, costly, and slow. To illustrate, the innovation timeline from invention to maturity for lithium batteries (based on the Li-ion shuttle concept) took approximately 20 years. This situation has given rise to a new breed of laboratories; namely, **self-driving laboratories (SDLs**) (also termed **Materials Acceleration Platforms (MAPs)**) that combine artificial intelligence (AI) with automated robotic platforms together with high throughput screening (off-line or in-line synthesis, characterization and analytics) to predict and assess materials' properties and performance. Concurrently, autonomous experimentation entails solving a multi-objective optimization problem across a high-dimensional condition space to develop materials with the tailored properties. Such automated closed-loop discovery scheme has brought a paradigm change in the materials R&D, accelerating (up to 10 times) the discovery and development of new functional materials while curtailing the infrastructure requirements and cost. Several multidisciplinary initiatives with participations from academia, governments, and industry have been formed in recent years; including, Materials Genome Initiative (USA), Centre for Accelerated Materials Discovery and Innovation (CAMDI, Canada) BIG-MAP of Battery 2030+ (EU-H2020), German-Canadian Materials Acceleration Centre (GC-MAC), DIADEM initiatives (France),) IEMAP program (Italy) and Accelerated Materials Development for Manufacturing, AMDM (Singapore), focusing mostly on organic PV materials, catalytic materials and "beyond Li" battery materials (see §2.1.1 for the current map of MAPs/SDLs in the EU).

To foster breakthrough technology (for energy), newly developed and highly functional materials must be shaped into *components* and integrated into *devices* with a minimum performance loss at each step. ***eDesign*** and ***Digital-Twin*** technologies are powerful computer-aided tools that are used to accelerate the device design and optimization processes. The former consists of virtual prototyping (*e.g.*, Computer-Aided Design - CAD, Computer-Aided Manufacturing - CAM, Computer-Aided Engineering - CAE), which allows the implementation of product design in a virtual environment by including process simulation and optimisation methods. This is often accompanied by rapid prototype fabrication iterative process for i) design verification and ii) process/product validation. The eDesign approach can also be extended to support the development of (new) materials and products from their early stage by predicting and analysing not only their performance, efficient use and reliability but also their manufacturability (including cost evaluations) before entering the production phase. The methods for carrying out a quantitative assessment of trade-offs for decision-making are established and are widely used in engineering/research labs as well as in industrial environment. Going another step further, *digital twins* add 'connectivity' dimensions to eDesign. A digital twin is a dynamic virtual copy of a device, together with underlying processes and key complex phenomena at various scale. Here, the physical prototype is connected to its virtual counterpart (*digital twin)* through wireless sensors for collecting real-time performance change under different operation scenarios, which will then be used as the baseline device calibration. The digital twin can also represent processes for fabrication of components or device assemblies using virtual reality software allowing immersive examination of system configurations that are impossible or highly costly to experiment in real-time.

Equally important, any given new technology (materials, products and processes) must satisfy the safety and sustainability conditions before it can be commercialised. Furthermore, regulatory bodies must be involved at early stages of the development process to prepare all the standards and indications that must be considered to enter the market. Indeed, a number of industrial, environmental, climate and energy priorities are proposed in the new EU's **Circular Economy Action Plan** (CEAP), in the **European Industrial Strategy**, calling for Safe-and-Sustainable-by-Design approach (SSbD) and the Chemical Strategy for Sustainability. The SSbD concept integrates safety, circularity, energy efficiency and functionality of materials, products, and processes throughout their life cycle in order to minimize environmental impacts, increase safety, reduce cost and increase societal wellbeing. Fuelled by the **EU Green Deal** goals and other international SSbD is a fast-developing field, where numerous methods and tools such as Life Cycle Sustainability Assessment (LCSA), Risk Assessment (RA) and Regulatory Preparedness (RP) are developed and continuously refined in all technology areas. Currently, there is a growing dynamic to include these SSbD tools and their associated databases in the eDesign process to optimize the functional materials selection, product design and manufacturing cost while respecting both functionality and sustainability requirements.

Combined together, EU-MACE aims to create a new form of alliance across the entire innovation/value chain of materials for renewable energy applications responding to the clean energy transition challenges, overcoming the fragmentation of functional/structural materials and technology development stages described above. **A systemic and inclusive research approach of the Action is applicable to all types of materials, and thus become a foundation for a future centre of excellence on advanced materials for energy**.

1.1.2. DESCRIPTION OF THE CHALLENGE (MAIN AIM)

From solar modules to batteries and energy-efficient buildings, advanced materials offer solutions to many low-carbon technologies and simultaneously provide high-quality job opportunities to researchers, innovators and manufacturers. At the same time, these very same materials occupy the dominant share of the technology cost. Therefore, the EU Green Deal's (EUGD) overarching goals (net-zero greenhouse gas emission by 2050, economic growth and no person and no place left behind) cannot be achieved without a ***systemic approach to accelerate the identification of disruptive technologies, their device level integration and de-risking along the whole production chain of low-carbon technologies based on advanced functional materials***. It implies streamlining the connections between different phases of the innovation/value chain from bottom-up research and technology push to market-pull guided by societal needs, *i.e.,* the sustainable development goals. The SDLs/MAPs described above is clearly a huge step in the right direction, accelerating materials screening, discovery and manufacturing. But how can we integrate these autonomous labs and platforms into the larger process of technology and value creation while ensuring the product/technology sustainability? Who are the key stakeholders and what role do they play? And how to organize, manage and operate such a systemic R&D scheme? These are precisely the questions and challenges tackled by EU-MACE. By identifying and gathering key stakeholders, the Action will demonstrate a model ecosystem addressing:

- **Accelerated device integration by identifying common ground and building on areas of overlap between digital and material competencies (horizontal link)**: Knowledge sharing and cooperation between existing SDLs/MAPs, and inclusion of key expertise for maximizing their operation efficiency and streamlining device integration process.
- **Market & society pull**: Upstream integration of advanced materials into functioning devices and scale-up production taking into account not only the performance (efficiency) requirements, but also the techno-economic issues, socio-economic impacts and regulatory bodies.
- **EU-Inclusiveness (bottom-up)**: Fostering the creation of a widespread international community based on gateways to SDLs/MAPs for the broadest EU research communities and accessing relevant knowledge bases of the latter (data, experimental & numerical techniques; theories, etc.).

The building and the operation of SDLs/MAPs are costly both in financial and human terms. For example, the government of Canada (via its R&D capacity at NRCan and NRC institutes) has invested 60 MCAD for the infrastructure and operation of 8 MAPs in 2017-2022 period. Once operational, the estimated running cost of these MAPs is 2MCAD/year/MAP, supported by various R&D funding programmes. Naturally, the European MAP/SDL initiatives are currently concentrated in high GDP countries (see Figure 2.1) and around large research centres with pre-existing infrastructures. The negative corollary of this geographical disparity is two-fold. First, it excludes a substantial fraction of EU researchers and small & medium enterprises from accessing these platforms and benefiting from their outcomes. Secondly, large amounts of valuable data and expert knowledge on *experimental* (*high-throughput synthesis & characterization*), *theoretical and numerical methodologies*, which could otherwise feed into the SDL databases to increase the simulation and selection capacities, are not incorporated in the SDLs' research loops. The **EU-Inclusiveness** approach is crucial for strengthening the EU society by aligning all national-funded initiatives and by providing knowledge, data and tools harmonised across Europe.

As the number of national and international initiatives and that of participating research groups in SDLs multiply, the demand for experts to develop and operate such systems, combining methodology skills (incl. *programming*), expertise in *robotics* and the *domain knowledge in the energy materials* of interest is also rising. In particular, the *advanced data management skills* are crucial for proper curation, annotation and storage of a broad range of experimental data, and for providing simple access to all users. High throughput material simulation schemes are also needed for curating materials data from different simulation sources like DFT, MD, phase field, micromechanical modelling, macroscopic modelling and machine learning and Bayesian methods. The coupling of experimental and computational data for materials design and screening requires the development of common ontology, interoperability protocols and visualisation/analysis tools (FAIR principle). Several large-scale initiatives on *Open Source Repositories* for materials data exist (Materials Genome Initiative and MaterialsMine in USA and MatNavi in Japan, for example). It is of the highest importance to join force with the existing platforms and to gain expert knowhow on handling data assembly and materials informatics applied to the high dimensional problems inherent in multi-functional materials due to their multi-phased nature and complex structures.

As described above, self-driving labs (SDLs) consist of software and robotic hardware components to orchestrate experiments and can be equipped with off-line or in-line characterization and analytics to assess properties and performance. Concurrently, autonomous experimentation entails solving a multi-objective optimization problem across a high-dimensional condition space to develop materials with the tailored properties. While the SDLs comprise accelerated discovery, all modelling and characterization tools need to be mapped to a particular technology-space. Integrating energy materials requires these bespoke processes to be well aligned from materials level to components and streamlined to device integration without losing performance at each step. Thus, the transfer of energy materials from R&D lab to industrial production requires human-centric knowledge and a seamless data flow to ensure the demonstrated performance at the component and device levels are maintained during up-scaling. Automation along this pipeline (Digital Twin, eDesign, baseline processing definition, etc.) hinges on metadata management to maximize data utility, improve data integration from diverse sources, ensure data quality, and enable quick data discovery and tracking. However, metadata management between SDLs and MAPs has not yet been sufficiently addressed. There is a limited interconnectivity with modelling, computational, or experimental modules beyond those readily integrated into the “closed-loop” hardware platform. Therefore, the “closed-loop” lab concept has found little traction in the integration of the know-how about advanced materials, where multiple functional properties need to be optimised through interdisciplinary multi-objective approaches (e.g. energy capacity, energy conversion efficiency, energy density, power output, operation range, cost, chemical stability, safety, etc.). The cooperation between multiple SDLs and the creation of geographically distributed multi-tenant MAPs (similar to *e.g.* FINALE project BIG-MAP for Li-ion batteries, or VIPERLAB for Perovskite PV cells) are needed to overcome this difficulty.

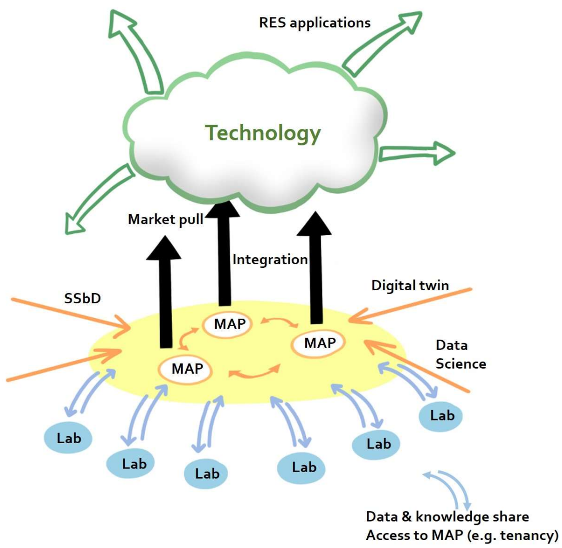
Simultaneously, the advanced material development must encompass several *sustainability* aspects: the safe-and-sustainable-by-design material approach, which is under the attention of the European Commission through several UNEP initiatives and H2020 & HEU-funded projects that incorporates sustainability and risk assessment but at early stages of the innovation processes; the Safe(r) Innovation Approach, which includes Safe(r)(ty)-by-Design and Regulatory Preparedness to establish the relevance of regulatory bodies involvement since the early stages of new material development. Some specific challenges include: Lack of common EU educational/training programmes including recent advancements concerning Safety and Sustainability assessment, Digitalisation, Entrepreneurship. Needs to educate skilled workers/managers, in particular at SMEs, able to correctly use and/or interpret the results form LCSA (able to choose the right tools for right technology by including territorial considerations, and the correct interpretation of the analysis results) that are today below market demand (identification of experts for each class of material and target technology. Appropriate matchmaking); Fragmentation of LCSA method and tools and databases needs to be customised according to territorial (national) requirements and harmonised at international level. Other methods and tools for SSbD need to evaluated and validated. EU-MACE network can contribute to the diffusion and standardisation of tools and methods; and Implementation of integrated LCSA+Risk Assessment tools at an early stage of material, process and product development for predictive analyses to be used for decision making purposes.

1.2. PROGRESS BEYOND THE STATE-OF-THE-ART

1.2.1. APPROACH TO THE CHALLENGE AND PROGRESS BEYOND THE STATE OF THE ART

EU-MACE aims to set an example of a future ecosystem enabling the fast-track discovery, development and integration of advanced materials into technology in key innovation markets for assisting the EU’s transition into a sustainable and autonomous society. This calls for coordinated multidisciplinary efforts from physics to materials science, engineering at different levels, and to social sciences, policymakers and all stakeholders in between.

<u>EU-Inclusiveness (bottom-up link)</u>: Continuous acquisition of the physical/chemical properties of the materials and their relationship to the microstructural features and synthesis routes are necessary for both understanding the fundamental physics of materials and expediting the screening and optimization process. This will be done by creating gateways to SDLs/MAPs to individual research groups and industries for ***accessing relevant knowledge bases from the widest EU research and innovation communities***. Simultaneously, it will open the access to the SDLs, creating opportunities to integrate new research methods into their activities either as platform users (tenancy) or by starting new initiatives, resulting in ***a wider uptake of powerful SDL approach in EU research and technology communities.***



<u>Accelerated device integration by unifying digital and materials competency (Increasing SDLs & MAPs capacities via horizontal collaborations)</u> As more initiatives are created at national and institutional levels across the EU, the communication between the platforms becomes crucial for optimizing the operation of each and avoiding unnecessary duplications. The bespoke high-dimensionality of multi-functional energy materials also complicates the simultaneous qualification of multiple properties using one MAP/SDLs. Furthermore, the future generation low-carbon or CO_2-neutral energy processes based on *new* advanced materials will differ from those in conventional processes. Therefore, the future material technology and components need to respond flexibly to new requirements without compromising the operational reliability and safety. Mutualisation of data and results, sharing of experimental and simulation methodologies and interpretation, analysis and decision making tools should lead to defining the best-practices for building a coordinated and flexible network of MAP/SDL platforms. To serve as a collaborative incubation centre for ***future new MAPs and cooperative multi-tenancy platforms*** (e.g. FINALE/BIG-MAP) responding to the growing needs for advanced materials-based technology should be the legacy of EU-MACE, continuing beyond the Action lifetime. Particular attention will be given to bringing in the key expertise from ***data-science*** (data curation and metadata standardization), ***device integrations*** (e.g., Digital-Twin, eDesign) and ***economic, environmental and social sciences*** (e.g., SSbD) domains. The existing material databases, MAP/SDL platforms, expert laboratories (experimental and numerical skills, LCSA, *etc*., within and outside the Action) will be assessed at the beginning of the Action for fostering synergies among Participants. Workshops will be designed to introduce the SDL paradigm to those who are new to the concept, to showcase the Participants' research focus, methodologies used, equipment, testing facilities, and target technology areas to facilitate collaborations and bridge gaps for scale-up production and device integrations. The training courses and interactions with SSbD experts will ***increase the common understanding of SSbD procedures***, ***towards embedding of LCSA tools into automated materials discovery and integration processes***.

<u>Market/society pull</u>: Upstream integration of advanced materials into functioning devices and scale-up production must take into account not only the time-of-service and (efficiency) requirements, but also the techno-economic and socio-economic impacts. Site visits, STSMs, workshops, training courses, online tutorial materials B2B platforms are foreseen to boost the exchanges with industries within (Partners: Data management, scale-up manufacturing of materials, and prototype building) and outside the Action. Showcasing our activities at international conferences and high-level meetings are also envisaged. Universities of the Third Age and more in general, citizens associations/initiatives will be involved in building up the public awareness and societal acceptance of the new R&D schemes promoted by EU-MACE. Tailor-made seminars (e.g., MOOC (Massive Open Online course) and YouTube) will be held for illustrating the topics addressed by the scientific communities and industries. Due to their informative nature, these seminars will be useful for addressing the importance of aligning national programs, sharing infrastructures, and facilitating ITC access. Selected educational contents (tutorials, demonstrations) maybe suitable for younger audience that can be disseminated using a virtual education platform such as FuseSchool (https://www.fuseschool.org/).

To implement the bespoke collaboration/cooperation approach, EU-MACE selects three types of multi-functional advanced materials with high application potential in the renewable energy technology sector.

***1. Perovskites* (and related lattice structures; e.g., rutiles, spinels and their sub-phases)** are highly researched materials for a wide range of applications due to their oxygen conductivity and non-stoichiometric oxygen vacancy formation during reduction. They can be described with the general chemical formula of $ABO_{3-\delta}$ (A: an inorganic or organic cation and B: a metal ion). Perovskites can be partly reduced and re-oxidized to a large extent without changing their crystal structure. A- and B-Site substitutions can be used to stabilise structural integrity or tune their reduction enthalpy, making them a versatile and extensively investigated material class for solar cells, electrodes for solid oxide fuel cells, ceramic membranes for H_2 separation at high temperature and for redox reactions. The latter makes them especially interesting for use in thermochemical cycles, since the avoidance of phase change during the reduction and the oxidation leads to improved structural stability and suppressed attrition. This property is crucial for particles, honeycomb structures and foams. A further advantage of perovskites is their fast reaction kinetics in the oxidation reaction even at low temperatures. Their composition can be tuned to match a wide range of different applications, and their properties can be adjusted by solid solution formation. This allows performing many redox cycles per unit time and reduces the amount of material necessary for a fixed O_2/N_2 production rate. Perovskites have already been applied in redox cycles for oxygen pumping, air separation, hydrogen and fuel production. The key characteristic of perovskites for different applications are their structural stability, thermodynamic properties and reaction kinetics. Withal, they constitute highly active areas of research amounting to over 60,000 published research articles in the past 3 years only.

All of these can be tailored by changing the chemical composition, however, for establishing a reliable structure-properties correlation and resolving the stability issues associated with different structures (e.g., quantum dots, thin layers, particles and foams) for accelerating the scale-up production and integration, shared databases on large-scale material screening are needed. Currently, several AI- and robotics-assisted SDLs for metallic *halide* perovskites exist, (e.g., MAOSIC (China), U. Toronto (Canada), ESCALATE (USA)), but 'closed-loop' automation for oxide perovskites with higher materials dimension remains rare (e.g., VIPERLAB see Figure 2.1). Thus, the development of SDLs for perovskites is of priority importance, either by creation of new MAPs or the incorporation of Perovskites in existing platforms as a 'tenant' material in order to advance the maturity of carbon-free, solar-based energy solutions (e.g., PV cells, fuel cells/electrolysers, and solar thermal applications and explore new application areas such as thermochemical cycles for ammonia production.

2. Metallic alloys: Despite technological differences, many low-carbon energy technologies (e.g., fuel cells and hydrogen, concentrated solar power, bioenergy, geothermal, and sustainable nuclear technologies) find a common ground in the use of metallic materials (alloys) that are resistant to harsh operating conditions. One challenge is related to the high operating temperatures which require multiple characteristics such as high thermal and thermomechanical stability, corrosion and oxidation resistance, sufficient strength and creep resistance and specific thermal conductivity. For each applications, these properties are tailored via development of new alloys through slow (traditional) trial-and-error processes. Recent advances in material modelling (the integrated computational materials engineering (ICME) and multiscale material modelling) have significantly improved the optimisation of a wide variety of material properties (e.g., lifetime endurance, wear and corrosion resistance, and fracture and fatigue durability) while reducing the cost and time-to-market of high-performance metallic materials (average time reduction of 50% for using the digital material virtual testing).

To rapidly meet the new demands in low-carbon energy market, metallic alloys can clearly benefit from AI orchestrated platforms, combined with the high throughput simulation/characterization methods. Material-specific challenges for SDL/MAPs network include: Understanding the degradation mechanisms under operate at harsh conditions (with special focus on combined loads); In-operando characterization and testing of materials and devices; Inclusion of life-cycle assessment, Development of new concepts like high entropy alloys and MAX-phases.

3. Additional multi-functional material will be chosen within the first year of the Action giving flexibility in the 3rd materials choice because of the fast evolving nature of the energy materials research and technology sector. At present, the candidate materials include: **flexible organic polymers** (energy storage, thermoelectrics, electrical and thermal insulation (cables and pipes), flexible electronics, robotics etc.), **Metal-Organic-Frameworks** (MOFs, for bifunctional electrocatalysts, hydrogen storage, water harvesting, supercapacitors, etc.) and **complex fluids and soft-materials** such as ionic liquids, nanofluids, molten salts, aerogels, foams, liquid crystals (for tribology, electrochemical energy storage, heat storage, cooling, etc.)

Sustainable advanced materials are the source and a trigger for innovation in many sectors critical for achieving EU Green Deal. The currently available research funding schemes at EU (Horizon EU), national and bilateral levels are in favour of fostering collaborative, open and systemic research approaches, which can greatly help create international platforms as we envision in EU-MACE. By combining responsible design principles with digital-assisted advanced materials production platforms and industrial technologies we purpose to turn the twin green and digital transitions in to reality.

1.2.2. OBJECTIVES

1.2.2.1. Research Coordination Objectives

Coordinate human/knowledge/infrastructure resources of the Action participants to facilitate collaborations. The Action will *inventory participants' laboratories, equipment, testing facilities (including automated high-throughput characterization) and HPC capabilities*, etc. The affiliation to the existing SDLs/MAPs structures, data repositories will also be assessed. The expert mapping will be extended beyond the Action perimeter, to include the lists of MAPs/SDLs, data repositories, Knowledge and Innovation Communities (KIC) promoting the exchange, knowledge-gap bridging and accelerate the advanced materials development and integration. To foster *inclusiveness* within European Research Area, the EU-MACE will advocate a platform sharing agenda with a specific time allocation for scientists from ITCs, in a tireless effort on meeting the core principle of 'not leaving anyone behind.'

Create a collaborative knowledge platform readily accessible through the Action website. A Web platform will be developed to store the expert & expertise lists mentioned above which will be accessible to the public. The platform will also host training material and seminar recordings produced by the Action. An internal (member's only) area of the platform will be used for sharing un-published data from experiments and simulations, software models, and benchmarks, among the Action participants. The platform will be simple by design, requiring minimum maintenance efforts to stay active beyond the Action duration.

Provide a R&D framework for accelerated material integration: the Roadmap. Recent and continued advances in digital technologies (multiphysics solvers, artificial intelligence, big data cybernetics, data processing and pipeline tools) and experimental techniques (robotics, nanotechnology) can bring next-generation multifunctional materials and their impact on society at unprecedented speed. Selecting the right tools and streamlining the workflow from the discovery phase to the final device level adapted for each material type and target technology still require innovation in the R&D framework. Building upon the SDL/MAP paradigm, EU-MACE will provide opportunities for researchers and innovators from all branches of advanced materials and device development, including manufacturing sustainability to identify the missing-links (in the 'closed-loop' approach) and the associated expertise/experts, promising innovation markets, relevant LCSA tools, etc. for building a truly systemic approach to advanced materials development and integration. The ***conclusions will be published as a roadmap to serve as a model for future EU centre of excellence for advanced materials***.

Coordinate strategic dissemination of activities and results will utilise both physical and digital means. The target audience of EU-MACE's workshops and seminars (both virtual and in-person) include companies, policymakers, certification bodies and the general public. The Action will also be presented at scientific conferences and industrial events to introduce our research concept to a wider audience. The involvement of policymakers (EU, member states, regional representatives) is of particular importance as the future R&D platforms envisaged by EU-MACE is costly, requiring a substantial investment of the member states. Technical/scientific review and dissemination articles will be made within EU-MACE. An active social media presence is foreseen (e.g. LinkedIn, Twitter) where events, outcomes, exchange or employment opportunities, news and other relevant information will be posted. Each Action member will contribute to the dissemination efforts, *e.g.* use of personal SNS accounts, institutional web-platform, talent labs, pro-active participation in local popular science events (e.g., EU Researchers' Night, Pint of Science, Science Week, Fête des Sciences, etc.).

1.2.2.2. Capacity-building Objectives

EU-MACE focuses on the following key capacity and critical mass building objectives.

EU-inclusiveness (see §1.1.2) for expanding SDL/MAP methodologies to the Inclusiveness Target Countries (ITC) and simultaneously increase the knowledge capacity by gathering resources from research and industrial groups distributed in larger geographical areas. The organisation of workshops and training schools in ITC is privileged. These efforts will lead to the creation of inclusive and interdisciplinary knowledge-sharing space for investigators from all innovation/value chains, naturally promoting new collaborations from several communities and countries: materials scientists, physicists, chemists, data scientists, device & process engineers, environmental & social scientists, technologies developers and manufacturers. The WG discussions and workshops will allow identifying and addressing strategic R&D gaps to "close the loop" of the R&D and innovation cycle, keeping focus on societal challenges.

Generation and gender balance. At the time of the proposal submission, the Action counts 23 % of YRI (Young Researchers and Innovators) and 40% of female members among the secondary proposers. The proportion of YRI will be increased to 40% (minimum target)within the first year of the Action. While *basic* materials science research can be assumed to be free of gender-bias, any extension to application and market opportunities should include a 'gender lens' in the decision-making processes to minimize the prejudice in the assumptions, interpretations and communication of the findings. For example in identifying a user-inspired market, or establishing safety guidelines. To this end, a minimum 25% (50%) of MC and WG leader positions will be attributed to YRI (female) members in the management committee and in WG task-leader positions.

Future generation preparedness. The Action promotes the active participation of YRI and PhD students in Short-Term Scientific Missions (STSM), training courses & workshops as well as in external conferences to increase their 'preparedness' to lead the 'systemic approach' pursued by EU-MACE and more widely by the EU. Fostering innovation and entrepreneurship is also of a great importance. The Action's training courses include: IPR management, Regulatory (Safety) preparedness, Soft-skills, to name a few. The active involvement of ECIs in MC positions will also provide hands-on experience in international collaboration management tasks (see WG4).

Continued growth (Further education). Adapting one's 'traditional' training to the fast-changing dynamics toward the digital-driven and holistic research approach is a formidable challenge faced by many senior investigators. EU-MACE acknowledges this difficulty and implement shorter STSM programme for senior members with transdisciplinary visions. The training courses will be open to them as well (up to 10% of attendees). Such opportunities will increase the acceptance-rate of 'new' methodologies and collaboration schemes, and speed up the implementation of SDL/MAP-like platforms across the EU.

Trans-national Education Programme Incubation. In the current dynamics of energy research, it is useful to generate a pool of young scientists whose academic knowledge spans all facets of advanced materials development prior to settling their PhD research agenda. Here, the Action will serve as an incubator for international education programmes such as ERASMUS-Mundus master project (*cf* §3.2.1). The workshops and seminars among the different members of the Action network will help define more precisely the core group of universities that will carry such international programmes.

2. NETWORKING EXCELLENCE

2.1. ADDED VALUE OF NETWORKING IN S&T EXCELLENCE

2.1.1. ADDED VALUE IN RELATION TO EXISTING EFFORTS AT EUROPEAN AND/OR INTERNATIONAL LEVEL

MAPs & SDLs in EU and beyond: The below cartography shows the major MAP/SDL like initiatives across EU today. The geographical distribution imbalance is clear. The first added value of the EU-MACE network will thus be the inclusions of research groups from regions where MAP-like initiatives are not available mutually benefiting from existing knowledge of individual groups while providing access to acceleration platforms. Outside EU, the well-established platforms and data-repositories are found in USA (Bayesian Experimental Autonomous Researcher-BEAR, SynFini, UW Soft Matter MAP, RAPID, Process optimizer for organic synthesis, molSimplify, MOFSimplify, Artificial Chemist, etc.), Canada (Opentrons pipetting robots (x2), The MACHIN, MAP for gold nanoclusters, Phase MAP, Organic laser MAP, ML for silicon and aluminosilicate atomistic simulations (MLSAAS), Minioni, Microfluidic Machine Learning (MFML) platform, High-throughput nanoindentation, Electrocatalysis MAP, etc.), China (PRIMITIV, Opentrons Liquid Handler, LISSY, Flow-based synthesis, etc.) Japan (MInt System, MaDIS, DICE, MatNavi, etc.) and others.

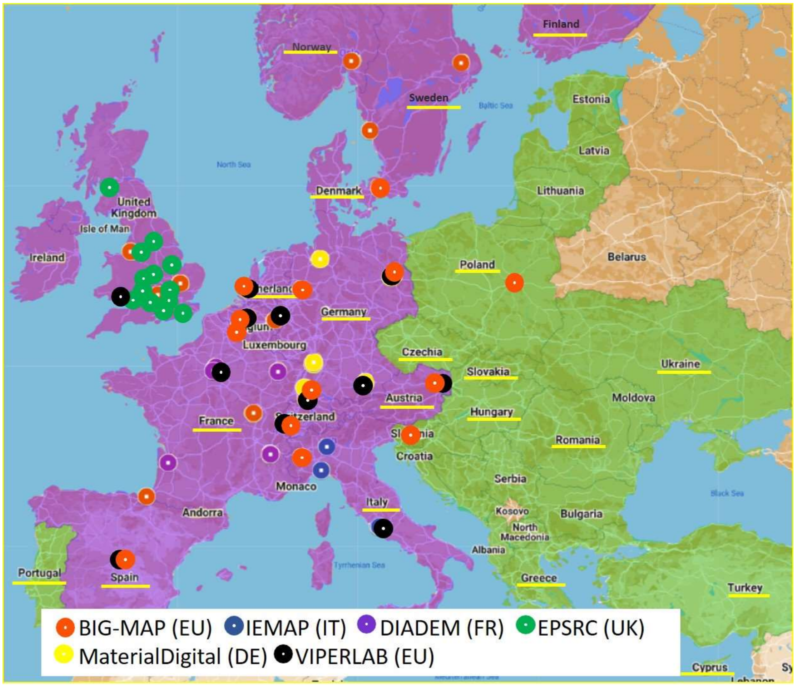


Figure 2.1: Distribution of Materials Acceleration Platforms in Europe.

Green zone: ITC countries. Purple zone: non-ITC countries. Yellow underline: EU-MACE member countries.

BIG-MAP (EU initiative on Battery 2030)

IEMAP (Italian Energy Material Acceleration Platform, Mission Innovation)

DIADEM (DIscovery Acceleration for the Deployment of Emerging Materials, French PEPR Initiative)

EPSRC (UK's Future manufacturing research hubs)

MaterialDigital (The Material Digitalization Platform, Germany)

VIPERLAB (Fully Connected Virtual and Physical Perovskite Photovoltaics Lab, EU)

International coordination actions/projects on advanced (energy) materials development with whom EU-MACE will liaise include, but not limited to:

COST-Actions: RENEW-PV (Inorganic Chalocogenides for PV), NETPORE (Porous semiconductors and oxides for energy storage), Hi-SCALE (High temperature superconductors), NanoUptake (Nanofluids for heat transfer), CompNanoEnergy (Oxide nanocrystals for water splitting).

CSA (on-going): stoRIES (Storage Research Infrastructure Eco-System, solutions for sustainable energy storage); SUNER-C (Accelerate innovation on solar fuels and chemicals); SAbyNA (Simple, robust and cost-effective approaches to guide industry in the development of safer nanomaterials and nano-enabled products); DIAGONAL (Development and scaled Implementation of sAfe by design tools and Guidelines for multicOmponent aNd hArn nanomateriaLs); EMMC (European Materials Modelling Council); SBD4NANO (Computing infrastructure for the definition, performance testing and implementation of safe-by-design approaches in nanotechnology supply chains); SABYDOMA (Safety by design (SbD) paradigm in industries); HARMLESS (Advanced high aspect ratio and multicomponent materials: towards comprehensive intelligent testing and Safe-by-Design strategies); SUNSHINE (Safe and sUstainable by desigN Strategies for HIgh performance multi-component NanomatErials) ASINA (Anticipating safety issues at the design stage of nano product development); IRISS (The InteRnatIonal ecosystem for accelerating the transition to Safe-and-Sustainable-by-design materials, products and processes); OntoCommons (Standardisation of data documentation across all domains related to materials and manufacturing)

EU-MACE also intends to interact with the Advance Materials Initiative 2030 to co-design a systemic approach to develop innovative advanced energy materials to offer faster, scalable, and efficient responses to the challenges and opportunities for Europe's society, economy, and environment.

Research, industrial and expert associations, platforms and societies with relevant member expertise and shared interests with EU-MACE are numerous. For example, The European Energy Research Alliance (EERA) and nearly all of its joint programmes (AMPEA, NM, DfE, E3S, PV, CCUS, etc.); The Energy Materials Industrial Research Initiative (EMIRI); The European innovation partnership (EIP) on raw materials; Mineral processing and extractive metallurgy for mining and recycling innovation association (PROMETIA), The European Technology Platform for Advanced Engineering Materials and Technologies (EuMaT); The European Technology Platform for Sustainable Chemistry (SusChem); The European Platform on Life Cycle Assessment (EPLCA); The EU NanoSafety Cluster; The Division for Sustainable Development Goals (DSDG, under the UN Department of Economic and Social Affairs (UNDESA)); The United Nations Environment Programme (UNEP); The Life Cycle Initiative; ANEC for Sustainability; The European Multifunctional Materials Institute (EMMI); The European Laboratory for Learning and Intelligent Systems (ELLIS); The European Materials Research Society (E-MRS) and a vast number of similar interest-groups/organizations at the national level.

Key stakeholders from and outside of the aforementioned initiatives have been informed in the conceptualization of the EU-MACE COST Action proposal. They will be formally invited to join the Action after the screening (mapping) phase by the working groups (see §4.1.1). The WG1/WG2 joint workshop (*c.f.* deliverable D1.2) will be the first occasion to invite external partners with whom the Action will create synergies and expand our influence.

2.2. ADDED VALUE OF NETWORKING IN IMPACT

2.2.1. SECURING THE CRITICAL MASS, EXPERTISE AND GEOGRAPHICAL BALANCE WITHIN THE COST MEMBERS AND BEYOND

EU-MACE gathers experts from a large spectrum of advanced materials R&D&I domains including AI and simulations, data-science and environmental & social sciences applied to materials. The starting network consists of 37 confirmed proposers from 18 countries (10 ITCs) of which, 15 female (40%), 9 ECIs (23%) and 2 industrial members. In addition to the experts' individual knowledge, EU-MACE benefits from their groups' numerical and experimental assets; e.g., high-throughput synthesis and testing facilities, high-performance computing clusters, large scale research facilities (synchrotron accelerators, for example) made available through members' affiliation to institutions and to SDL/MAP platforms. The industrial presence (data management and device design) is less than 10% in the starting network composition, for which targeted dissemination & exploitation activities (3.2.2) are to be held to secure critical mass for building a holistic and inclusive network toward technology development. The innovation uptake and technology deployment hinges heavily on the socio-economic and regulatory constraints, which vary enormously from one territory to another. Therefore, it is important that policymakers and regulatory bodies from the EU member states and associated countries are aware of the latest research and technology advancements, and involve the S&T sector into their decision-making processes for emerging new technology markets. A wide geographical area represented by the Action participants will facilitate the communication and dissemination of our progress to the regional government bodies, and stimulate regional, national and inter-governmental endorsement for creating future systemic research structures for accelerated materials integration into technology.

2.2.2. INVOLVEMENT OF STAKEHOLDERS

The success of EU-MACE and its long-lasting impact (united EU, next generation MAP, new training methodologies, etc.) relies on the active involvement of the key stakeholders. A dissemination plan detailed in 3.2.2, identifies several such stakeholder groups (Table 3.1) and the measures to reach them. These stakeholders include: Research community of the core of EU-MACE actions with equitable representations of gender, generation and regional diversities. Scientific (includes social sciences) societies and EU research communities related to advanced materials and renewable energy (see 2.1.1) will be solicited. Industrial participants will play a key-role in identifying the innovation markets based upon the research output on both technical and SSbD merits. Tutorial/training courses and STSM hosting of ECIs are to take place. In order to increase the industrial presence within the Action, industry associations, technology clusters and industrial end-users will be invited to participate in the Action workshops and training course. The organization of bilateral events coupled to EU-MACE's workshops and training schools with these stakeholder groups will be a privileged communication pathway for effectively disseminating our actions to the relevant professionals and groups. It will also serve for validating and refining the envisaged systemic research approaches. Policymakers and regulatory bodies are involved through their invitation to the Action's workshops and bilateral events throughout the Action.

Several material acceleration and data-repository platforms have been identified as potential collaborators of EU-MACE (North America and Asia). Their representatives will be invited to join our Action as third parties after the official approval by the MC. Such international collaborations will increase the impact of the Action's outcomes and expand the access to a diverse pool of expertise across research institutions, academia, and industry from these countries. Lastly, the Action is open to all who adhere to our systemic materials research vision. Through dissemination actions (*cf* §3.2.2), the Action will attract future participants from countries currently without access to MAP/SDL platforms, in particular, COST near-neighbour countries, leading to possible future collaborative RIA projects under the HEU programme.

3. IMPACT

3.1. IMPACT TO SCIENCE, SOCIETY AND COMPETITIVENESS, AND POTENTIAL FOR INNOVATION/BREAK-THROUGHS

3.1.1. SCIENTIFIC, TECHNOLOGICAL, AND/OR SOCIOECONOMIC IMPACTS (INCLUDING POTENTIAL INNOVATIONS AND/OR BREAKTHROUGHS)

EU-MACE aims to establish a new systemic and comprehensive R&D&I scheme for accelerated development of safe and sustainable advanced materials and technology for energy, thereby strengthening European research and innovation capacities. It will thus directly contribute to the ongoing effort to reach a climate neutral Europe by 2050, improving the quality of life of all European citizens. Significant impacts of EU-MACE will be the increased European science and industrial leadership and the reduction of the European dependence for the supply of raw materials reducing material use and substituting the most critical materials. Some specific examples of breakthroughs and potential for innovation are listed below.

Impact	***Potential for innovation/Breakthroughs***
Scientific (Research & Education)	
EU leadership in materials science and low-carbon energy research infrastructure and education (short-mid-long term)	• Creation of new, inclusive and collaborative MAPs/SDLs at national and multinational levels with increased participation from ITCs • Strategize the R&D funding framework for advanced materials used in clean energy and mobility technologies at EU level (by influencing the European R&D policy-making process) • Open access web portal (maintained beyond the Action cf §1.2.2.1) provides 1-step lists of MAPs/SDLs, experts and open data repositories for continued collaboration and assistance to all stakeholders • Novel systemic R&D framework for accelerated advanced material development and integration, including improved data-curation and standardization methodologies • Deeper research acumen on systemic approach among ECIs as future leaders of advanced materials R&D *and* among senior researchers for faster adaptation of digital & automation tools in the widest EU regions
Technological (& Industry)	

EU leadership in low-carbon energy technology and innovation market
 	
(short-mid-long)
	• Faster innovation timeline via unification of digital and materials competency (including safe & sustainability by design tools) with reduced cost-to-market
	• Contribute to EU's twin green & digital transition
	• Reinforce EU industrial leadership in strategic energy technologies
	• Increased capacity for low-carbon energy production based on new technologies (mid-term) Examples:
	  ◦ **Perovskites**: accelerated <u>*PV-cell*</u> uptake (via existing supply chain). 20% higher efficiency w/r/t Si-cells. <u>*Thermochemical air separation*</u> with 40% less energy demand w/r/t state-of-the-art cryogenic distillation
	  ◦ **Metallic alloys**: reduced reliance on rare elements in High Entropy Alloys (HEA) and superalloys (HESAs) without performance compromise. Extended maximum operational temperatures by hundreds of K and/or lifetime by several tens of %.

Socioeconomic	
EU Green-Deal and Improved EU autonomy & Resilience	• Reduced environmental footprint (safe & sustainable) • Job creations in key energy and materials industries • Safeguard EU autonomy by reducing the reliance on critical materials • Mitigate regulatory constraints across wider EU regions

3.2. MEASURES TO MAXIMISE IMPACT

3.2.1. KNOWLEDGE CREATION, TRANSFER OF KNOWLEDGE AND CAREER DEVELOPMENT

Knowledge creation & transfer

EU-MACE gathers expert skills, resources and visions from a network of specialists pertaining to the entire value chain of advanced materials development and their integration into renewable energy applications, focusing on three pilot materials (see WGs 1-2-3). New knowledge will arise from the discussions in the WG meetings, short-term visits, workshops and dissemination events organized throughout the Action involving both internal and external stakeholders. The knowledge created by the

Action will be used to define the strategic guidance for a systemic research approach that will serve as the basis of a future *EU center of excellence on advanced materials for energy*.

Bottom-up knowledge: Creating new, and/or enriching existing data and knowledge-bases by contributions from individual research groups (materials data, synthesis & characterization techniques, numerical methods, theoretical models, etc.) will improve the AI-assisted materials design, automated characterization schemes and the result interpretation and optimization of MAPs. In return, the individual researchers will gain access to large-scale MAPs, thus acquire the operational knowhow of such research infrastructures. In addition, researchers will be able to enrich their skills with new ones, which can be technical and related to the use of new infrastructures, but also organizational skills associated with new concepts to drive research in material science.

Horizontal knowledge: Interactions between existing MAPs participants will give rise to coordinated research dynamics (e.g., metadata standardization) around common pilot materials for multiple renewable energy applications, leading to the creation of *new* international MAP initiatives.

Technology push vs. market & society pull: New collaborations between materials scientists with data-scientists, device developers (including digital-twin expertise), manufacturers and techno-economic and socio-economic experts will accelerate the advanced materials integration into viable and sustainable renewable energy technologies. The direct involvement of companies and industrial associations (not yet members) will provide a discussion arena for researchers and industries to jointly examine the state-of-the-art materials performance and development processes (technology push) against the technical limitations of existing technologies and the bottlenecks in the scale-up manufacturing processes (market pull). The constraints associated with intellectual property rights and confidential business information can also be scrutinized, defining a legal framework for IPR co-ownership.

Trans-national education programmes: One of the objectives associated with the implementation of EU-MACE is to create the appropriate scientific and academic environment for the setting up of an ERASMUS-Mundus type master project related to the accelerated and innovative design of materials for energy. The emergence of this project is realistic insofar as several partners of this COST project have a strong university anchoring. In addition, the EU-MACE network aims to federate academic and industrial actors on material issues related to the energy production technologies of the future. In order to carry out research within these institutions, it is crucial to build up a pool of young scientists whose academic skills will be both specialized and transverse in order to be able to grasp all the facets of research in materials science with the modern tools of "artificial intelligence" and "big data". Within the framework of this project, the Action also wishes to consider societal issues related to the energy transition, which is at the heart of the Action and which will also be a major theme of the master's degree program to be carried out in the future. From a practical point of view, the seminars and workshops to be held among the different partners of the Action network should help us to define more precisely the core of universities that will carry this ERASMUS program, the typical second year courses and the industrial and institutional partners likely to contribute to the training of the students.

Transfer to public: The Action will establish, and continuously update an open-access materials' expert database with information on research groups involved in MAPs, data repositories that ensure FAIR, security, and TRUST standards of data access, rendering the use and interoperability possible across the EU and beyond. Additionally, the course materials and workshop presentations will be made freely accessible on the Action website.

Career development

Through proactive participation in the management tasks, ECIs will acquire a wide set of skills and experience for their future career in science & technology research and management; e.g., developing new research projects, proposal preparation, event organization and the operation of international networks, to name a few. The direct interactions (STMSs, WG meetings and workshop attendances) with MAPs and industries, as well as the training courses (soft-skills, entrepreneurship, social science, data science, etc.) will deepen their research acumen, providing a clear understanding of the interconnection between the different stages of materials research and its relation to the societal challenge. It should be remarked, however, that a large number of senior researchers are still unfamiliar with the SDL operation schemes in Europe today, and the notion of 'systemic research approach' also remains abstract to many, regardless of their age-groups. EU-MACE, through its interdisciplinary and inter-sectoral network will thus provide continued growth (further education) opportunities to all generations of researchers and investigators.

3.2.2. PLAN FOR DISSEMINATION AND/OR EXPLOITATION AND DIALOGUE WITH THE GENERAL PUBLIC OR POLICY

The Action logo, website, dissemination materials, media tool-kit (introductory video, mission statement, etc.) and contents will be designed to clearly reflect our Action identity; *i.e.*, to create a new systemic research approach for accelerated integration of advanced materials for clean energy applications. The Action's results and progress will be disseminated to various stakeholders using appropriate channels (see Table 3.1), overseen by the Communication & Dissemination team (see Implementation section). The target audience outside the Action includes international research communities, students and educators (including undergraduate university levels), EU and national energy communities, industry associations and technology clusters, professional boards, policymakers, regulatory and standardisation bodies, and the public. (See 2.1.1. for key stakeholders identified).

The website, and different social network service (SNS) accounts will be set up and running within the first 6 months. Multiple SNS platforms will be used, each intended for specific target groups. Twitter will be used for quick public announcements (e.g., Workshops or Training courses, participant's publications) while LinkedIn will focus more on exchange opportunities. YouTube channel will store tutorial materials and recorded seminars from workshops and bilateral presentations, suitable for students as well as industrial audiences. The use of a virtual reality SN platform (Metaverse) will also be considered for introducing immersive experience on various simulation methodologies used in the materials development and integration processes by the network members (target audience, students). Other dissemination media include a regular e-news (with e-mail alerts) posted on the Action webpage and press releases (communicating main achievements). The Action website will have both public and restricted areas; the latter will be used for internal communications and as an information repository for the Participants with contents such as Task calendar, meeting minutes and internal reports.

Finally, the scientific and methodological outcomes resulting from new collaborations among the Action members will be accessible to a wider community of researchers through conferences and journals articles and on Action media outlets.

Stakeholder group	*Materials/activities*	*KPI (TND: target not defined)*
Action Participants	i. Kick-off meeting ii. WG meetings iii. Action meetings iv. Training Schools v. Workshops vi. Final meeting (open) vii. Members' only website	i. 50 participants ii. 4/WG/year iii. 1/year iv. 3 (every 18 months) v. 3 (every 18 months) vi. 100 participants vii. TND (internal communications)
Researchers	i. Expert and MAP/SDL lists (Open access) ii. Training schools iii. Workshops iv. Review reports v. Roadmap papers vi. Journal & conference articles	i. > 200 (experts), > 50 (platforms & repositories ii. See above iii. See above iv. 1/WG/year v. 2 (mid-term and final) vi. 1/Participant/year
Students & teachers	i. Tutorial material (Web, MOOC, FuseSchool, etc.) ii. Training schools iii. Seminar recordings iv. Twitter/Meta	i. TND ii. Concurrent with workshops iii. Concurrent with training schools iv. TND
Ind. Associations, EU energy communities, Sci. societies	i. Expert and MAP/SDL lists (Open access) ii. Workshops/seminars iii. Conf. presentations iv. B2B matchmaking v. LinkedIn/Twitter	i. See above ii. See above iii. 1/WG/year iv. TND v. TND
Policymakers, regulatory bodies	vi. Roadmap papers vii. Action presentation meetings (incl. bilateral events)	vi. See above vii. Twice/year
General public & All	i. Web page ii. YouTube (TikTok) iii. Twitter/Meta iv. Popular science events v. e-news vi. Press-releases	i. Unique visits: 2000 ii. 1 post/WG/trimester 1000 views iii. TND iv. > 1/WG/year v. 1/trimester vi. TND

4. IMPLEMENTATION

4.1. COHERENCE AND EFFECTIVENESS OF THE WORK PLAN

4.1.1. DESCRIPTION OF WORKING GROUPS, TASKS AND ACTIVITIES

The Action Work Plan will be organized through five working groups (WGs), three of which are devoted to specific class of materials (**WG1:Perovskites, WG2: Metallic Alloys** and **WG3: New materials**) and two are on overarching activities; *i.e.*, **WG4: Training** and **WG5: Dissemination & Communication** (see Fig. 4.1). The Action Management Committee (**MC**) is responsible for the coordination, implementation and management of all Action activities and for appropriate grant allocation to achieve the Actions' objectives. Following the COST rules, WG leaders (**WGL**) and Core Group (**CG**) members will be elected at the first Kick-off meeting. To facilitate the work of the MC, the daily coordination work of the Action will be performed by a CG that includes: **Action Chair**, **Action Vice-Chair**, **WGs Leaders** and other action coordination positions such as the **STSM Grant coordinator**, **ITC Conference Grant coordinator, Training Programme coordinator** and **Science Communication coordinator**. A dedicated committee will be set up to assist the coordination of each action. The gender and generation balance as well as fair representation of ITC/ non-ITC countries will be used as nomination criteria for all leadership positions.

EU-MACE's objective is to establish a winning strategy for digitally-assisted fast-track advanced materials and technology development (from material discovery to device integration) that is applicable to all types of functional materials. As such, many 'Goals' (G1 through G3) and 'Tasks' (T1 through T5) are common to all technical WGs as depicted in Fig 4.1. It is of at most importance that the task results are shared between WGs through joint meetings.

WG1/2/3 Common Tasks:

T1: Expert & SDL/MAP mapping: The compiled list of experts, existing materials acceleration and self-driving lab platforms (see §2.1) needs to be updated as new initiatives and projects are created in EU member states and elsewhere.

T2: Material integration framework: The complementarity of existing MAPs and missing links toward technology integration (see §1.1.2 & 1.2.1) will be identified. Liaising with experts with required knowledge, leading to the creation of *new* as well as *multi-MAP* and *multi-user* platforms with an added capacity of device integration.

T3: SSbD implementation: The integration scheme of social science perspectives (life-cycle, circular economy, environmental, social acceptance) both in the early concept stages of materials development and in the device manufacturing phase will be studied.

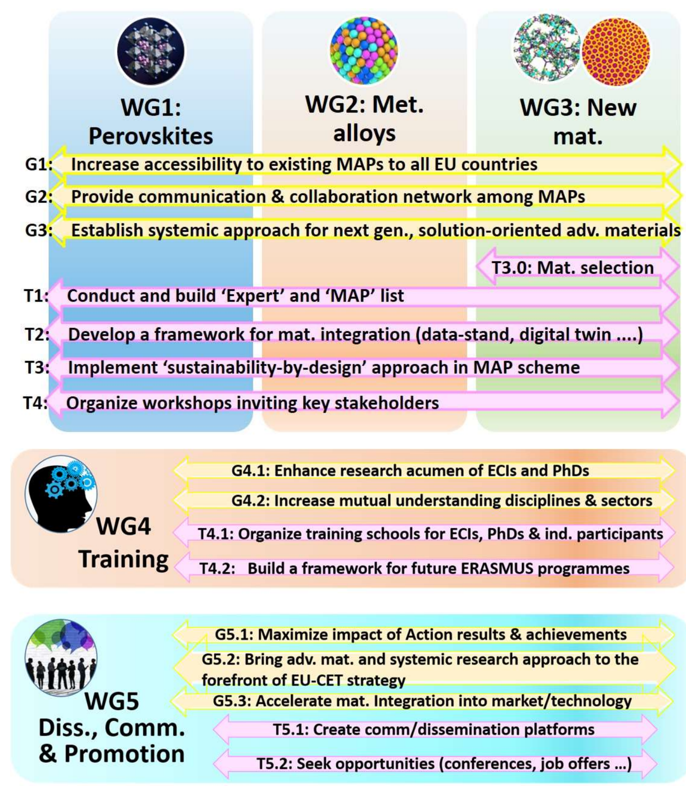


Figure 4.1: WG organization and interactions

T5: Interdisciplinary Workshop organizations. One/year covering at least 2 WGs. A 2.5 day event will consist of 'technical sessions' showcasing individual research groups' work, presentation of existing MAP/SDL initiatives, round-table discussions on 'future MAP' concepts. Key stakeholders (§ 2.2, 3.2.2) will be invited to these events. WGLs will coordinate with the Training Prog. coordinator for the construction of training courses (T 4.2).

The MC members will **select new functional material** (**T3.0**) as the Action's 3rd pilot material (WG3) based on the application potential as well as on the evolution of available research initiatives (*cf* § 1.2.1).

WG4 Task (over seen by Training Programme coordinator)

T4.1: Training courses for ECIs, PhDs and Masters' students will be held during the annual workshop event. These courses will focus on the transversal skills; metadata management, digital twins and device building, industrial level scale-up production, sustainability-by-design, national policy, *etc.* All courses will be made available on-line (open science) and made into tutorial videos accessible by the public. The final EU-MACE Conference will consist in an open wrap-up event to present the Action's main achievements and a roadmap (white paper) dealing with an efficient structure and operational scheme for the future centre of excellence on advanced materials for energy.

T4.2: Academic partners will hold round-table discussion on future ERASMUS programme topics that reflect EU-MACE's systemic research approach for materials R&D&I.

WG5 Tasks (overseen by Science Communication coordinator):

T5.1: Create and maintain website, social network accounts. Prepare dissemination materials (factsheets, review papers, technical notes, and educational material). B2B matchmaking platform. The web-platform will be used for e-newsletter (on website), research roadmap (W1-3), tutorial videos (from T4.1: training schools), and workshop presentations.

T5.2: External conferences, summer schools, internship and job opportunities will be compiled (website's members area) as a part of career development plan. Funding/cooperation opportunities (e.g., Horizon-EU calls) will be included in the database to assist members in designing new collaborative research projects.

The following tasks/activities encompassing all WGs are overseen by the MC & CG members.

MC/CG meetings (2/year): Progress monitoring based on the reports from WGs and organise network activities for the next period, ensuring implementation of COST policies, approval of participation of additional institutions from either COST or non-COST countries and management of the network budget. Additionally, identification of European and national funding and developing consortia to apply for funding for new research projects is envisaged.

Short-Term Scientific Missions (STSM): STSM (target 10/year) will allow *new* collaborations to be fostered among the Action members. Training in new techniques will be fostered and access to equipment not available in network affiliates home institutions. An STSM committee will assess applications and supported applicants will have travel and subsistence costs of their visit covered by the network. Priority will be given to ECIs and PhD students. Very short-term missions will be provided to senior researchers with transversal visions (see §1.2.2.2 under Continued Growth)

Inclusiveness Target Countries Conference grants (ITC-CG): Grants to support conference attendance of PhD students and ECIs from ITC countries. Some conditions apply, such as the adequacy of presentation (oral or poster) contents with respect to the Action objectives, the notoriety of the event, etc. Approval will be given by the ITC-CG panel and will cover expenses related to the conference.

Administrative and organizational support: The MC and CG institutions from member countries will provide support to WGLs for workshop organization on logistics (venue selection, payment procedure, etc.) and on the technical contents (invited speaker selections, programme definition, etc.)

4.1.2. DESCRIPTION OF DELIVERABLES AND TIMEFRAME

Deliverable and description ("DT.#" are transversal deliverables coordinated by the CG/MC; while "D1.#", "D2.#", "D3.#"and "D4.#" are related to WGs 1 to 4)		**Year**	**QTR**
DT1	Experts & MAP (incl. similar structures, data repositories, etc.) lists - updated yearly.	1	2
DT2	Position paper based on Action results (WG actions, bilateral meetings, workshops, STSMs etc.) – updated yearly.	1	4
DT3	Roadmap on advanced materials development & integration in renewable energy sector (final version in year 4). Includes subsections dedicated to specific materials	2	4
D3.1	Selection of 3rd pilot materials (Task 3.0)	1	3
D4.1	Publication of training course materials and tutorial videos - 3 months after each workshop/training school organization	2	2
D4.2	Report on future ERASMUS programme scheme	4	4
D5.1	Action logo, website (public and members' only) and social networks accounts available – updated regularly with news, summaries, demos, announcements	1	2

D5.2	B2B platform for matchmaking between industry/research, researcher/SDL, etc.	2	4
D5.3	Dissemination actions - continuous	1-4	Cont.

4.1.3. RISK ANALYSIS AND CONTINGENCY PLANS

Risk Description	***Contingency Plan***
Delay in WGs' tasks, deliverables, or milestones (L)	Redistribution of WG tasks and revision of associated Action timeline (for +3 months delay). All WG Participants provide help to the WG leaders. The MC will provide support, replace inactive WG leaders in her/his coordination tasks. If necessary, find new participants to the Action.
Partners are unable to organise planned events or events delayed (M)	For +2 months delays, local organisers will report to the MC to find solutions to limit the delay within 3 months. The MC may reschedule/reallocate the event at another Participant's site.
Difficulty of identifying or inviting experts with necessary skills for advancing EU-MACE objectives (L)	MC & CG members will seek and solicit non-EU experts with required skills. Active search of interested new partners will be frequently encouraged by the Action chair and CG
Inaction or limited interactions in WGs (L)	MC and WG leaders will cooperate to define common objectives (scientific, technology or training) to stimulate STSMs. Follow-up actions from this STSMs will be required for consolidating the achieved advances.
New MAP or similar projects & platforms pursued by groups outside Action (M)	MC will monitor the evolution of new research trends, and integrate the representatives from such new projects & platforms into our Action

4.1.4. GANTT DIAGRAM

References

1. “MATERIALS 2030 MANIFESTO” Advanced Materials 2030 Initiative, 2022,https://www.ami2030.eu/wp-content/uploads/2022/06/advanced-materials-2030-manifesto-Published-on-7-Feb-2022.pdf

2. “Assessing Emerging Technologies—Methodological Challenges and the Case of Nanotechnologies” T. Fleischer, et al., Technol. Forecast. Soc. Change 2005, 72 (9), 1112, https://doi.org/10.1016/j.techfore.2004.10.005

3. “The Matter Simulation (R)evolution,” A. Aspuru-Guzik et al., ACS Cent. Sci. 2018, 4 (2), doi: 10.1021/acscentsci.7b00550.

4. “The Role of Machine Learning in the Understanding and Design of Materials” S. Moosavi, et al., J. Am. Chem. Soc. 2020, 142 (48), 20273–20287 doi: 10.1021/jacs.0c09105.

5. “The evolution of Materials Acceleration Platforms: toward the laboratory of the future with AMANDA,” J. Wagner et al., J. Mater. Sci. 2021, 56 (29), 16422–16446, doi: 10.1007/s10853-021-06281-7.

6. “Materials Acceleration Platforms: On the way to autonomous experimentation,” M. M. Flores Leonar et al., Curr. Opin. Green Sustain. Chem. 2020, 25, 100370, doi: 10.1016/j.cogsc.2020.100370.

7. “Accelerating materials discovery using machine learning,” Y. Juan, et al. J. Mater. Sci. Technol. 2021, 79, 178–190, doi: 10.1016/j.jmst.2020.12.010.

8. “Progress and prospects for accelerating materials science with automated and autonomous workflows,” H. S. Stein and J. M. Gregoire, Chem. Sci., 2019, 10 (42) 9640–9649, doi: 10.1039/C9SC03766G.

9. “Brokering between tenants for an international materials acceleration platform,” M. Vogler et al., 2022, preprint, doi: 10.26434/chemrxiv-2022-grgrd.

10. “The Digital Twin Technology and Its Role in Manufacturing” V. S. Magomadov, IOP Conf. Ser. Mater. Sci. Eng. 2020, 862 (3), 032080. https://doi.org/10.1088/1757-899X/862/3/032080.

11. “e-Design: Computer-Aided Engineering Design” K.-H. Chang, Academic Press, 2016, http://booksite.elsevier.com/9780123820389.

12. “Opportunities for machine learning to accelerate halide-perovskite commercialization and scale-up,” R. E. Kumar, et al., Matter, 2022, 5 (5) 1353, doi: 10.1016/j.matt.2022.04.016.

13. “The Perovskite Database Project: A Perspective on Collective Data Sharing,” E. Unger and T. J. Jacobsson, ACS Energy Lett., 2022, 7 (3), 1240, doi:10.1021/acsenergylett.2c00330.

14. “Robot-Accelerated Perovskite Investigation and Discovery | Chemistry of Materials.” https://pubs.acs.org/doi/10.1021/acs.chemmater.0c01153?ref=pdf.

15. “High-entropy alloys,” E. P. George, D. Raabe, and R. O. Ritchie, Nat. Rev. Mater., 2019, 4 (8), 8, doi: 10.1038/s41578-019-0121-4.

16. “New multiphase compositionally complex alloys driven by the high entropy alloy approach,” A. M. Manzoni and U. Glatzel, 2019, Mater. Charact., 147, 512, doi:10.1016/j.matchar.2018.06.036.

17. “Digital twin in energy industry: Proposed robust digital twin for power plant and other complex capital intensive large engineering systems,” A. K. Sleiti, J. S. Kapat, and L. Vesely, Energy Rep., 2022, 8, p3704, doi: 10.1016/j.egyr.2022.02.305.

18. “Metrics-based dynamic product sustainability performance evaluation for advancing the circular economy,” B. M. Hapuwatte, K et al., J. Manuf. Syst., 2022, 64, p275, doi:10.1016/j.jmsy.2022.06.013.

19. “LCA Compendium—The Complete World of Life Cycle Assessment” Series ed. W. Klöpffer and M. A. Curran, SpringerLink, https://link.springer.com/article/10.1007/s11367-016-1041-9.

20. “Comparing the European Commission product environmental footprint method with other environmental accounting methods,” S. Manfredi et al., Int. J. Life Cycle Assess., 2015, 20 (3), 389, doi:10.1007/s11367-014-0839-6.

21. “Nanosafety research in Europe – Towards a focus on nano-enabled products,” V. Pomar-Portillo, et al.,NanoImpact, 2021, 22, 100323, doi: 10.1016/j.impact.2021.100323.