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TECHNICAL ANNEX

# S&T EXCELLENCE

## Soundness of the Challenge

### DESCRIPTION OF THE STATE OF THE ART

*Summary: Advanced 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 strong materials innovation ecosystem for driving the clean energy transition. In response, self-driving laboratories (SDL) (also known as 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 the 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 of technology challenge. 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. To this end, EU-MACE will become an ecosystem aiming to accelerate materials development at the user end, gathering researchers and stakeholders well-versed in the state-of-the-art digital and material competences combined with market/social pull. Our inclusive & systemic approach will lay the foundation for future center of excellence for advanced functional materials to assist transition toward a united and stronger EU. (this paragraph will be moved to summary section outside the Annex)*

Innovation in the clean energy technology sector critically depends on rapid materials breakthroughs[[1]](#footnote-2). However, the historically 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 future labs; namely, self-driving laboratories (SDLs) (also termed ‘Materials Acceleration Platforms (MAPs)’ for SDLs applied to materials) 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 (by how much?). Several multidisciplinary initiatives with participations from academia, governments, and industry have been formed in recent years; including, [Materials Genome Initiative](https://www.mgi.gov/) (USA), [BIG-MAP of Battery 2030+](https://battery2030.eu/battery2030/projects/big-map/) (EU-H2020), [German-Canadian Materials Acceleration Centre](https://gcmac.ca/) (GC-MAC), [DIADEM](https://www.cnrs.fr/en/diadem-exploratory-priority-research-programme-and-infrastructure-linking-materials-and-ai) initiatives (France) and Accelerated Materials Development for Manufacturing , [AMDM](https://www.a-star.edu.sg/imre/research-departments/electronic-materials-department/accelerated-materials-development-for-manufacturing-(amdm);%20https:/www.youtube.com/watch?v=s2zwBUVriKU&list=PLGVe6BxyFHNVt9kAJpMRHE5MpUMZOypF3&index=25) (Singapore) to name a few (see Figure 2.1 in §2.1.1 for current map of MAPs), focusing mostly on organic PV materials, catalytic materials and “beyond Li” battery materials. PLEASE GIVE ONE MORE SPECIFIC EXAMPLE OF (nonEU) MAP SUCCESS STORY!

Waiting: input on digital-twin description & verification on SSbD

In order to bring rupture (energy) technology, these newly developed, highly functional materials must be shaped into *components* and then integrated into *devices* with a minimum loss of performance at each step. eDesign and Digital-Twin technologies are powerful computer-aided tools 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 implementation of product design in a virtual environment by including optimisation methods. This is often accompanied by rapid prototyping techniques (e.g., additive manufacturing) for design verification. eDesign thus supports the development of (new) materials and products from their early stage by predicting and analysing not only their efficiency and reliability but also their manufacturability (including cost evaluations) before entering the production phase. The methods for carrying out quantitative assessment of trade-offs for decision making are established and are widely used in engineering/research labs as well as in industrial environment. Digital twin adds ‘connectivity’ dimension to eDesign. 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. Then the digital twin is tested virtually (simulation) for accurately predicting the operational limits without pushing the prototype to its breaking point. This allows the early identification of operational bottlenecks, constraints and weak points, and reduces the amount of both time and cost required in the device design phase.

Equally important, any given new technology (materials, products and processes) must satisfy the safety and sustainability conditions before it can be considered for commercialisation. Indeed, a number industrial, environmental, climate and energy priorities are proposed in the EU’s new action plan for the circular economy (CEAP) and in the European industrial strategy, calling for Safe-and-Sustainable-by-Design approach (SSbD). The SSbD concept integrates safety, circularity, energy efficiency and functionality of materials, products, and processes throughout their life cycle in order to minimize the environmental footprint. 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, overcoming the fragmentation of functional materials and technology development stages described above. A systemic research approach proposed here is applicable to all advanced materials responding to the clean energy transition challenges.

Should we evoke the geographical disparity and United-EU inclusiveness here? Should we emphasize more that we build methodology and not a technology itself?

### DESCRIPTION OF THE CHALLENGE (MAIN AIM)

From solar modules to advanced batteries and energy efficient buildings, advanced materials offer solutions to much of low-carbon technologies and simultaneously provide high-quality job opportunities to researchers, innovators and manufacturers. However, advanced materials occupy the dominant share of the cost of technologies. Therefore, accelerating the innovation in advanced materials holds the key to achieving ‘Climate neutral’ Europe, *i.e.*, the EU Green Deal (EUGD). The EUGD’s overarching goals (net-zero greenhouse gas emission by 2050, economic growth and no person and no place left behind) calls for a ***systemic approach to accelerate the development (a better word?) solution-oriented low-carbon technologies based on functional materials***. This implies streamlining the connections between different phases of the innovation/value chain from ‘bottom-up research and technology’ push to ‘market-pull’ guided by the societal needs. The SDLs/MAPs described above is clearly a big step in the right direction accelerating materials discovery and screening. But how can we integrate these autonomous labs and platforms into the larger process of technology and value creation? Who are the key stakeholders and what role do they play? And how to organize 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, we will demonstrate a model ecosystem addressing specifically; **EU-Inclusiveness**: Creating gateways to SDLs/MAPs for the widest EU research communities and accessing relevant knowledge base of the latter (data, experimental & numerical techniques; theories, etc.). **Accelerated device integration by unifying digital and materials competency** (Horizontal link, Interrelation.. better word?): 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 and socio-economic impacts.

The building and the operation of SDLs and MAPs are costly both in financial and human terms. For example, Canada has invested 75 M€ to build and operate which MAPs (how many? Yearly investment?). 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 methodical (incl. *programming what else?*) skills, expertise in *robotics* and the *domain knowledge in the energy materials* of interest (@Holger @Kourosh, did I understand this correctly?) 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 facile access to all users. The coupling of experimental and computational data for materials design and screening requires the development of common ontology, interoperability and visualisation/analysis tools (FAIR principle). Several large-scale initiatives on *Open Source* repository for materials data exist (Materials Genome Initiative, MaterialsMine and another example from Japan?). It is of the highest importance to join force with the existing platforms and to gain expert knowhow on handling data assembly and informatics applied to the high dimensional problems inherent in multi-functional materials (due to their multi-phased nature and complex structures).

As described in the previous section, 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 of accelerated discovery, all modelling and characterization tools needs to be mapping to a particular technology space. Integrating energy materials requires these bespoke processes to be well aligned (@Kourosh changed from “integrated.” Is it ok?) 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 (need to mention tools and procedures; e.g., digital twin, eDesign, baseline processing definition… is this the good place?) 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 semi-automated labs and the materials acceleration platforms 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” future labs concept has found little traction advanced materials integration, where multiple functional properties need to be optimized, 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* (e.g., FINALE project from BIG-MAP for Li-ion batteries) are needed to overcome this difficulty. (comment: We chose perovskites and metallic alloys thus the electrochemical energy conversion example appears at odds.)Therefore, the “closed-loop” future labs concept has found little traction in the field of electrochemical energy conversion and storage, encompassing hydrogen fuel cells and electrolysis cells. This is mainly due to the fact that electrochemical devices are multilayer assemblies, with each layer having to provide a complex array of properties and functions.

**@SSbD core group**: Insert specific challenges for implementing or merging “safety & sustainability by design” approach and tools into the digital and/or automation scheme of accelerated technology based on functional materials. Possible elements listed below.

- The availability of skilled workers able to correctly use LCSA tools (choosing the right tools for right technology and territorial considerations, and the correct interpretation of the analysis results) is below market demand (identification of experts for each class of material and target technology. Appropriate matchmaking).

- Lack of common understanding (Educational/training programmes including recent advancements concerning Safety & Sustainability assessment and management to address this issue).

- Fragmentation of LCSA analysis tools and databases (within the scope of EU-MACE? i.e., networking and discussion among LCSA specialists to set harmonization path?)

Combined together, EU-MACE will set an example of future ecosystem leading fast-track discovery, development and integration of advanced material into technology in key innovation markets for assisting the EU’s transition into sustainable and autonomous society.

## Progress beyond the state-of-the-art

### APPROACH TO THE CHALLENGE AND PROGRESS BEYOND THE STATE OF THE ART

General Approach: Creation a new holistic R& D&I scheme by joining forces of the state-of-the art SDL platforms, the widest pool of materials data, synthesis and characterization techniques, theories, digital skills and SSbD tools for accelerating the integration beyond materials discovery…. This calls for coordinated multidisciplinary efforts from physics to material science, engineering at different levels and to social science… (fix).

|  |  |
| --- | --- |
| **EU-Inclusiveness**: 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 ***accessing relevant knowledge base 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.*** | Figure 1.1: Approach to the Challenge |

**Accelerated device integration by unifying digital and materials competency (Increasing SDLs capacities via horizontal collaborations (interrelations))** As more initiatives are created at national and institutional levels across EU, the communications between the platforms become crucial for optimizing the operation of each and avoiding the unnecessary duplications. The bespoke high-dimensionality of multi-functional energy materials also complicates the simultaneous qualification of multiple properties using one MAP/SDLs (see section above for more explanation). Mutualisation of data and results, sharing of experimental and simulation methodologies and interpretation/analysis/decision making tools should lead to defining the best-practices for coordinated network of MAP/SDL platforms. To serve as a collaborative incubation center 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 to last beyond the Action lifetime. Particular attention will be given to bringing in the missing (?) 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 skill, LCSA, etc., within and outside the Action) will be assessed at the beginning of the Action for promoting synergies among Participants. (need to give specific examples of numerical tools, software?) 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***.

**Market/society pull**: Upstream integration of advanced materials into functioning devices and scale-up production taking into account the performance (efficiency) requirements, but also the techno-economic and socio-economic impacts. Site visits, STSMs, workshops, training courses, 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. Need more elements on this branch of networking approach + progress beyond the state of the art… to be added later. All suggestions welcome!)

To put bespoke collaboration/cooperation approach into practice, 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 ABO3-δ. 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 stabilize 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* 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 O2/N2 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 (or none? If there are, which?). 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 (e.g. thermochemical cycles for ammonia production). (from Dorottya).

2. Metallic alloys (Dario & Pekka) – waiting for inputs

3. New mutli-functional material will be chosen within the first year of the Action. We give ourselves this flexibility in the 3rd materials choice because of fast evolving nature of the energy materials research and technology sector. At present, the candidate materials include: organic polymers (for which applications?), MOFs (for which applications?) and complex fluids (such as ionic liquids and nanofluids for tribology, electrochemical energy storage, and whatelse???). – list their potential applications and their long-term impacts in reducing CET & other characteristics.

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 foster collaborative, open and systemic research approach, which can greatly help create international platforms as we envision in EU-MACE. By combining responsible design principle with digital-assisted advanced materials production platforms and industrial technologies we can hope to bring the twin green and digital transitions in to reality.

### Objectives

#### 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 key stakeholder contacts (scientific, industrial and civil societies) what else to include? the world promoting the exchange, knowledge-gap bridging and accelerated the development and integration of advanced materials. How to introduce ‘inclusiveness’ here?

**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, requiring minimum maintenance efforts such that it stays 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, xxx add more examples) 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 opportunity 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 truly systemic approach to advanced material development and integration. The ***conclusions will be published as a roadmap to serve as a model 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 are planned 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, pro-active participation in local popular science events (e.g., night of researchers, pint of science, Fête des Sciences, etc.).

#### 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, we count XX % of ECI and 15% of female members among the secondary proposers. The proportion of ECI will be increased to 40% (minimum target) by the Kick-off meeting. While *basic* materials science research can be assumed to be free from gender-bias, any extension to application and market opportunities should include a ‘gender lens’ in the decision making processes to ensure, or 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, minimum 25% (50%) of MC positions will be attributed to ECI (female) members in the management committee and in WG task-leader positions.

**Future generation preparedness**. We promote the active participation of ECI 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 an important aspect. The proposed training courses (see WG4) 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.

**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 opened (up to 10% of attendees). Such opportunities will increase the acceptance-rate of ‘new’ methodologies and collaboration scheme, and speed up the implementation of SDL/MAP-like platforms across the EU territory.

**Trans-national Education Programme Incubation**. It is desirable that the building up a pool of young scientists whose academic skills will be both specialized and transverse to grasp all the facets of advanced materials development to start before the students choose their respective PhD research subjects (okay, need to rephrase this). Here, the Action will serve as an incubator for international education programmes such as ERASMUS-Mundus master project (see §3.2.1 for more detail). The workshops and seminars planned among the different partners of the Action network will guide define more precisely the core of universities that will carry such international programmes.

# NETWORKING EXCELLENCE

## Added value of networking in S&T Excellence

### ADDED VALUE In relation to existing efforts at European and/or international level

The below cartography shows the major MAP/SDL like (and Data-repositories?) initiatives across EU today. The geographical distribution inequality is clear. The first added value EU-MACE network is thus the inclusions of research groups from regions where MAP-like 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.

|  |  |
| --- | --- |
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The added dimension in terms of material types, and application domains are summarized in Table 3.1 below

**Suggested Table format. Showing on which materials and applications the existing MAPs work on, compared to EU-MACE participants expertise/research focus. add more apps/mat and Turn the table by Pi/2…? Wait for everyone’s contribution reconsider presentation format to include non-MAPable fields: sustainability, energy systems, etc.**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Appl. Focus  **→** | Solar cell | | Energy storage | | structure | | sustainability | | Energy systems | | Device/products | | | Scale-up manuf. | | |
| Material  **↓** | MAP | EU-MACE | MAP | EU-MACE | MAP | EU-MACE | MAP | EU-MACE | MAP |  | | existing | EU-MACE | | existing | EU-MACE | |
| Perovskites\* | 3 | 12 |  |  |  |  |  |  |  |  | |  |  | | 2 | 1 | |
| CC alloys |  |  | 1 | 5 | 3 | 4 | 0 | 10 |  |  | | 2 | 5 | |  |  | |
| Organic pol. | 5 | 3 |  |  |  |  |  |  |  |  | |  |  | |  |  | |
| xxx |  |  |  |  |  |  |  |  |  |  | |  |  | |  |  | |
| MOF |  |  |  |  |  |  |  |  |  |  | |  |  | |  |  | |
| Complex fluids |  |  |  |  |  |  |  |  |  |  | |  |  | | 0 | 1 | |
|  |  |  |  |  |  |  |  |  |  |  | |  |  | |  |  | |

\*Includes metallic halide perovskites

The international ‘coordination’ actions/projects (COST-Action and Horizon 2020/EU CSA projects) on advanced (energy) materials development with whom EU-MACE plans to liaise include:

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). Are there more?

CSA (on-going): STORIES (spell, + 1line description), SUNER-C (accelerate innovation on solar fuels and chemicals) and what else?.

International research, industrial and expert associations and societies with relevant member expertise and shared interests with EU-MACE are numerous: The examples are, 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), European Materials Research Society (E-MRS), European Technology Platform for Advanced Engineering Materials and Technologies (EuMaT) European Multifunctional Materials Institute (EMMI), European Material Modelling Council (EMMC)

Representatives from bespoke EU platforms, projects, associations and societies are already included in the EU-MACE (breach of anonymity?) and many others have been informed. Several non-EU structures have been notified of EU-MACE initiative. 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 (deliverable D1.2) will be the first occasion to invite, external partners with whom we will create synergies and expand our .

@must add societies, networks, CSA’s on SSbD, social science, environmental science, etc. on materials and energy technologies here

## ADDED VALUE OF NETWORKING IN IMPACT

### 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 29 research groups and 3 industrial partners across 16 countries (8 ITCs). Over 40% of proposers are female and 10 (9?) ECIs. 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 (scale-up manufacturing, data management (Dorottya, is this ok?) and device design) is ~10% in the starting network composition, for which targeted dissemination & exploitation activities (3.2.2) are planned to secure critical mass for building a holistic and inclusive network toward technology development. The innovation uptake and technology deployment, however, hinges more heavily on 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.

### 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 consisting the core of EU-MACE actions with equitable representations of gender, generation and regional. Scientific (includes social sciences) societies and EU research communities related 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 hosting STSM of ECIs are planned. 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 general Kick-off meeting, workshops and bilateral events throughout the Action. Roadmap papers to be produced, will be the culmination of results from WGs and interactions among all stakeholders, aiming to support new policies for creating future center of excellence for advanced materials for energy (not necessary?).

Lastly, several material acceleration and data-repository platforms have been identified potential collaborators of EU-MACE (North America and Asia). The representatives will be invited to join our Action after the official approval by the MC. Such international collaboration will allow us to increase the impact of the Action’s outcomes, and gain access to a diverse pool of expertise across research institutions, academia, and industry from these countries.

# IMPACT

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

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

Impacts will be summarized in the table below. For text, see previous version Table 3.1 to be completed

|  |  |
| --- | --- |
| ***Impact*** | ***Potential for innovation/Breakthroughs*** |
| Scientific | |
| New and improved data procuration and standardization methodologies |  |
| Roadmap for improved advanced material development and integration schemes | Sustainability, too. |
| Inclusive collaborative knowledge platform | Open science, equal research access |
| Deeper research acumen for new generation of researchers |  |
| Technological | |
| Improved technology push and market pull |  |
| Environmental |  |
| Socioeconomic | |
| Systemic solution for faster integration of next generation advanced materials for clean energy transition |  |
| EU Autonomy |  |
| United EU |  |

## MEASURES TO MAXIMISE IMPACT

### 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 systemic research approach that will serve as the basis of 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 scheme and the result interpretation and optimization of MAPs. In return, the individual researchers will gain access to large-scale MAPs, 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 relate 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 technology. The direct involvement of companies and industrial associations (not yet members) will provide discussion arenae 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 important 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, we also wish 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 that we plan to carry out in the future. From a practical point of view, the seminars and workshops planned 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 MAPs, data repositories that ensure FAIR, security, and TRUST standards of data access, use and interoperability will be possible across 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 develop 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 network to name a few. The direct interactions (short-term visits, 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, giving a clear understanding of the interconnection between the different stages of materials research and its relation to the societal challenge. We remark, 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.

### 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 new systemic research approach for accelerated integration of advanced materials for clean energy applications. Our results and progress will be disseminated to various stakeholders using appropriate channels (see Table 3.1), overseen by Communication & Dissemination team (see Implementation section). For selected dissemination materials and content productions (e.g., webpage design, promotional video recordings, etc.) a professional services will be used (in principle, this is eligble). The target audience outside the Action includes international research communities, students and teachers (including undergraduate university levels), EU and national energy communities, industry associations and technology clusters, professional boards, policymakers, regulatory and standardisation bodies, and the general public. (See 2.1.1. for key stakeholders identified).

The website, and social media accounts (Twitter and LinkedIn) will be set up and running before the kick-off meeting. Twitter will be used for quick announcements (e.g., Workshops or Training courses, participant’s publications) while LinkedIn will focus more on exchange opportunities. Other dissemination media include a regular e-news (Action updates) posted on the Action webpage and press-releases (communicating main achievements). The Action website will have both public and restricted areas, the latter of which will be used for internal communications and information repository for the Participants such as Task calendar, meeting minutes and internal reports.

The action results and progresses will be accessible to a wider community of researchers through conferences and journals articles published by Participants…. BUT we focus on new research approach rather than science & engineering results, where can we publish our results? We need to be featured by EMIRI, and other international associations! –

|  |  |  |
| --- | --- | --- |
| Stakeholder group | Materials/activities | KPI (TND: target not defined) |
| Action Participants | 1. Kick-off meeting 2. WG meetings 3. Action meetings 4. Training Schools 5. Workshops 6. Final meeting (open) 7. Members’ only website | 1. 50 participants 2. 4/WG/year 3. 1/year 4. 3 (every 18 mos) 5. 3 (every 18 mos) 6. 100 participants 7. TND (internal communications) |
| Researchers | 1. Expert and MAP/SDL lists (Open access) 2. Training schools 3. Workshops 4. Review reports 5. Roadmap papers 6. Journal & conference articles | 1. How many researchers/labs? 2. See above 3. See above 4. 1/WG/year 5. 2 (mid-term and final) 6. 1/Participant/year? |
| Students & teachers | 1. Tutorial material (Open Access) 2. Training schools 3. Seminar recordings |  |
| Ind. Associations, EU energy communities, Sci. societies who else ? | 1. Expert and MAP/SDL lists (Open access) 2. Workshops 3. Conf. presentations 4. B2B matchmaking | 1. See above 2. See above 3. 1/WG/year 4. TND |
| Policymakers, regulatory bodies | 1. Roadmap papers 2. Action presentation meetings (*e.g.* bilateral events *cf*. §2.2.2) | 1. See above 2. Twice/year |
| General public & All | 1. Web page 2. Soc. Network (LinkedIn) 3. Twitter 4. e-news 5. Press-releases | 1. Total visits: how many? 2. 200+ followers. 1 post/WG/month 3. How many followers and tweets? 4. 2/WG/year 5. TND |

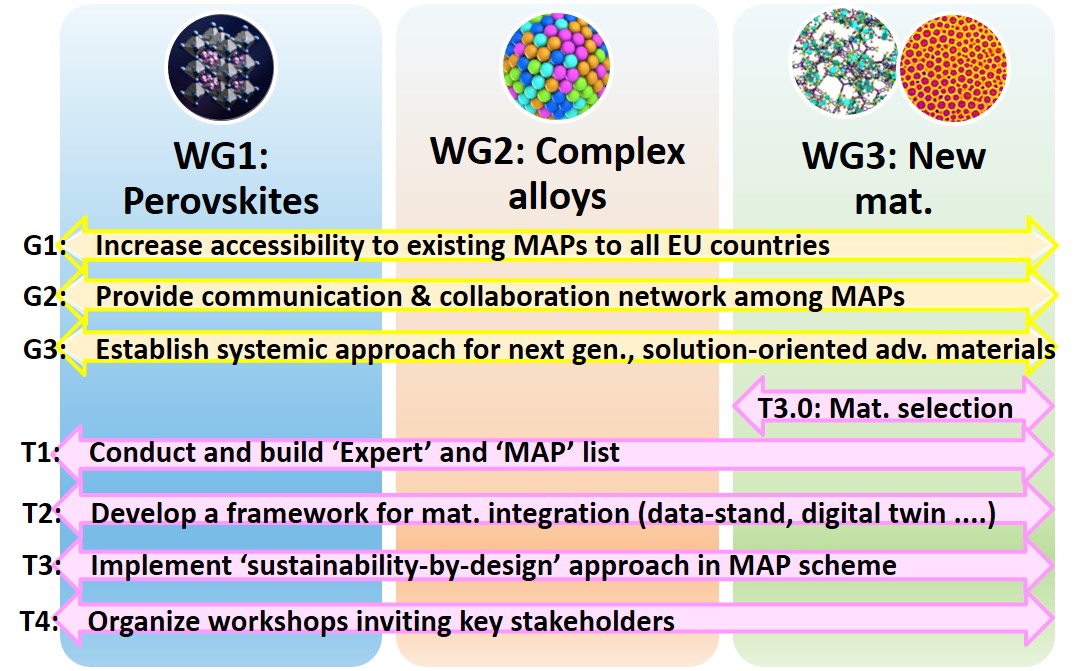
# IMPLEMENTATION

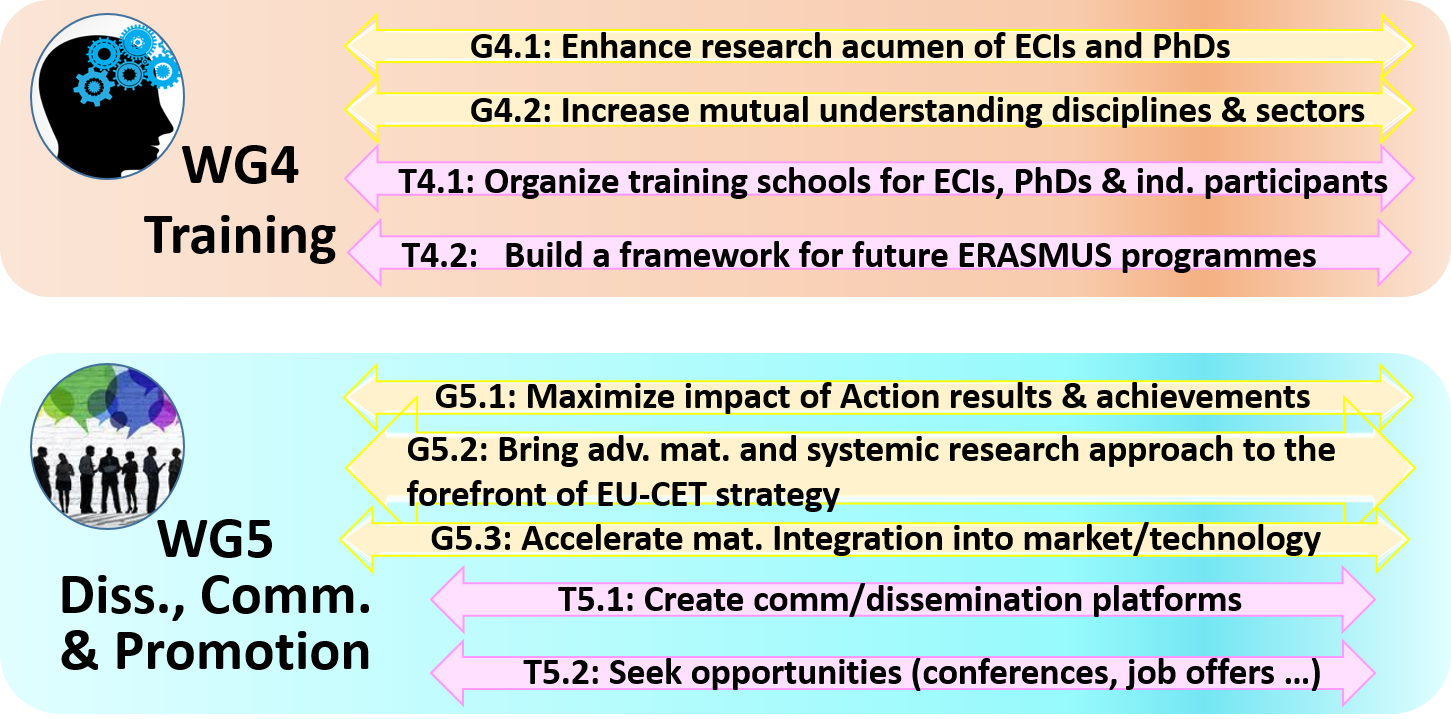
## COHERENCE AND EFFECTIVENESS OF THE WORK PLAN

### 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: CCA and WG3: ‘New material’) and two on overarching activities; i.e., WG4: Training and WG5: Dissemination & Communication (see Fig. 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**, **WGL** 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 thru G3) and ‘Tasks’ (T1 thru T5) are common to all technical WGs as depicted in Fig 4.1. The description of tasks are given below.





**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.

**T5: Interdisciplinary Workshop organizations**. 1 workshop/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 (accelerated materials integration)’ concepts. Key stakeholders (section 2.2/3.2.2) will be invited to these events. WGLs will coordinate with the Training Programme coordinator for the construction of training courses (Task 4.2).

The MC members will **select new functional material** (**T3.0**) as the Action’s 3rd pilot in WG3 where we will apply all above tasks and goals. The selection will be based on the application potential, the existing research initiatives (see ss 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 general public.Final EU-MACE Conference: an open wrap-up event to present the Action’s main achievements and the roadmap (whitepaper) on the efficient center of excellence strucuture and operation scheme for on advanced materials for energy.

**T4.2**: Academic partners will hold round-table discussion on future ERASMUS programme topics that reflects 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, educational material). B2B match-making 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. Find funding/cooperation opportunities (e.g., Horizon-EU programme) will be included in the database to assist members build new collaborative research projects.

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 policy, and approval of participation of additional institutions from either COST or non-COST countries and management of the network budget. Additionally, it will identify European and national funding and developing consortia to apply for funding for new research projects.

**Short-Term Scientific Missions (STSM)**: STSM (target 10/year) will allow *new* collaborations to be fostered among the Action members. Training new techniques and give network affiliates access to equipment not available in their own institution. 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 sec. XXX, 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.

**Workshop organization assistance:** The MC and CG members 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.) --- is this useful?

### 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 | Expert and MAP (includes similar structures, data repositories, etc.) to be updated yearly. | 1 | 2 |
| DT2 | Action results report (yearly) | 1 | 4 |
| DT3 | Roadmap on advanced materials development & integration in renewable energy sector (final version in year 4) | 2 | 4 |
| D3.1 | Selection of 3rd pilot materials (Task 3.0) | 1 | 3 |
| D4.1 | Publication of training course materials (?) 3 months after the 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 | 1 | 2 |
| D5.2 | B2B platform | 1 | 4 |
| D5.3 | Publication of tutorial videos | 2 | 2 |
| D1.1 | Review paper on Perovskite (metallic alloys, 3rd mat) devices, applications and perspectives in clean energy transition? | 3 | 4 |
| D5.5 | Position paper/brief report on the results of the interdisciplinary workshops | yearly |  |
| D4.3 | Do WE NEED MORE DELIVERBALES? NOT COUNTING MEETINGS |  |  |

### 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? |
| *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 |

### GANTT Diagram

Gannt goes here

1. materials make up nearly 80% of the cost of clean energy technologies. (I need source!! IEA?) [↑](#footnote-ref-2)