



Agenda

- 13:30 14:00 Introduction and Information on
 - Relevant call topics
 - EMMC activities
 - EMMC services for projects

 Gerhard Goldbeck (EMMC Executive Secretary)
- 14:00 16:00 Presentations of project ideas and organizational member contributions (about 10 minutes each)
 Chaired by Gabriele Mogni (Materials Square)
- 16:00 16:30 Discussions at tables in the Airmeet Lounge



Pitch presentations overview

- 14:00 14:10 Emerging Technology Identification and Forecasting System; Burak Dindaroglu, Izmir Institute of Technology
- 14:10 14:20 Characterization and modelling of plastics/composites materials; Guillaume ZIETEK, Technical Center for Plastics and Composites, France (IPC)
- 14:20 14:30 Circularity and Sustainability through Digitized Material Development CircuMat; Tobias Rosnitschek, University of Bayreuth
- 14:30 14:40 Coupling dynamic systems theory and symbolic regression to reduce time to development of materials for high temperatures in renewable energy technologies, Pavel Praks, IT4Innovations National Supercomputing Center, VSB Tech. Univ. of Ostrava, Czechia and Vladislav Kolarik, Fraunhofer-Institute for Chemical Technology (ICT)
- 14:40 14:50 Digital Twin of multiscale characterization pyramid from lab to production, Javier Zurbitu, Ikerlan
- 14:50 15:00 Smart Adaptive Material and Processes modelling for emerging digital production schemes; Amir Horr (AIT)
- 15:00 15:10 Involvement of Virtual Lab in future EMMC-lead Horizon Calls and Projects, Gabriele Mogni (Materials Square)
- 15:10 15:20 Yoav Nahshon, Dirk Helm (Fraunhofer IWM)
- 15:20 16:00 Further OM pitches and discussion



Overview of (some) relevant calls

- HORIZON-CL4-2023-RESILIENCE-01-23: Computational models for the development of safe and sustainable by design chemicals and materials (RIA)
- HORIZON-CL4-2023-RESILIENCE-01-39: Coordination and knowledge sharing across materials development communities (CSA)
- HORIZON-CL4-2023-DIGITAL-EMERGING-01-12: Adaptive multi-scale modelling and characterisation suites from lab to production (RIA)
- HORIZON-CL5-2023-D2-01-03: Advanced digital twins for battery cell production lines (Batt4EU Partnership)
- HORIZON-CL4-2023-HUMAN-01-54: Green and digital skills and training needs for a just transition (CSA)



Computational models for the development of safe and sustainable by design chemicals and materials

HORIZON-CL4-2023-RESILIENCE-01-23

- 4 projects of €6-7m each
- Produce innovative modelling software for the development of chemicals and materials (including advanced materials) building on high-throughput chemicals and materials characterisation facilities and relevant models and make it available and interlinked through open platforms accessible to SMEs and industry;
- Develop predictive computational models and software ...;
- Enable the integration of materials modelling, safety and sustainability assessment tools and databases into a single workflow. Apply AI techniques for data search and missing data, including statistical analysis (sensitivity and uncertainty), in all the areas covered: modelling of the functionality, safety and sustainability assessment (including life cycle assessment);
- Address information exchange on chemicals and materials along value chains ...;
- Make developed models on chemicals, materials and their production process FAIR[6], ...,
- The interoperability for data sharing should be addressed, including synergies with other European projects addressing ontologies for data documentation, for example projects resulting from topic DT-NMBP-39-2020 (ONTOCOMMONS including EMMO ontology);
- Projects should build on or seek collaboration with existing projects and develop synergies with other relevant European, national or regional initiatives, funding programmes and platforms, such as projects resulting from the topics HORIZON-CL4-2021-RESILIENCE-01-08, HORIZON-CL6-2023-ZEROPOLLUTION and/or HORIZON-CL4-2023-RESILIENCE-01-39. Proposals should allocate the necessary resources for collaboration with other relevant projects.



Coordination and knowledge sharing across materials development communities (CSA)

HORIZON-CL4-2023-RESILIENCE-01-39

- 1 project of €2m)
- Establish an inventory of relevant existing collaborative materials data and information systems.
- Network the identified data and information systems and make them accessible and usable.
- Establish common methodologies for data acquisition and knowledge generation:
 - · Modelling, including data- and physics-based materials modelling
 - Characterisation, including multi-scale, multi-technique, in/on-line
 - Materials synthesis and fabrication technologies including autonomous robotics platforms
 - Machine learning and AI-based methods
- Develop a common language for data documentation and exchange on advanced materials and related manufacturing processes through widely agreed vocabularies, taxonomies as well as relevant domain ontologies based on the Industry Commons Ontology Commons EcoSystem (OCES) and the Elementary Multiperspective Material Ontology (EMMO),
- Demonstrate easy access to reliable data and information/knowledge by connection of identified databases with the ontologies,
- Integrate data and methods for life-cycle assessment and take into account the safe and sustainable by design framework for chemicals and materials.
- Establish a cost overview and a business plan for the sustainability for a digital knowledge sharing system
- Establish training schemes to facilitate skills development, reskilling and upskilling
- Proposals should build on or seek collaboration with existing projects and develop synergies with other relevant European and national initiatives, funding programmes and platforms, in particular with the "Materials 2030 Roadmap" and any follow up actions.



Adaptive multi-scale modelling and characterisation suites from lab to production (RIA)

• HORIZON-CL4-2023-DIGITAL-EMERGING-01-12:

- 4 projects of €5-7m each
- Develop integrated methodologies of multi-scale and multi-technique characterisation, combined with respective multi-scale modelling and machine learning to
 - improve the reliability and quality of data;
 - understand scaling relationships in the behaviour of advanced materials;
 - develop complex structure-property correlations in advanced materials;
 - ensure complete coverage of conditions in industrial environments.
- Integrate modelling and characterisation, in particular by
 - Developing modelling methods that provide the capabilities to virtually characterise materials and enhance the interpretation of the results of particular characterisation methods in order to guide and refine experiments;
 - Developing accurate, validated physics-based models, in areas where these capabilities are a bottleneck, by utilising a combination of characterisation and machine learning to generate material and application specific parameters and equations (called materials relations, ref. CWA 17284.)
- Demonstrate the functionality of the suites for the development of certain advanced materials for the green transition.
- Validate the methodologies and provide benchmarks, i.e. clear documentation of capabilities that can serve as a standard point of reference for industrial application.
- Research should build on existing standards or contribute to standardisation. Documentation and interoperability for data sharing should be addressed, based on the **OntoCommons EcoSystem (OCES)**.
- Projects should build on and seek collaboration with existing projects and develop synergies with other relevant European, national
 or regional initiatives, funding programmes and platforms. In particular, projects funded under this call should collaborate under the
 umbrella of the EMMC and EMCC and interact closely with topic HORIZON-CL4-2023-RESILIENCE-01-39 (CSA).
- TRL 3-5



Advanced digital twins for battery cell production lines (Batt4EU Partnership)

HORIZON-CL5-2023-D2-01-03

2 projects of €7m each

- Developing digital twins of battery cell manufacturing routes at pilot line level that incorporate appropriate models
- Design robust digital tools integrating multi-physics, data-driven models and hybrid modelling.
- Flexible Digital Twins capable to evolve to different battery chemistries, new disruptive materials as well as new
 manufacturing processes (the model would be chemistry neutral so easily adaptable to new disruptive materials and
 chemistries).
- Verify the transferability from pilot to production plant level.
- Propose applications that will enable to overcome single process considerations towards process chain perspectives.
- Implementation of the sensorisation of the manufacturing plant and automatisation of the data acquisition.
- Ensuring greater interoperability, by implementing available data standards[1], e. g., Modelling-Data (MODA) and Characterisation Data (CHADA), as well as, a common semantic framework, like The European Materials Modelling Ontology (EMMO) and the battery interface ontology (BattINFO).
- Promote the control and decision making of the manufacturing chain.
- Aspects like safety and security, **explainability of models** as well as contributions to sustainability of battery production will be addressed.



Green and digital skills and training needs for a just transition (CSA)

ExpectedOutcome:

- Reduce skills gaps that hold back the green and digital transitions.
- Support collective action on skills development by companies and providers of education and training,
- Support the training of advanced ICT-specialist skills or other key digital technologies' skills that would contribute to industrial leadership and strategic autonomy and rely on advanced specialised know-how, and to reaching the digital decade targets[4].



General guidelines for EMMC involvement

https://emmc.eu/news/support-and-services-provided-by-emmc-in-horizon-europe-work-programme/

- 1. Project beneficiaries who lead relevant tasks (e.g. modelling, ontology) should foresee the budget to become Organisational Members of EMMC for the duration of the project. As Organisational Member they will be able to lead an EMMC Task Group that can be set up as an environment for collaboration with other relevant projects.
- 2. EMMC as contractor supporting inter-project collaboration
 - To support inter-project coordination, EMMC tasks may include the following
 - Organise projects coming together: support clustering, fostering interaction and improving synergies
 - Inter-project coordination regarding EMMC objectives and cooperation with wider stakeholder community (other EMMC members etc)
 - Support road-mapping activities in materials modelling and digitalisation
 - Produce project related outcome documents and ensure their dissemination within the project and support their publication to wider stakeholder community
 - Run (online) workshop(s)
 - Support the interactions with EMCC

The estimated cost of contract is in the region of €12000 per project. It is recommended to specify the cost in category "other direct costs" (within costs of other goods and services)



MODA, CHADA and EMMO

- Useful resources for project proposals https://emmc.eu/moda/
- EMMC is governing body for EMMO developments: <u>https://github.com/emmo-repo/EMMO</u>
- EMMC manages a github for project collaborations: https://github.com/EMMC-ASBL/



Materials 2030 Roadmap

- Elaborated by the Advanced Materials Initiative AMI2030
- EMMC leads Working Group 1: Materials Digialisation



Advanced Materials 2030 Initiative

https://www.ami2030.eu/roadmap/

Inclusive governance a new form of cooperation

MATERIALS DIGITALISATION

New research and dev. methologies

Merging computational and experimental material science with data science

MATERIALS SCALING UP

Common manufacturing technologies & conditions for the producion and processing of advanced materials

MATERIALS PRIORITY AREAS

The basis for the development of a novel European strategic agenda

Connecting "Blue sky" research with market demands

Evidence-based policy recommendations

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WG1 Materials Digitalization

Gerhard Goldbeck (EMMC), Philippe Jacques (EMIRI)



Create game changing tools and FAIR data interchange in a materials data space

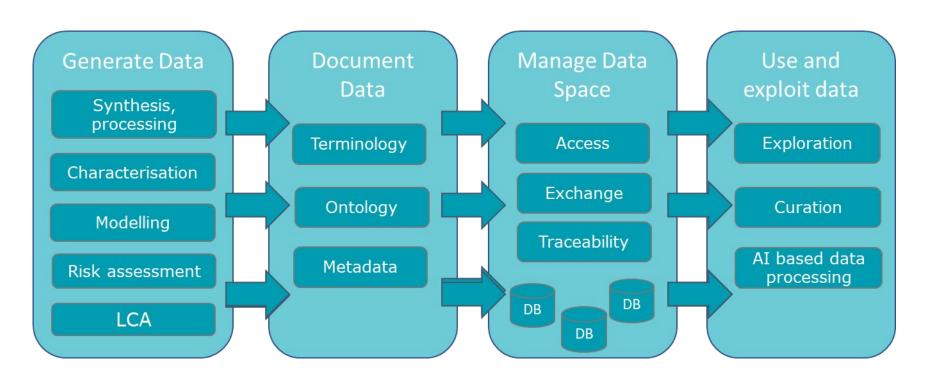
- Digitalise and integrate materials investigation technologies
- Harmonised and interoperable data across all domains
- Federated data space with trusted data access and exchange
- Created value from data using digital and AI strategies

Generate

Document

Manage

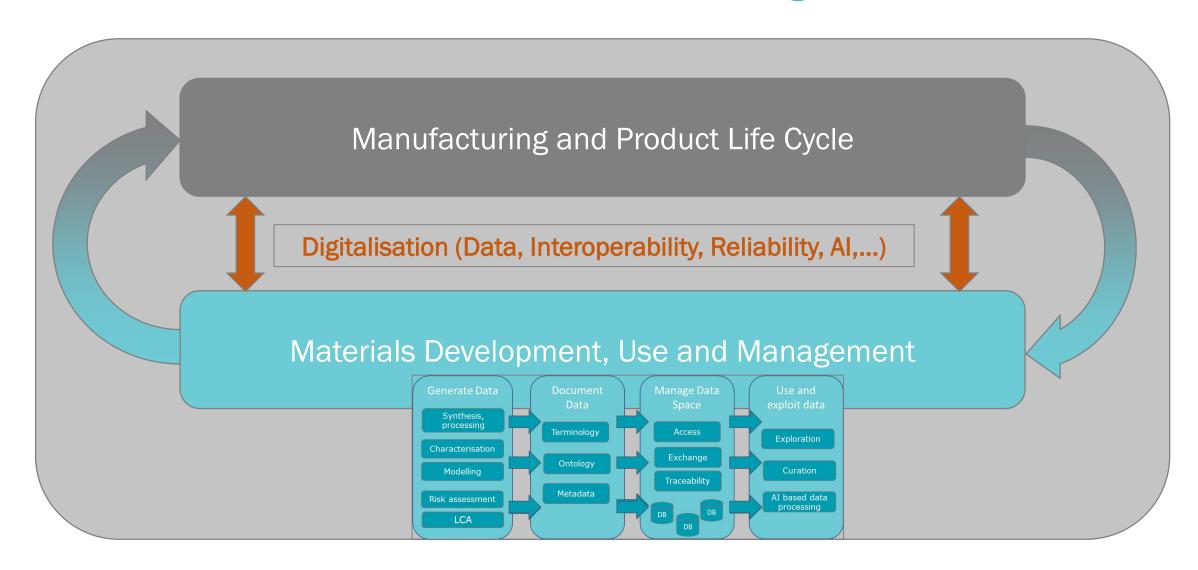
Exploit





A Common Materials Data Space

interconnected with Manufacturing and PLM





Actions to digitally integrate and iterate data and knowledge activities throughout the life cycle

1. Generate new data with harmonised and digitalised techniques

Digital and innovative methodologies for generating materials data and knowledge, including modelling, characterisation, production and testing technologies

2. Document data for FAIRness and in support of materials standards

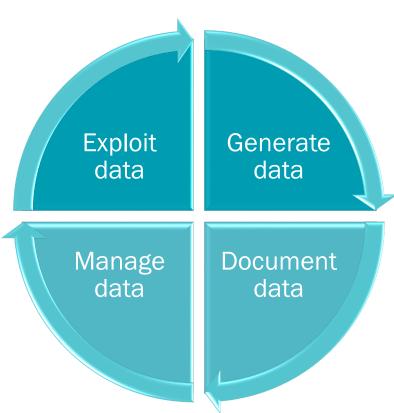
Develop and disseminate a common (standardised) language (ontology) for data exchange and knowledge management in materials R&D

3. Common materials data space with trusted management, data access and exchange and distributed data repositories

Provide reliable and easy access to and exchange of generated data/information/knowledge for all stakeholders

4. Use and exploit data supported by semantic and AI strategies

Provide powerful tools for interrogation and processing data





Coordination and knowledge sharing across materials development communities (CSA)

- Strongly linked to AMI2030
- Proposal coordinated by EMMC

