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Open data and industry-driven environment for materials characterisation and modelling combing physics and data-based approaches

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About

The Horizon Europe project MatCHMaker officially started on 1 December 2022 and will last until 31 May 2026. The full project title is Open data and industry-driven environment for multiphase and multiscale Materials Characterisation and Modelling combining physics and data-based approaches. The project is coordinated by the French Alternative Energies and Atomic Energy Commission (CEA). Ten partners and two affiliated entities from 8 European countries are involved to advance sustainable industry. Together, we contribute to the European Green Deal decarbonising the EU economy while improving people's quality of life.

Why "MatCHMaker"?

"MatCHM" in the MatCHMaker project refers to Materials Characterisation and Modelling. Advanced material characterisation methods, computational data-based modelling and physics-based models are seen as the three main pillars of material design optimisation towards the decarbonisation of industries. The project aims to contribute to the integration and interoperability of complex characterisation and modelling data and workflows matching the needs of the EU manufacturing industry. Knowledge transfer, data sharing and full interoperability between characterisation and modelling "communities" will be facilitated using data-related standards and creating an open repository with a direct connection to design and manufacturing processes.

Requirements on multiphase and multiscale materials from the industrial sectors of construction, energy and mobility will be translated into innovation challenges. The tasks will be addressed by an integrated approach in a reproducible and efficient way. The expected result is to reduce development costs, time and risks for advanced materials, contributing to a sustainable and low-carbon economy.

Objectives



Accelerate advanced materials development

Develop a model-based innovation process to accelerate the materials' design, validation, characterisation methods and computational modelling

Traceability, Integrity and Interoperability

Enhance the interoperability and integration of characterisation and modelling data and workflows through a semantic approach



Open Data Repository

Create an open data repository based on semantic representation to connect design and manufacturing processes







Applications

Use Case I Construction



Decrease CO2 emissions in cement production



To decrease CO2 emissions from cement production, substituting conventional cement with supplementary cementitious materials (SCM) is key. Currently, the European cement sector still heavily incorporates by-products of the steel and coal industries. Looking ahead, the challenge lies in finding the maximum replacement level of these alternatives while maintaining or improving the performance.

Use Case II Energy

Solution Emission-free hydrogen production with the highest efficiency

To advance hydrogen production without CO2 emissions, electrolyser technologies could meet the demands in various capacities. The goal will be to produce more hydrogen while consuming less electricity which not only reduces the running costs but also the capital expenditure to install the necessary renewable production capacity.

Towards this goal, MatCHMaker aims to improve the performance and mechanical robustness of electrochemical cells implemented in Solid Oxide Electrolysis Cells (SOEC) via advanced modelling and characterisation.



Use Case III Mobility



Emission-free power in multiple mobility applications



Analytical and computational tools enable a better understanding of degradation in fuel cells. The MatCHMaker aims to develop new future highperformance material by enhancing analytical and computational analysis in this use case.

The focus lies on improving the durability and performance of proton-exchange membrane fuel cells (PEMFC) for mobility applications.





Online Presence

In line with the open science concept, MatCHMaker wants to promote outreach activities in science communication to all stakeholders and the general public. Alongside the project <u>website</u>, MatCHMaker joined <u>LinkedIn</u> to further connect with the scientific community and everyone interested in the domain of the project. In the near future, MatCHMaker will continue this effort by extending its online presence on other social media platforms, so stay in the loop!

Synergies: EMMC and Sister Projects

The <u>4th EMMC International Workshop 2023</u> took place again in Vienna, Austria, after holding it online during the pandemic in 2021. Plenary talks and sessions covering the EMMC focus areas (modelling development, interoperability, digitalisation, software, impact on industry and policy) and discussion rounds were accompanied by presentations from the scientific community, EU projects and exhibitors.

MatCHMaker partners from AIMEN, CEA, Heidelberg Materials, SINTEF and TU WIEN attended inperson and connected with other EU projects and participants across disciplines.

Our Project Coordinator Ludovic Jason (CEA) presented the MatCHMaker project and discussed the challenges and chances together with the other Horizon Europe sister projects <u>AddMorePower</u> <u>Horizon</u>, <u>D-STANDART Project</u>, <u>Knowskite-X</u>, <u>CoBRAIN Project</u>.

We look forward to more collaborations and synergies within the framework of the EMMC and other relevant projects leading to a wider impact!



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We are looking for long-term partnerships!

Materials' microstructure is fundamental for our understanding of the material's properties. Quantitative characterisation of microstructures is therefore essential for the optimisation of the performance of materials. Machine learning algorithms are promising for image analysis yet are still scarcely applied in our field. In cement research, e.g., clustering algorithms enabled a better understanding of the kinetics of recycled concrete paste carbonation.

We will continue in this direction and are gathering more data to make our codes more robust and transversal, and are looking for partnerships and synergies going beyond the lifecycle of the project.

If you are part of an EU project or know one interested in expanding an image database, building case studies and algorithms on all classes of materials, please contact us!

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