

## **Press Release**

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# Accelerating battery innovation with AI-driven materials discovery

#### Max Planck team receives 1.5 million euros as part of the European project FULL-MAP

To meet the urge for the development of new batteries with a higher longevity, an increased capacity in energy storage and refraining from critical or scarce elements, the European Commission now granted 20 million euros for the development of a materials acceleration platform. Artificial intelligence, machine learning and multi-scale modelling will be combined with experimental results to discover and develop next-generation battery materials. The Max Planck Institute for Sustainable Materials (MPI-SusMat) will receive 1.5 million euros to develop theoretical and experimental frameworks and workflows for accelerated materials discovery.

### Merging artificial intelligence with experimental data

"The project aims to automate laboratory processes and conduct high-throughput integrating essential elements for thorough. sequential experiments by experimentation based on smart decision-making supported by artificial intelligence and machine learning", says Dr. Chuanlai Liu, head of the group Computational Energy Storage Materials at MPI-SusMat. Liu will develop the physics-informed neural network models to study battery performance and ageing mechanisms at both the meso-scale and cell level, the design of electrode microstructures, the optimization of cycling conditions, and the synthesis of electrodes and electrolytes. "My group will enable and develop high-resolution characterization workflows as well as multiscale operando characterization", explains Dr. Yug Joshi, leading the group Microstructure and Interfaces of Battery Materials at MPI-SusMat.

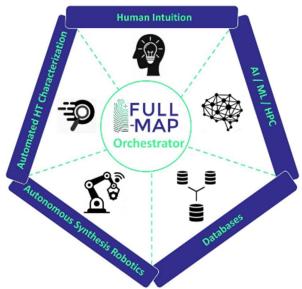
#### **European-wide collaboration**

The project brings together a diverse consortium of 33 partners from 12 European countries, coordinated by the Vrije Universiteit Brussel. This multidisciplinary team includes partners from academia and industry merging expertise in artificial intelligence, materials design and commercialisation. The aim is to ensure that both environmental criteria and economic factors are met.





**Figure 1:** The project Full-Map brings together a consortium of 33 partners from 12 European countries to develop a materials acceleration platform for the discovery of next-generation battery materials. Photo: Thierry Geenen.



**Figure 2**: The project Full-Map combines artificial intelligence and machine learning with experimental databases and automated workflows, thereby merging expertise from academia and industry. Photo: Full-Map.

Materials science is facing major challenges: The steel industry alone contributes eight percent of global carbon dioxide emissions. Each year, e-waste, equivalent to 350 mega cruise ships, is discarded or incinerated rather than recycled, despite containing valuable metals. At the Max Planck Institute for Sustainable Materials (MPI-SusMat), we are exploring climate-neutral, resource-conserving approaches to produce, utilize, and recycle essential materials for modern societies. We seek to produce metals using hydrogen instead of fossil fuels, extend material lifespans, enhance recyclability, and minimize waste. When developing materials that fulfil these requirements, we are increasingly relying on artificial intelligence to make the process significantly more efficient. The institute conducted its research under the name Max-Planck-Institut für Eisenforschung GmbH until 2024.

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Contact: Yasmin Ahmed Salem, M.A. Press and Public Relations Officer E-Mail: <u>y.ahmedsalem@mpie.de</u> Tel.: +49 (0) 211 6792 722 <u>https://www.mpi-susmat.de</u>

