DE-centralised Cloud labs fOr inDustrialisation of Energy materials

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Integrated characterization and modelling toolkits | Delivering WP2 results

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The objective of Work Package 2 (WP2) was to establish a **correlative workflow of characterisation and modelling methods** according to the **knowledge graph developed in WP1** and apply it to a **first demonstration case**. To do so, a comprehensive **multimodal characterisation framework** has been established by combining imaging, electrochemical, physico-chemical, and modelling techniques to analyse catalyst layers, gas diffusion layers, and membrane electrode assemblies. Techniques such as X-ray tomography, electron microscopy, neutron scattering, rheology, permeability analysis, and nano-indentation have been integrated into shared **workflows linking material structure to transport and electrochemical performance**. Extensive work has also been done to identify and integrate **in-situ and operando characterisation methods** capable of analysing electrochemical cells during operation.

An **integrated multi-scale modelling workflow** has been implemented to connect raw material properties, ink formulations, manufacturing parameters, and microstructural data to PEFC performance prediction. Transport, electrochemistry, and microstructure models have been coupled within a Python-based environment coordinated by a dynamic workflow manager, enabling automated interaction between simulations and experiments.

A digital backbone for workflow orchestration has been established through the implementation of the **knowledge graph** and an **Integration Readiness Level (IRL) framework**. More than **80 characterisation, modelling, and manufacturing methods** have been evaluated in terms of maturity, interoperability, resource requirements, and integration complexity, enabling AI-assisted workflow selection and optimisation.

Finally, the integrated workflows have been successfully demonstrated for **PEFC baseline cases** using varying ionomer-to-carbon ratios in cathode catalyst layers. In total, **39 methods from 8 partner institutions have been connected** through a dedicated data platform that monitors workflow execution, parameter exchange, and logical toolchain connectivity. Large, consistent datasets have been generated and the modelling workflow has successfully reproduced experimental PEFC performance trends, while also identifying remaining gaps toward full predictive capability.

Together with these achievements and from the lessons learned, WP3 will further drive the development of the DECODE platform for its application in the explorative cases in WP4.