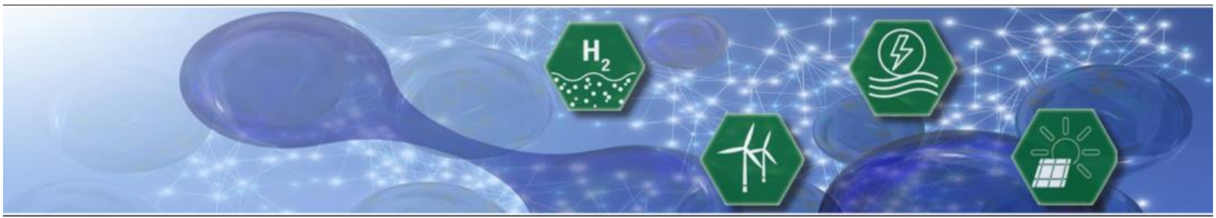
NOUVEAU



NOVEL ELECTRODE COATINGS AND INTERCONNECT FOR SUSTAINABLE AND REUSABLE SOEC

UPDATES ON ACTIVITIES at M33

The consortium of NOUVEAU is running for 33 months! In this fifth Newsletter, we will guide you through our **EMMC clustering webinar activity** with other European projects working on similar topics. Joint webinar '**Advances in Materials Modelling: From Atoms to Industrial application**" aim to connect with similar initiatives: **FreeMe, MOZART, NICKEFFECT** and to establish a strong cross-project liaison, driving forward European advancements in computational materials science, electrochemistry, and industrial process optimization by implementing shared strategies and methodologies.

In addition, we would like to highlight our fifth **NOUVEAU consortium meeting**, which took place at the **Coatema Coating Machinery GmbH** in Dormagen. We also present the project progress of **Forschungszentrum, IMDEA Energy, VITO,** and **QSARLAB.**

Enjoy the reading!

Joint Webinar "Advances in Materials Modeling: From Atoms to Industrial application"

Together with NOUVEAU, the sister projects NICKEFFECT, MOZART, and FreeMe have founded the 4SEE CLUSTER. The 4SEE Cluster is a collaborative initiative focusing on safe and sustainable-by-design metallic coatings and engineered surfaces.

As a cluster event, on June 18, 2025 with the collaboration of NOUVEAU project and EMMC a joint webinar will be co-organized. For registration, please visit Joint Webinar of NOUVEAU project and sister projects | EMMC

During this collaboration, project representatives will deliver **short talks** outlining their approaches to **materials modeling**, with a focus on: Density-functional theory(DFT),
Machine-learned interatomic potentials
Process optimization
Multiscale modeling
Electrochemical plating processes

These topics align with cutting-edge research in computational materials science, electrochemistry, and industrial process optimization, fostering knowledge exchange across different domains.
Key Outcomes of the Collaboration:

- Identifying and addressing bottlenecks in atomic modelling
- Enhancing the transferability of workflows and methodologies between projects
- Facilitating the exchange of standardization approaches across related sectors

This initiative is a significant step toward revolutionizing metallic coatings and engineered surfaces, strengthening European leadership in sustainable and advanced material solutions.

For detailed agenda please visit the link: Joint Webinar of NOUVEAU project and sister projects | EMMC

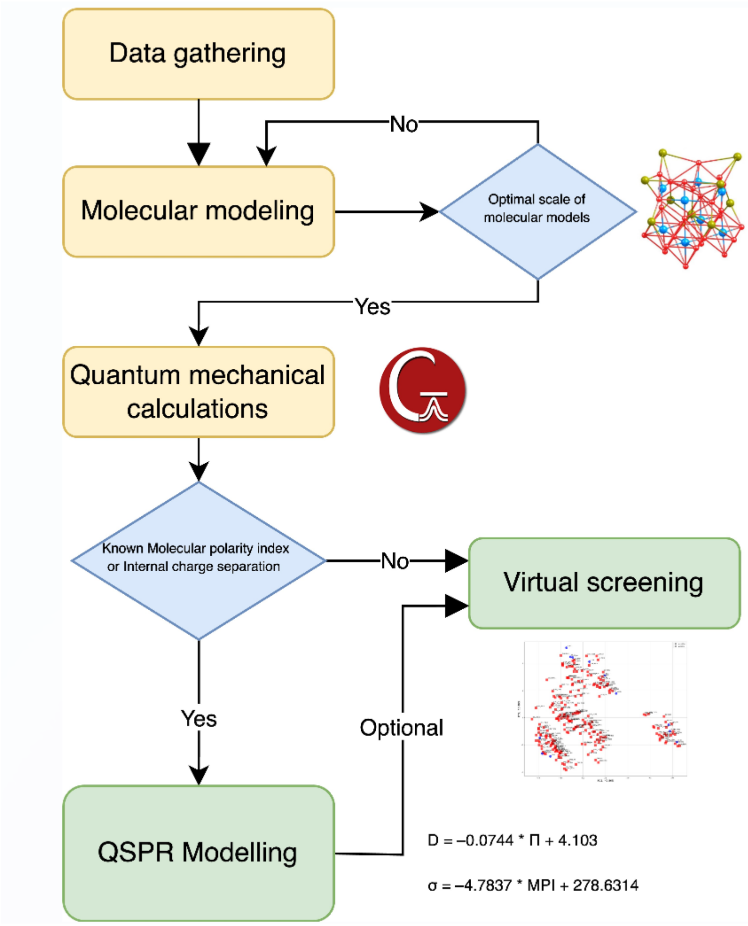
Consortium meeting in Dormagen

On 10-11 April the 5th consortium meeting of the NOUVEAU project took place in a hybrid mode, both in Dormagen, Germany, and online. During the meeting hosted by Coatema Coating Machinery GmbH, partners had the opportunity to summarize the achievements of the project's third year and discuss next steps.

UPDATES ON ACTIVITIES

A Computational Strategy for SSbD: Virtual Screening and Predictive Modeling in SOEC Material Design": QSARlab

All the knowledge generated over the past year QSAR lab built 165 molecular models of possible structures of SOEC anodes based on the brown millerite structure. All the knowledge generated, was used to create Safe and Sustainability by Design tools, integrated with Life Cycle Sustainability to make them safer, greener and economically feasible.



The Integrated Testing Strategy (ITS) developed within WP2 provides a comprehensive, data-driven approach for the design of SOEC materials in accordance with Safe-and-Sustainable-by-Design (SSbD) principles. This innovative, data-driven framework leverages advanced computational techniques—including Virtual High Throughput Screening (vHTS), quantum mechanical modeling (DFT), molecular dynamics (MD), and machine learning-based QSPR models—to guide the design of SOEC materials in line with Safe-and-Sustainable-by-Design (SSbD) principles

Initially applied to anode materials, ITS has already accelerated the discovery of high-potential candidates while minimizing reliance on costly experimental testing. As the project progresses, the strategy is being expanded to cathodes and electrolytes, with potential applications extending to alternative hydrogen production technologies.

Upcoming activities in WP3 and WP4 will focus on the experimental validation of selected materials, while further developments aim to incorporate multi-objective optimization and explore pathways for industrial scalability and integration.

Understanding NOUVEAU progress from a sustainability perspective

The Systems Analysis Unit of IMDEA Energy is leading the sustainability assessment and benchmarking of the novel solutions proposed in NOUVEAU from a life cycle perspective. The study explores coating technologies and innovative manufacturing processes relevant to the project, such as the synthesis of a lanthanum-free anode and the development of novel interconnects.

In particular, IMDEA Energy is leading the sustainability benchmarking of a NOUVEAU solid oxide electrolysis cell at two different levels. First, at the stack level, a life cycle sustainability assessment and a material criticality analysis were conducted, where the results were benchmarked against a conventional solid oxide electrolysis cell stack and presented remarkable improvements. For instance, a 10% climate change reduction and a 13% cost decrease were recorded. Furthermore, at the hydrogen production level, the focus was placed on the environmental life cycle assessment of the novel stack coupled with photovoltaic electricity and industrial waste heat, finding a carbon footprint below 3 kg CO_2 eq/kg H_2. Additionally, NOUVEAU-based hydrogen was benchmarked against conventional hydrogen from steam methane reforming.

IMDEA Energy presented these findings at the European PhD Hydrogen Conference (EPHyC 2025) in Trieste (Italy) in April 2025. The presentation entitled “Towards an enhanced Assessment approach for safe and sustainable-By-design hydrogen-related products” , focused on the sustainability study of NOUVEAU case study.

All in all, the benchmarking results for the NOUVEAU-based products indicate important improvements in a wide range of sustainability aspects regarding both stack manufacturing and hydrogen production.

Interconnect coatings with Cr reduction and system integration: modelling effect of component geometry on substrate steel oxidation behaviour

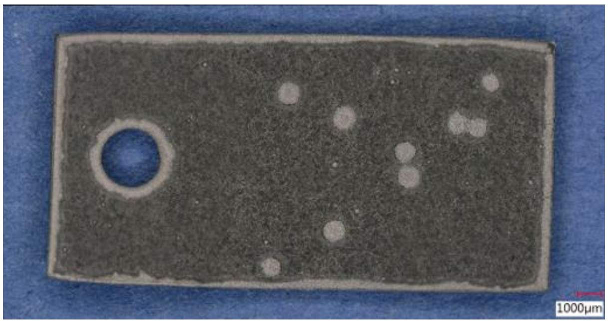


Fig. 1. Photo of AISI430 steel specimen after exposure in air for 3000 hours at 900°C

Under accelerated oxidation conditions, the investigated ferritic stainless steels exhibit a tendency for breakaway oxidation (formation of fast-growing iron-rich oxides) at the sample edges (Fig 1). According to our suggestion, this effect corresponds to a higher surface-to volume ratio at the sample edges, limiting the chromium flux to the surface.

To quantify this behavior, Forschungszentrum Jülich (FZJ) developed a 2D kinetic-thermodynamic model accounting for chromium diffusion and geometrical factors that may promote the onset of breakaway oxidation. Application of the model to an Fe-17.5Cr alloy reveals significantly deeper chromium depletion at the edges (Fig. 2), with chromium levels dropping below 13% after 3 hours of exposure, compared to 15–16% on the flat surface.

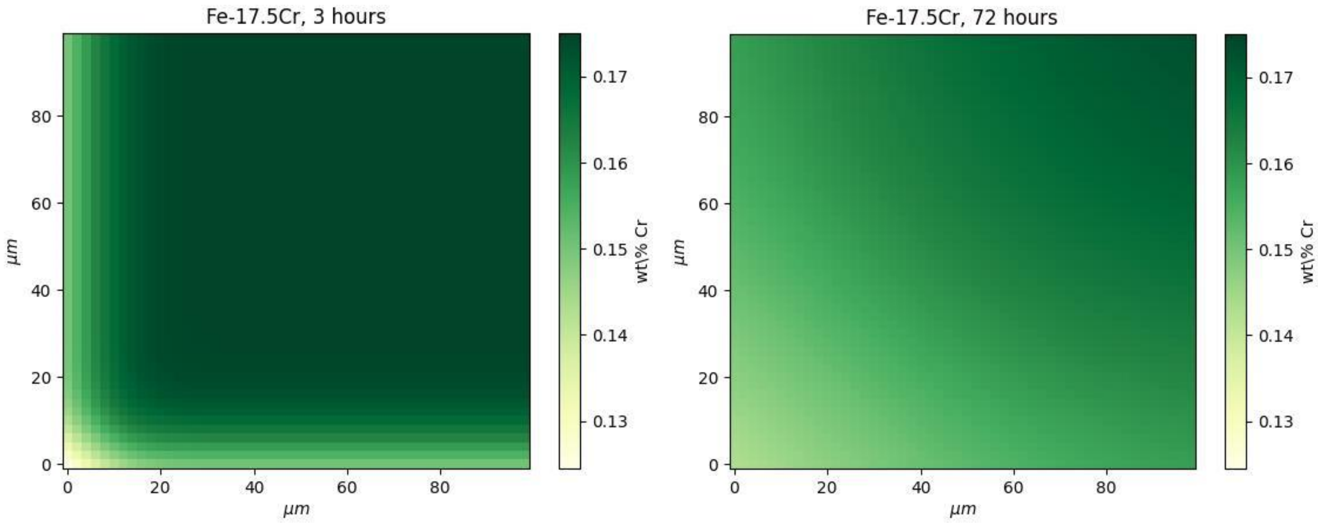


Fig. 2. Chromium concentration distribution in Fe-17Cr steel exposed to air at 900°C after 3 and 72 hours of exposure, based on model calculations. The point (0,0) corresponds to the sample edge.

These modelling results indicate that edges of steel components—such as interconnects with gas channels in SOECs—are particularly vulnerable to breakaway oxidation. Consequently, component geometry must be considered in material selection and lifetime assessment.

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