Conducting research for a changing society: This is what drives us at Forschungszentrum Jülich. As a member of the Helmholtz Association, we aim to tackle the grand societal challenges of our time and conduct research into the possibilities of a digitized society, a climate-friendly energy system, and a resource-efficient economy. Work together with around 7,500 employees in one of Europe's biggest research centres and help us to shape change!

The Institute of Energy Technologies – Theory and Computation of Energy Materials (IET-3) conducts multidisciplinary research to advance hydrogen technologies. We explore both theoretical and computational approaches, ranging from fundamental electrochemical processes to the data-driven optimization of innovative materials. Our Artificial Materials Intelligence (AMI) division leverages AI-powered analysis, and sophisticated knowledge graph-based tools to accelerate the entire materials development cycle—from basic characterization to device-scale applications.

We are looking to recruit a

Master Thesis / Project Opportunity - Development of Autonomous Multi-Agent Performance Prediction Framework for PEM water electrolysis

Your Job:
Join AMI, the Artificial Materials Intelligence division at the IET-3 at Forschungszentrum Jülich to develop an Autonomous Multi-Agent Performance Prediction Framework for PEM water electrolysis. As an MSc student, you will design and implement a suite of AI "agents" (autoencoders, statistical models, LSTMs and LLM-based rule engines) that process historical and live sensor data (voltage, current, temperature, pressure, flow) to forecast electrolyzer efficiency, degradation and stability. You will build data pipelines, refine predictive rules through a review-and-correction loop, and integrate an Aggregator Agent to fuse all outputs into one robust performance prediction-advancing explainable, self-improving AI for sustainable hydrogen production.

Your tasks in detail:
1. Data Preparation & Preprocessing
- Collect and clean historical and live PEM electrolyzer sensor streams (voltage, current, temperature, pressure, flow) from our partners.

We look forward to receiving your application until 16.06.2025 via our **Online-Recruitment-System!**
Questions about the vacancy?
Get in touch with us by using **our contact form.**
Please note that for technical reasons we cannot accept applications via email.
www.fz-juelich.de

- Segment data into fixed□length windows, normalize values, and engineer features (e.g., rolling means, deltas).

2. Agent Implementation

- Statistical Agent: Develop regression/control□chart methods to capture trends and threshold breaches.
- Forecasting Agent: Implement LSTM/Transformer networks for time□series performance forecasting.

3. Rule-Based Agent: Encode expert□driven and LLM-generated prediction rules into a modular, executable library.

- Rule Management & Refinement
- Rule Generation Agent: Use templates or LLM prompts to propose new performance□prediction rules when agents disagree or fall below accuracy targets.
- Review Agent: Monitor inter-agent conflicts, false positives/negatives, and flag poor predictions for rule updates.
- Correction Agent: Validate, debug, and sanitize new or modified rules (syntax, logic, coverage) before deployment.

4. Collaboration & Documentation

- Work closely with project supervisors and partner labs to share progress, datasets, and interim results.
- Maintain clear, up-to-date documentation of data pipelines, model code, rules library, and evaluation results.
- Present findings in regular meetings and contribute to thesis chapters or conference papers as needed.

Your Profile:

- Enrollment in a Master's Program; Fields such as Data Science, Computer Science, Materials Science, Engineering, Physics, or a related domain.
- Proficient in Python; experience or eagerness to learn ML libraries (PyTorch, TensorFlow, scikit-learn),
- Familiarity with time-series analysis and forecasting methods (LSTM/Transformer).
- Experience with rule-based and LLM-driven systems is a plus.
- Passion for sustainable energy solutions, with an emphasis on hydrogen materials.
- Creative problem solver who enjoys interdisciplinary research and collaborative teamwork.
- Proficient in English (written and spoken).
- Comfortable engaging with international and cross-functional teams.

Our Offer:

Hands-On multi-Agent AI Project

- Play a central role in developing a novel, high-impact performance prediction system for PEM water electrolyzers.

Cutting-Edge Research Environment

- Access to modern HPC infrastructure, AI toolkits, and an internationally recognized research community.

Professional Development

- Build critical skills in time-series data workflows, multi-agent architectures, and rule-based/LLM-driven model development—highly sought after in both academia and industry.

Flexible MSc Thesis Structure

- Typical duration of 6–12 months aligned with Master's project requirements.
- Potential to co-author research papers or present findings at conferences, depending on project progress.

Support & Guidance

- Supervision from experienced researchers in a highly collaborative setting.
- Opportunity to network with experts at FZ Jülich, and other Helmholtz centers

In addition to exciting tasks and a collaborative working atmosphere at Jülich, we have a lot more to offer: https://go.fzj.de/benefits

We welcome applications from people with diverse backgrounds, e.g. in terms of age, gender, disability, sexual orientation / identity, and social, ethnic and religious origin. A diverse and inclusive working environment with equal opportunities in which everyone can realize their potential is important to us.

Further information on diversity and equal opportunities: https://go.fzj.de/equality