This Thesis will be partly conducted in two different institutes in Jülich. The Institute for Energy and Climate Research - Electrochemical Process Engineering (IEK-14) at Forschungszentrum Jülich with more than 20 years of experience in electrochemical energy conversion, is at the forefront of innovative solutions for clean and sustainable energy conversion devices. PEM water electrolysis is one promising technology for supplying the growing demand for green Hydrogen. At the Institute of Energy and Climate Research – Theory and Computation of Energy Materials (IEK-13) we contribute to fundamental understanding of electrochemical phenomena, development and characterization of tailored material solutions, and testing and optimization of new energy technologies. We are advancing the discovery and integration of energy materials by using AI to streamline the development workflow. This involves deep learning for materials characterization, inverse molecular design for targeted syntheses, and the development of ontologies and graph databases to enhance data utilization.

We are offering a

PhD Position – New insights from existing PEM water electrolysis data: Optimizing data analysis using Machine Learning

Your Job:
Currently insights into electrochemical systems are generally gained by defining a research question, designing an experiment which is suitable to answering this question, executing the experiment and analyzing the results in order to answer the research question. It is likely, however, that the results can also be used to answer other questions and therefore existing results are an unused asset that can help accelerating research on electrochemical systems. The focus on the thesis work is on recovering these data and define what data are needed and how they have to be structured and
stored. These data will then be used to find out what additional insights can be generated by using suitable analysis algorithms. This work is part of the EU-funded project “Decode – Decentralized Cloud Labs for Energy Materials” in cooperation with partners from academia and industry from several European countries. Your tasks in detail:

• Conduct cutting-edge research to develop and validate advanced AI methodologies for the characterization, modelling, and simulation of energy materials
• Contribute to the FAIR-ification of data, establishing systematic data collection and metadata extraction protocols to enhance machine learning-based software applications for materials science
• Develop code and utilize machine learning to support the automation of characterization and fabrication processes
• Ensure the integration and effectiveness of AI and ML algorithms in high-throughput and automated systems, addressing challenges related to data quality and operando characterization
• Collect data from already existing experiments on PEM water electrolysis and conduct some additional experiments
• Define useful data and store data and meta-data in a suitable RDM repository
• Define additional questions that may be answered based on existing data
• Analyze data using ML algorithms
• Communicate results and needs to partners within the Forschungszentrum and within the EU-project

Your Profile:

• Master's degree with excellent marks in Engineering or Chemistry, Physics or Informatics
• Experience with experimental work and characterization techniques
• Demonstrated experience in programming, particularly in Python, with a robust understanding of data extraction and machine learning models
• An analytical thinker with proven problem-solving abilities and a commitment to pushing the boundaries of interdisciplinary collaboration
• Experience in research data analysis
• Willingness to learn and ability to think outside the box
• Excellent cooperation, communication, and teamwork skills
• Collaborative working in multicultural and interdisciplinary team
• Independent, self-motivated, and responsible
• Fluency in English is mandatory
• Fluency in German is advantageous

Our Offer:

We work on the very latest issues that impact our society and are offering you the chance to actively help in shaping the change! We offer ideal conditions for you to complete your doctoral degree:

• An interesting, forward-looking, and socially relevant dissertation topic
• Interdisciplinary collaboration on a project in an international, committed, and collegial team environment
• Well-equipped laboratories in one of the largest research centers in Europe
• State-of-the-art research
• Flexible working arrangements
• 30 days of annual leave as well as an arrangement for bridging days (e.g. between Christmas and New Year's Day)
• Fun and social working atmosphere
• Further development of your personal strengths, e.g. through an extensive range of
training courses; a structured program of continuing education and networking opportunities specifically for doctoral researchers via JuDocS, the Jülich Center for Doctoral Researchers and Supervisors: https://www.fz-juelich.de/en/judocs

- Targeted services for international employees, e.g. through our International Advisory Service

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

The position is for a fixed term of 3 years. Pay in line with 75% of pay group 13 of the Collective Agreement for the Public Service (TVöD-Bund) and additionally 60 % of a monthly salary as special payment („Christmas bonus“). Further information on doctoral degrees at Forschungszentrum Jülich including our other locations is available at: https://www.fz-juelich.de/gp/Careers_Docs

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.