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. To achieve our ambitious goals, we bring to bear a diverse spectrum of methods and tools, from physical-mathematical theory and quantum mechanical simulations to continuum modelling. Our research program presents linkages for model evaluation by comparison with experiments, knowledge transfer to material design and development, and testing and analysis from materials to device level. Complementarily, we are developing an artificial intelligence-based platform for data analytics as well as materials design and development.

We are offering an interesting

**PhD Position – Theory and Simulation of Electrocatalyst Materials for Water Electrolysis**

**Your Job:**
Economically viable and environmentally friendly hydrogen-based energy technologies, such as fuel cells and electrolyzers, are of enormous strategic importance. Efficiently catalyzing the oxygen evolution reaction (OER) remains key challenge for the wide-spread commercialization of water electrolysis technologies. Owing to its excellent catalytic activity and stability, iridium oxide is the state-of-the-art anode catalyst for the OER in proton-exchange membrane water electrolyzers (PEMWE), but the price and scarcity of iridium are matter of concern. Employing quantum-mechanical methods, the newly hired PhD candidate will simulate and predict properties of mixed metal oxides as electrocatalysts for the OER. Computational workflows will be developed for automated processing of compositional libraries for relevant classes of mixed oxides. Basic materials descriptors towards combined activity and stability will be identified. AI-powered data analytics and inverse design approaches will be employed to predict...
materials combinations for optimized performance as PEMWE anode electrocatalysts. Computer simulations will be performed on latest supercomputer resources of the Jülich Supercomputing Centre (JSC). The work will make an essential contribution to the German-Canadian Materials Acceleration Centre (GC-MAC, https://gcmac.de).

Your Job:
- Development of computational workflows for simulating relevant properties of mixed metal oxides as electrocatalysts for water oxidation.
- Contribution to the elucidation of structure–composition–property relationships of mixed oxides towards application as anode electrocatalysts for water electrolyzers.
- Laying the foundation for the descriptor-based design of oxide electrocatalysts employing machine-learning methods, to be tested and exploited through collaboration with experimental partners (in synthesis and characterization).

Your Profile:
- M.Sc. degree in physics, chemistry, materials science, or related field
- Knowledge and competences in physical and chemical theory and molecular simulation methods
- Experience in computer programming
- Basic knowledge of electrochemistry and electrochemical energy technologies
- Intrinsic motivation and self-sufficiency
- Self-organized and independent work style
- Excellent collaboration and communication skills
- Highly proficient in spoken and written English and German

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:
- A highly motivated working group and an international and interdisciplinary working environment in one of the largest research institutions in Europe
- Excellent scientific and technical infrastructure
- Support from the scientists at IEK-13, who have a high level of expertise in theoretical electrochemistry and materials modelling
- Continuous professional support from your scientific supervisor
- Open discussion culture
- Diverse opportunities to develop professional skills
- Comprehensive training programme to best prepare you for a career, for example in academia or industry
- Network with leading global partners in academia and industry
- Excellent prospects and career opportunities in a dynamic technology sector
- Attractive flexitime organisation and a wide range of options for balancing work and family life
- Comprehensive company health management programme
- Optimal conditions for balancing work and private life as well as a family-friendly company policy
- The opportunity to work flexibly (in terms of location), e.g. homeoffice
- Targeted services for international employees, e.g. through our International Advisory Service
- 30 days of annual leave and provision for days off between public holidays and weekends (e.g. between Christmas and New Year)
- Opportunity to develop your strengths, e.g. through a comprehensive training programme; a structured programme including continuing professional development
and networking opportunities specifically designed for Jülich’s doctoral researchers by the Jülich Center for Doctoral Researchers and Supervisors (JuDocS):
https://go.fzj.de/JuDocs
• Working for one of the best employers in Germany - 6th place in the Glassdoor award for employee satisfaction:
  https://www.glassdoor.de/Award/Beste-Arbeitgeber-Deutschland-LST_KQ0.29.htm

The employment of doctoral researchers at Jülich is governed by a doctoral contract, which usually has a term of three years. Attractive 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

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.