



We are offering several

## **PhD positions for new programs in physical theory, modeling and simulation of energy materials**

Several PhD opportunities are available in the [IEK-13](#), a newly founded subinstitute in the Institute for Energy and Climate Research of the Forschungszentrum Jülich GmbH. IEK-13 pursues a program in theory, modeling, and simulation of complex functional materials for emerging energy technologies, such as fuel cells, batteries, electrolysis cells, and CO<sub>2</sub> reduction cells. Goals of the program are to increase fundamental understanding of vital electrochemical phenomena, support the development of tailor-made materials solutions and diagnostic approaches, and develop model-based tools for the evaluation and optimization of next-generation devices. To expedite this agenda, we make use of a broad inventory of tools, including calculations based on quantum mechanical density functional theory, molecular dynamics simulations (ab initio, classical, and coarse grained), Monte Carlo simulations, theory of transport phenomena in disordered media, kinetic theory, theoretical approaches of non-equilibrium thermodynamics, and continuum modeling.

Our research program offers ample interfaces for model evaluation by comparison to experiments, knowledge transfer to materials science laboratories, and testing and analytics of innovative materials in functional energy devices. The scientific program is complemented by the development of a Virtual Materials Intelligence platform.

In this playing field, there is a need for highly-qualified theory and modeling experts, whom we are offering to train and put at the forefront of exciting developments.

**Your job:**

You will conduct independent theoretical and/or computational research in one of the three major thrust areas of the institute, which focus on computational materials science, theoretical chemical physics, and physical modeling and diagnostics. Your general tasks will include gaining expert-type knowledge (context and perspective) in the field of study through extensive literature study, acquiring and expanding theoretical knowledge and mathematical/computational skills to formulate and solve insightful physical models, analyzing results, and communicating them effectively to collaborators and the scientific community at large.

**Your topic as a PhD student will be one (or a combination) of the following:**

**Topic 1:**

[Apply for topic 1 here](#)

- Develop a methodology for first principles theory and computation of electrochemical interfaces and reactions, using a combination of density functional theory, theory of electrochemical interfaces, and microkinetic modeling
- Apply the methodology to decipher crucial electrochemical reactions in fuel cells, electrolysis cells, and CO<sub>2</sub> reduction cells
- Develop criteria (descriptors) for selection and design of highly performing and stable electrocatalytic materials

**Topic 2:**

[Apply for topic 2 here](#)

- Study self-assembly and network formation in charged polymer materials, using mean-field theory and molecular dynamics simulations
- Rationalize physico-chemical properties in solutions, membranes and inks formed from charged polymer materials
- Study basic mechanisms of structural change that lead to aging, degradation, and failure

**Topic 3:**

[Apply for topic 3 here](#)

- Develop models of nanoprotic and -ionic materials and devices and solve them using continuum mean-field theories and classical dynamical density functional theory
- Analyze model solutions in view of the dynamic response of capacitor and electroactuator devices

**Topic 4:**

[Apply for topic 4 here](#)

- Develop advanced models of high-performance electrodes in fuel cells, electrolysis cells, and batteries
- Integrate interface models and agglomerate models into porous electrode models
- Address the following question: How can performance and lifetime be optimized for a wide range of operating conditions?

**Topic 5:**

[Apply for topic 5 here](#)

- Contribute to the development of a platform for modeling and intelligent diagnostics of dynamic phenomena in energy devices
- Develop models and methods for diagnostic purposes, implement and test them (in close collaboration with experimentalists)

**Topic 6:**

[Apply for topic 6 here](#)

- Contribute to the development of a Virtual Materials Intelligence platform (cognitive technology for autonomous materials R&D)

**Your profile:**

- Curiosity-driven, open-minded, aspiring, and goal-oriented personality
- Excellent university degree in physics, (electro-)chemistry, materials science, engineering science or other relevant discipline
- Strong interest and previous experience in theoretical and computational physics and mathematical modeling
- Knowledge of programming languages (e.g., Python, C++) and simulation software
- Fluent in spoken and written English
- Excellent organizational skills and ability to work independently
- Excellent cooperation and communication skills

**Our offer:**

- Vibrant and internationally well-connected research environment
- Excellent scientific and technical support
- Barrier-free, thought-provoking, and stimulating communication and cooperation
- Mentoring and structured guidance to develop scientific skills and research competencies
- Cross-sectional skill training for career in science, business, or research management
- Flexible working hours and mindfulness of work-life balance
- Degree completion within 3 years
- Degree in natural sciences (Dr. rer. nat.) or engineering (Dr. Ing.)
- Salary and social benefits in conformity with the provisions of the Collective Agreement for the Civil Service (TVöD). Salary grade 13 (75%) TVöD-Bund

If you are interested in more than one topic, you are welcome to apply for different topics. Please note, that you will have to apply individually for each topic that you are interested in.

Forschungszentrum Jülich aims to employ more women in this area and therefore particularly welcomes applications from women. We also welcome applications from disabled persons.

We look forward to receiving your application until August 31, 2019, via our online recruitment system.