Batteries move our world and are ubiquitous – they start the engine of our cars, they move the hands of your clocks and allow us to take pictures with our cell phones. The Helmholtz Institute Münster Ionics in Energy Storage (IEK-12) as part of the Institute of Energy and Climate research focusses on electrolyte research as a key area for future battery concepts. Major research activities comprise the development, characterization, and theoretical understanding of more sophisticated battery electrolytes. Our subinstitute is located within the branch office in Münster of Forschungszentrum Jülich in close cooperation with the University of Münster and RWTH Aachen University - in this way fostering joint research efforts while promoting this important forward-looking field of electrochemical energy storage.

We are offering a

**PhD position - Simulation of electrolytes at interfaces, using advances computational techniques**

**Your Job:**
Join the EU-funded BIG MAP project to develop new theoretical approaches to accelerate the design of significantly improved battery materials. Further information on the project can be found here: https://battery2030.eu/research/research-projects/big-map/

Your tasks in detail:
- You perform molecular dynamics simulations. The information about the force fields is either taken from standard packages, from quantum-mechanical input or from machine-learning based methods, thereby using a multiscale modelling framework.
- You write analysis programs to extract the relevant formation from the microscopic trajectories
- You strongly interact with experimental groups, working on high throughput screening (HTS) techniques and develop concepts of optimal experimental design to
establish a forward-backward loop between theory and experiment

- You take part in regular project meetings with the involved partners from research and industry

Your Profile:
- Completed Master’s degree in physics, chemistry, materials science, or a comparable field of study
- Competences in computer simulations. Knowledge of at least one programming language and basic experience with Unix-like operating systems are required
- Experience with machine-learning approaches is a plus
- Willingness to get familiar with different theoretical/computational tools
- Strong cooperation and communication skills required for internal and external project partners, including business trips
- Structured and independent way of working
- Ability to work together in an international and interdisciplinary team

Our Offer:
- Excellent scientific development opportunities at the Helmholtz Institute Münster as well as cooperation opportunities with our other research locations in Aachen and Jülich
- Opportunity to undertake a doctorate at the Department of Chemistry of the WWU Münster upon fulfillment of the requirements
- Chance of participating in (international) conferences and project meetings as part of your work
- Usually a contract for the duration of 3 years
- Pay in line with 50 % of pay group 13 of the Collective Agreement for the Public Service (TVöD-Bund)

Place of employment: Münster

Forschungszentrum Jülich promotes equal opportunities and diversity in its employment relations.
We also welcome applications from disabled persons.