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 6,400 employees in one of Europe's biggest research centres and help us to shape change!

With computer-aided research, we provide at the Institute of Energy and Climate Research- Theory and Computation of Energy Materials (IEK-13) essential contributions to the fundamental understanding of electrochemical phenomena, the development and characterization of tailored material solutions, and testing and optimization of energy technologies.
High entropy (HE) metal oxides are a new class of cathode materials for Li- and Na-ion based energy storage systems. Owing to their compositional flexibility and fast ion transport, Li transition metal oxides (LTMO) with cation-disordered rocksalt (DRX) structures are interesting compounds for the battery applications. In such a multi-compound system, thermodynamically driven structural arrangement of cations determines performance of the material including energy density and rate capability. Atomistic simulations are powerful tools to predict electrochemical capabilities of novel DRX compounds.

We are offering a

PhD Position - Simulation-guided design of high entropy cathode materials for Li-ion batteries

Your Job:
Within the the Computational Materials Modeling group of the IEK-13 (leader: Dr. Piotr Kowalski) we perform atomistic modeling-based investigation of materials properties using world-class supercomputing facilities of Forschungszentrum Jülich and RWTH Aachen University. Our work is undertaken in close partnership with the modeling group of the IEK-1 (Institute of Energy and Climate Research - Materials Synthesis and Processing, leader: Dr. Payam Kaghazchi).

This project aims at development of a self-consistent approach to simulate and design DRXs as cathode materials for Li-ion batteries. The successful candidate will apply state-of-the-art methods of atomistic modeling and electronic structure calculations to

The job will be advertised until the position has been successfully filled. You should therefore submit your application as soon as possible. We look forward to receiving your application 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

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audit berufundfamilie

simulate local atomic ordering and crystal structure (by IEK-13), as well as redox mechanism (by IEK-1) in novel HE-LTMO-DRX cathode materials. The computational approach will be validated by calculation of parameters that describe ionic conductivity and chemical stability followed by their comparison with experimental data provided by our experimental partners. Such a characterization will allow for the development of a reliable computational methodology that could be applied to design a multi-cation LTMO system with a high rate performance and stability. The developed approach will be used in the future to design novel HE materials from first principles calculations.

Your tasks in detail:

- Simulation of high entropy materials using ab initio calculations and thermodynamic modeling
- Performing calculations using supercomputers
- In-depth analysis of the computed data vs. current state of the knowledge
- Participation in national and international conferences, meetings and workshops
- Coordination of the project with internal and external partners
- Publication and presentation of research results in relevant journals and at international conferences

Your Profile:

- Successfully completed scientific master's degree in chemistry, physics, materials science, computational science or similar discipline
- Strong interest in the high-performance computing
- Basic knowledge in computational quantum chemistry will be of advantage
- High motivation for pursuing a PhD within 3 years
- Excellent organizational skills
- Ability to show initiative, work independently
- Excellent cooperation and communication skills and ability to work as part of a team,
- Fluency in spoken and written English.

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:

- Vibrant international and interdisciplinary working environment in one of the largest, research centers in Europe
- Outstanding scientific and technical infrastructure, including excellent supercomputing infrastructure
- Opportunity to participate in (international) conferences and project meetings
- Continuous scientific mentoring by your scientific advisor
- Research topic on energy materials of high importance to society
- Excellent opportunity for professional development, including training courses and participation in mentoring of students
- An attractive doctoral degree programme within doctoral researchers' platform JuDocs https://www.fz-juelich.de/judocs and HITEC interdisciplinary Doctoral Training in Energy and Climate Research: https://www.fz-juelich.de/hitec/DE/_node.htm.
- Targeted services for international employees, e.g. through our International Advisory Service

The position is initially for a fixed term of 3 years. Pay above average 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: www.fz-juelich.de/gp/Careers_Docs

Forschungszentrum Jülich promotes equal opportunities and diversity in its employment relations.

We also welcome applications from disabled persons.