**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Energy and Climate Reserch, Materials Synthesis and

Processing (IEK-1)

http://www.fz-juelich.de/iek/iek-1/EN/Home/home node.html

Prof. Dr. D. Fattakhova-Rohlfing, Dr. Frank Tietz, Supervising scientist:

Dr. Enkhtsetseg Dashjav

University for Registration: University Duisburg-Essen (UDE)

Solid state lithium batteries Research Field:

Position: PhD Student X Joint PhD Student □

#### Research Area:

Solid-state batteries is one of the most dynamically developing technologies with a promise of greatly increased storage capacity and improved safety as compared to classic batteries with liquid electrolytes. Particularly, ceramic oxide- and phosphate-electrolyte based batteries attract attention due to their chemical and electrochemical stability and the industrial relevance. The practical realization of such batteries is however still hampered by the lack of suitable processing techniques and the general understanding of material compatibility - the challenges that are going to be addressed in this project. This project aims at the design of full Lisolid state battery based on the phosphate electrolyte and cathode materials, as well as the development of scalable routes to their processing. Besides the materials development and material and microstructural characterization, the project will include the development of ceramic processing technologies as well as the electrochemical characterization.

## Specific Requirements:

- Master degree in chemistry or physics or materials science with good performance in university and post-graduate period
- Good written and spoken English knowledge or German
- Basic knowledge of inorganic material synthesis and processing, microstructure design and electrochemistry

Duration of stay:

36 months

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

September 2019

Language Requirement: Excellent command of English, written and spoken, A German

language course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. D. Fattakhova-Rohlfing, Dr. F. Tietz,

Dr. E. Dashjav, Forschungszentrum Juelich GmbH, Institute of Energy and Climate Research (IEK-1), 52425 Jülich, Germany: d.fattakhova@fz-juelich.de), (f.tietz@fz-juelich.de),

(e.dashjav@fz-juelich.de)

**Helmholtz Centre:** Forschungszentrum Juelich GmbH – www.fz-juelich.de

Department/Institute: Institute of Energy and Climate Research, Troposphere (IEK-8)

http://www.fz-juelich.de/iek/iek-8/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. Thomas F. Mentel

University for Registration: University of Cologne

Research Field: Aerosol Monitoring

Position: PhD Student X Joint PhD Student □

#### Research Area:

Impact of clouds, and hereby aerosol cloud interactions are the largest uncertainties in understanding radiative balance of the Earth. These uncertainties are a large obstacle for the predictive power of climate models. In Jülich we are in the unique situation to have a Meteorological tower on the site and the continuously operating Jülich Observatory for Cloud Evolution (JOYCE). We are operating an aerosol mass spectrometer, aerosol size distribution and cloud condensation nuclei measurements at the Meteorological tower in three heights. The goal is to provide long term simultaneous observations of aerosol composition (aerosol mass spectrometry) and microphysical properties (CCN activity) over several seasonal cycles. The thesis project will provide a unique set of observations and interpretations. By analysis of aerosol composition and CCN activity these properties will be related to regional and local aerosol sources.

#### Specific Requirements:

- Master degree in Physics, Chemistry, Meteorology, or Environmental sciences
- The PhD work requires good skills in experimental work, programming and statistical analysis of data, as well as willingness to cooperate in teams.
- Experience in mass spectrometry or measurement of aerosols are welcome
- We expect that the candidate can communicate her/his results in oral and written form in English.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Juelich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Thomas F. Mentel, Forschungszentrum Juelich,

Institute of Energy and Climate Research (IEK-8), 52425 Juelich,

Germany; E-Mail: t.mentel@fz-juelich.de

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute:

Institute of Bio- and Geoscience, Biotechnology (IBG-1)

http://www.fz-juelich.de/ibg/ibg-1/EN/

Supervising scientist: Dr. Eric von Lieres

University for Registration: RWTH Aachen University

Research Field:

Model-Based Analysis and Optimization of Preparative Chromatography

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

Chromatography is the most important unit operation for the industrial purification of biopharmaceutical products. Our group has developed the Chromatography Analysis and Design Toolkit (CADET) and provides it to the scientific community as open source code (https://github.com/modsim/CADET). CADET runs on multiple platforms and is currently extended and applied to various applications of both academic and industrial relevance. This particularly includes rational process analysis (identify mechanisms and model parameters), process optimization (improve devices and operating conditions), scale up (transfer process knowledge from laboratory to production scale), and experimental design (maximize measured information).

### Specific Requirements:

We seek a qualified and highly motivated PhD student for process modeling, data analysis and for extending the CADET framework to novel applications. A solid background in modeling and simulation and some experience in biotechnology applications are essential for the project. Programming skills in MATLAB/Python and/or C++ are required, and specific knowledge of separation techniques and would be beneficial. Good command of the English language is necessary.

**Duration of stay:** 

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

September 2019

Language Requirement: Excellent command of English, written and spoken. A German language course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Eric von Lieres, Forschungszentrum Jülich, Institute of

Bio- and Geosciences (IBG-1), 52425 Jülich, Germany; E-Mail:

e.von.lieres@fz-juelich.de

Helmholtz Centre: Forschungszentrum Julich GmbH – www.fz-juelich.de

**Department/Institute:** Institute of Bio- and Geoscience, Agrosphere (IBG-3)

http://www.fz-juelich.de/ibg/ibg-3/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. Harrie-Jan Hendricks-Franssen

University for Registration: RWTH Aachen

Research Field: Hydrology / Simulation Sciences

Position: PhD Student X Joint PhD Student □

#### Research Area:

TerrSysMP-PDAF is an integrated model for simulations from the deep subsurface into the upper atmosphere coupled to a data assimilation framework. Currently it is able to assimilate groundwater level, soil moisture and river stage data and it will be extended in the near future to assimilate further data types. In this PhD-project it is planned to further exploit the existing set-up of the coupled land surface-subsurface model for the EURO-CORDEX domain (Europe) including data assimilation capacity to create a reanalysis for the land surface-subsurface over the European continent. In a first step, an ensemble of coupled land surface-subsurface model runs at 12km resolution over Europe is made, driven by atmospheric reanalysis data. It is checked whether the ensemble can reproduce enough spread in model states. In a second step, crucial hydrological observations will be assimilated for a time period of 20 years in the 21st century. These observations include remotely sensed soil moisture, water storage, river discharge and leaf area index. Independent verification data will be used to check the quality of the data assimilation to make sure that the characterization of hydrological states and fluxes improved compared to the open loop run. In the third step the reanalysis is established for the land surfacesubsurface over the 20 years period and the analysis of the reanalysis in terms of changes in water storage in aquifers and the unsaturated zone and changes in fluxes like groundwater recharge, evapotranspiration and river discharge.

#### Specific Requirements:

- The candidate should have a MSc in one of the earth sciences (for example meteorology, hydrology, soil science or environmental engineering) with a focus on quantitative methods or have a MSc in informatics or physics with a strong interest in geosciences.
- Solid background in mathematical statistics and model simulations is important.
- Background in computer programming and analysis of large datasets is of advantage.

Duration of stay: 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: Excellent command of English, written and spoken. A German language

will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Harrie-Jan Hendricks-Franssen,

Forschungszentrum Julich GmbH, Institute of Bio- and Geoscience (IBG-3), 52425 Jülich, Germany; h.hendricks-franssen@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute for Advanced Simulations (IAS), Computational Biomedicine

(IAS-5 / INM-9)

http://www.fz-juelich.de/ias/ias-5/EN/Home/home\_node.html

Supervising scientist: Dr. Vania Calandrini

University for Registration: RWTH Aachen University

Research Field: Modeling Neuronal Information Processing

Position: PhD Student X Joint PhD Student

### Research Area:

Neurotransmission is driven by molecular signaling cascades, mediating very complex processes, such as memory, learning, mood etc. These signaling processes involve tens to hundreds of molecules (proteins, neurotransmitters, chemicals) in highly crowded environments, such as cell membrane and cytosol, that have to diffuse, meet and interact at the correct time at the correct place. Knowing how key physicochemical features, such as compartmentalization, membrane composition, diffusion processes, mutations, crowding or electric fields, combine together and shape over time and space neuronal signaling would provide important hints on the human brain functioning.

The PhD will dissect the interplay among these aspects through the implementation of a mesoscale stochastic model of collective phenomena relevant to neuronal cascades using mean-field-like approaches based on statistical mechanics methods and higher-resolution forcefield-based deterministic simulations.

### Specific Requirements:

We encourage applications from candidates with a Master degree in Physics (preferred), Chemistry, Applied Mathematics, or Computational sciences. We are seeking for a candidate familiar with Brownian dynamics and/or molecular dynamics simulation methods applied to biophysical systems, soft matter, or statistical mechanics problems, and with a strong interest in simulation and theoretical work in statistical physics. Teamwork attitude and ability to communicate effectively in English are required.

Duration of stay: 4 years

Work Place: INM-9/IAS-5, Forschungszentrum Jülich

Earliest Start: October 2019

Language Requirement: Excellent command of English language, both written and verbal. A

German language course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Vania Calandrini, Forschungszentrum Jülich,

IAS-5 / INM-9, 52425 Jülich, Germany; E-Mail: v.calandrini@fz-

juelich.de

**Helmholtz Centre:** Forschungszentrum Juelich – www.fz-juelich.de

Department/Institute: Juelich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz

Zentrum (MLZ), Garching (near Munich)

http://www.fz-juelich.de/jcns/EN/Home/home\_node.html

Supervising scientist: Dr. Yixi Su, Prof. Dr. Thomas Brueckel

University for Registration: RWTH Aachen University

Research Field: Condensed Matter Physics, Materials Physics

**Research Project:** Crystal growth and neutron scattering studies of quantum materials

Position: PhD Student ☑ Joint PhD Student □

### Research Area:

Quantum materials have become a focus of intense research owing to the remarkable possibilities to realize emergent quasiparticles such as magnetic monopoles, Weyl and Majorana fermions. Realization and eventual manipulation of those exotic quasiparticles in condensed matter may lead to applications for future information and quantum technology such as decoherence-free quantum computing. We are seeking highly motivated PhD students to work on the single crystal growth and neutron scattering studies of quantum materials with the focus on frustrated quantum magnets and correlated topological materials. The main aim is to elucidate the interplay between lattice structure, magnetism and unusual transport properties in quantum materials. Typical tasks of the potential candidates would include single-crystal growth mainly via the flux method, characterizations of physical properties via SQUID and PPMS, and determinations of crystalline and magnetic structures via neutron and x-ray diffraction. As one of the leading neutron science centers in the world, the Jülich Centre for Neutron Science JCNS operates many advanced neutron scattering instruments at some of the most powerful neutron sources in the world such as FRM II (Garching, Germany), ILL (Grenoble, France) and the SNS (Oak Ridge, USA), which can be ideally used for this project. You will be located at the JCNS institute at the MLZ in the Munich area, where you can also take advantage of working and studying in the stimulating science campus of Technical University Munich (TUM), and of living in the beautiful city of Munich.

### Specific Requirements:

The candidates are expected to hold a Master degree in condensed matter physics or in materials physics with excellent grades. Experience and training in magnetism and magnetic material research are highly desired. Very good knowledge of English is required. You are expected to work in a young and dynamic team including a number of PhD students and postdocs, both independent- and team-work are important. Additional allowance is possible for excellent candidates.

**Duration of stay:** 4 years for PhD

Work Place: Juelich Centre for Neutron Science JCNS at MLZ, Garching near Munich

Earliest Start: September 2019

Language Requirement: Very good knowledge of English language, written and spoken. A

German language course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Yixi Su, Juelich Centre for Neutron Science JCNS at

MLZ, Forschungszentrum Juelich, Lichtenbergstr. 1, 85747 Garching,

Germany (e-mail: y.su@fz-juelich.de)

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Jülich Supercomputing Centre

http://www.fz-juelich.de/ias/jsc/EN/Home/home\_node.html

Supervising scientist: Dr. Paul F. Baumeister

University for Registration: RWTH Aachen University

Research Field: Interdisciplinary: Physics + Applied Mathematics + Computer Science

Position: PhD Student ☑ Joint PhD Student □

#### Research Area:

The aim of this PhD project is to assess the viability and performance of a novel real-space Green's function (Gf)-based approach towards density functional theory (DFT). The design of new materials with outstanding properties and potential application to data storage or quantum computing requires large-scale DFT calculations on current supercomputers. It has been shown that linear-scaling DFT algorithms exist in the framework of density matrix methods and, even allowing to treat metallicity, on the base of Green's functions. With the use of very efficient basis sets featuring small numbers of numerically adopted atomic orbitals the computational workloads of these methods can be tackled easily by state-of-the-art computers comprising high-performance hardware. The drawback of limited atom-centered basis sets is a moderate accuracy when it comes to force calculations. Structural relaxation, however, is a key to the predictive power of DFT for the design of realistic materials. DFT on equidistant real-space grids comes at higher cost factors but gives access to plane-wave accuracy for total energies and forces.

## **Specific Requirements:**

The ideal candidate is trained in physics, preferentially theoretical solid state physics, theoretical chemistry or similar, augmented by mathematical analytical skills from the fields of partial differential equations and linear algebra.

Experience with a high-level programming language like C, C++, F90 or equivalent are a valuable asset. In addition, any sort of software engineering skills from the area of scientific software development are welcome. Personal interest in current and future computer architectures and first experience with programming vectorized and accelerated processors like GPUs would be of great benefit.

The candidate should best have an open-minded character and should tend to solve conflicts by communication. Strong presentation skills are desirable. Furthermore, a self-contained working style as complement to regular discussions with the supervisor is preferable. The candidate should bring an ambitious desire to work in an interdisciplinary environment at one of Europe's top-tier supercomputing facilities and embrace also challenges that reach beyond her/his fields of expertise.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Paul F. Baumeister, Forschungszentrum Jülich, Jülich

Supercomputing Centre, 52428 Jülich, Germany

p.baumeister@fz-juelich.de

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH - www.fz-juelich.de

Department/Institute:

Institute of Energy and Climate Research, Photovoltaics (IEK-5) http://www.fz-juelich.de/iek/iek-5/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. Thomas Kirchartz

University for Registration: Duisburg-Essen

Research Field:

**Photovoltaics** 

Position:

PhD Student X

Joint PhD Student

#### Research Area:

Solar cells made from lead-halide based perovskites have been shown to enable efficiencies > 20 % using a solution-based fabrication process. However, the materials currently lack stability and are insufficiently well understood in many respects related to electrostatics and charge carrier recombination in these materials. We are looking for candidates that support our research efforts on fabricating and characterizing layers of lead-halide perovskites. In particular, we are interested in improving material stability e.g. by using stable methyl-ammonium-free combinations of cations. In addition to quality and stability of the active layer, we are also interested in band gap tuning for tandem applications as well as tuning of interfacial layers for increased open-circuit voltages and fill factors. Characterization of solar cells and films using transient and steady-state photoluminescence methods will be used to better understand the losses due to recombination and due to resistive effects. Depending on the profile of the applicant a slightly different focus of the project is possible and candidates with a background in physics or in chemistry are both encouraged to apply.

#### Specific Requirements:

The successful candidate should have a background in physics, chemistry, materials science or electrical engineering and be familiar with the fabrication and characterization of semiconductor devices and semiconducting materials (ideally solar cells).

**Duration of stay:** 

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start:

September 2019

Language Requirement: Excellent command of English, written and spoken. A German language will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Thomas Kirchartz, Forschungszentrum Jülich,

Institute of Energy and Climate Research (IEK-5), 52425 Jülich,

Germany; t.kirchartz@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

**Department/Institute:** Ernst Ruska-Center (ER-C) for microscopy and spectroscopy with

electrons, Physics of Nanoscale Systems (ER-C-1 / PGI-5) http://www.fz-juelich.de/er-c/er-c-1/DE/Home/home\_node.html

Supervising scientist: Prof. Dr. Rafal Dunin-Borkowski, Dr. Marc Heggen, Dr. Xiankui Wei

University for Registration: Rheinisch-Westfälische Technische Hochschule Aachen (RWTH

Aachen)

Research Field: In-situ electric-field (scanning) transmission electron microscopy

Position: PhD Student □ √ Joint PhD Student □

#### Research Area:

Rechargeable batteries are in great demand for applications such as electric vehicles and stationary energy storage devices. Solid-state batteries are currently attracting attention for use as next-generation energy sources, as a result of their lack of leakage, non-volatility, non-flammability, separator-free design and wide working temperature range. In particular, all-solid-state batteries that make use of earth-abundant Na provide an attractive and low-cost alternative to lithium batteries. The proposed project involves in-depth research into all-solid-state sodium batteries using *in-situ* (scanning) transmission electron microscopy. By investigating dynamic charging-discharging process in the presence of an electric field, changes in microstructure, composition and valence state in the parent phases will be characterized at the atomic scale. The possible presence of novel interfacial phases will also be investigated. The results will provide guidance for the design of future sodium battery materials.

### Specific Requirements:

The applicant should have a Master degree in physics, materials science, chemistry or a related field, with excellent academic performance. A basic knowledge of transmission electron microscopy, condensed matter physics, batteries and electrochemistry is expected. The applicant should have good hands-on experimental skills, enthusiasm for scientific research and be proficient in English.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Rafal Dunin-Borkowski), Dr. Marc Heggen and

Dr. Xiankui Wei, Forschungszentrum Jülich GmbH, Ernst Ruska-Center (ER-C-1/PGI-5), 52425 Jülich, Germany; E-mail: r.dunin-borkowsky@fz-

juelich.de; m.heggen@fz-juelich.de; x.wei@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Bio- and Geosciences, Agrosphere (IBG-3)

http://www.fz-juelich.de/ibg/ibg-3/EN/Home/home\_node.html

Supervising scientist: Dr. Bei Wu, Prof. Dr. Wulf Amelung

University for Registration: University of Bonn

Research Field: Si fertilization in paddy soils with purpose of organic rice cultivation

Position: PhD Student √ Joint PhD Student □

Research Area:

With the purpose of sustainable rice cultivation, conversion of conventional paddy fields to organic rice farming is necessary. Because pesticides are no longer allowed to be used in the converted paddy fields, one of the key questions is how to protect rice from being affected by pathogens to ensure a reasonable yield. In addition, as Cd and As are common inorganic pollutants in paddy fields and can be accumulated in the rice products, the question of how to eliminate such contaminations in organic rice rises. Literature and pioneering field practices have shown that, together with other strategies such as organic fertilization, Si fertilization cannot only protect rice from pathogen infection, but also hamper heavy metal/metalloids translocation and accumulation in rice. However, many questions still remain open, such as how does the rice take up Si? What is the Si-fertilization use efficiency? What strategy should be applied regarding Si-fertilization? Therefore, this PhD project aims at answering these questions and applies the optimized Si-fertilization strategy in paddy fields. This project is closely linked with our project of sustainable rice cultivation in the Mekong Delta in Vietnam supported by German Federal Ministry of Education and Research. The successful thesis will be graded by Prof. Wulf Amelung and will be defended at the Faculty of Agriculture of the University of Bonn.

#### Specific Requirements:

Master's degree in Soil Sciences, Agricultural Sciences, or Environmental Sciences. Good at inorganic analytical chemistry and soil-plant analyses. Experiences with Si fertilization and analyses of Si by inductively coupled plasma mass spectrometry (ICP-MS), familiar with paddy ecosystems are advantageous. Fluent in English writing and communication.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Bei Wu, Forschungszentrum Jülich, Institute of Bio-

and Geosciences (IBG-3), 52425 Jülich, Germany

E-mail: b.wu@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH - www.fz-juelich.de

Department/Institute: Institute of Neuroscience and Medicine, Medical Imaging Physics

(INM-4), http://www.fz-juelich.de/inm/inm-4/EN/Home/home\_node.html

Supervising scientist: Dr. J. Scheins, Prof. Dr. N. J. Shah

University for Registration: RWTH Aachen University

Research Field: Positron Emission Tomography (PET), Neuorimaging, PET/MR hybrid

scanners

Position: PhD Student X Joint PhD Student a

#### Research Area:

The Institute of Neuroscience and Medicine (INM-4) is currently developing a second generation Positron Emission Tomography (PET) scanner as hybrid PET/MR system for advanced neuroscience research. The new scanner involves cutting-edge technology with a 3-layer detector block design, digital silicon photomultipliers (SiPMs) and a highly flexible data acquisition platform, thus offering novel opportunities for improvements of PET image quality. In this context, the applicant is going to work in the field of iterative PET image reconstruction based on our in-house PET Reconstruction Software (PRESTO). As major goal, accurate point spread function (PSF) maps of the scanner should be derived from measurements based on the extended detector information provided by the novel PET scanner generation. In a second step, the obtained PSF maps have to be efficiently integrated into the reconstruction process using PRESTO with subsequent performance validation.

The INM in Juelich provides a world-wide highly reputed research in neuroscience and a unique environment to support breakthrough discoveries. Among a 3Tesla Tim Trio MR/BrainPET system, it runs a Siemens 7T MR Terra scanner, which is foreseen to host the new PET system.

The successful applicant will participate in interdisciplinary research related to the development, validation and application of the new strategies in fully-3D iterative PET Image Reconstruction for challenging new PET scanner hardware.

#### **Specific Requirements:**

Required: excellent educational records in the related field, good programming skills (preferred C++) and data processing skills, solid knowledge of mathematics and statistics Assets: experience with PET data acquisition and iterative image reconstruction, good knowledge of English language, basic knowledge on FPGAs, GPU programming Preferred applicant's background: physics, informatics, maths or related.

**Duration of stay:** 4 years

Work Place: Research Centre Juelich, Germany (near Cologne)

Earliest Start: October 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. J. Scheins, Prof. Dr. N. J. Shah, Forschungszentrum

Jülich, Institute of Neuroscience and Medicine (INM-4), 52425 Jülich,

Germany; j.scheins@fz-juelich.de

Helmholtz Centre:

Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute:

Institute of Energy and Climate Research, Electrochemical Process

Engineering (IEK-3)

http://www.fz-juelich.de/iek/iek-3/EN/Home/home node.html

Supervising scientist: Dr. Heidi U. Heinrichs, Prof. Dr. Detlef Stolten

University for Registration: RWTH Aachen University

Research Field:

Energy system analysis

Position:

PhD Student √

Joint PhD Student □

### Research Area:

Title: Assessing the global development of bioenergy demand and trade Background: Globally traded renewable energies and thereby produced raw materials ('renewable resources') show the potential to become the new global commodity of the 21st century. How this will impact global trade and future energy systems is still an open question and forms the motivation of this proposed research topic.

Your task: Your research will focus on the global demand of bioenergy and possible trade pathways. For this you will determine the development of the global demand of bioenergy in a spatially and temporally detailed way and take emerging technologies in the field of bioenergy as well as the impact of possible climatic effects into account, too. Finally, you will assess the current and potential future global trade of bioenergy and combine this with your findings from the demand analysis.

## Specific Requirements:

- Very good academic records in agricultural economics, energy engineering, energy systems engineering, renewable energy engineering, sustainable energy supply or a comparable field
- Advanced knowledge in technologies related to bioenergy processing and demand
- Knowledge in energy systems modelling is beneficial
- Interest in renewable energy, energy systems and future energy markets
- High individual motivation, good analytical skills and fluent command of English
- Experience of programming in GIS and Python is beneficial

**Duration of stay:** 

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

October 2019

Language Requirement: Excellent command of English, written and spoken (CEFR level C1 or higher). A German language course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Detlef Stolten, Forschungszentrum Jülch,

Institute of Energy and Climate Research (IEK-3), 52425 Jülich,

Germany; d.stolten@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Energy and Climate Research, Electrochemical Process

Engineering (IEK-3)

http://www.fz-juelich.de/iek/iek-3/EN/Home/home\_node.html

Supervising scientist: Dr. Heidi U. Heinrichs, Prof. Dr. Detlef Stolten

University for Registration: RWTH Aachen University

Research Field: Energy system analysis

PhD Student √ Position: Joint PhD Student

#### Research Area:

Title: Assessing the global sustainable bioenergy potential and trade Background: Globally traded renewable energies and thereby produced raw materials ('renewable resources') show the potential to become the new global commodity of the 21st century. How this will impact global trade and future energy systems is still an open question and forms the motivation of this proposed research topic.

Your task: Your research will focus on the global production potential of bioenergy and possible trade pathways. For this you will determine the sustainable global potential in a spatially and temporally detailed way and take emerging technologies in the field of bioenergy as well as the impact of possible climatic effects into account, too. Finally, you will assess the current and potential future global trade of bioenergy and combine this with your findings from the potential analysis.

## Specific Requirements:

- Very good academic records in agricultural economics, energy engineering, energy systems engineering, renewable energy engineering, sustainable energy supply or a comparable field
- Advanced knowledge in agricultural constraints of bioenergy and technologies related to bioenergy processing
- Knowledge in energy systems modelling is beneficial
- Interest in renewable energy, energy systems and future energy markets
- High individual motivation, good analytical skills and fluent command of English
- Experience of programming in GIS and Python is beneficial

**Duration of stay:** 

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start:

October 2019

Language Requirement: Excellent command of English, written and spoken (CEFR level C1 or

higher). A German language course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Detlef Stolten, Forschungszentrum Jülch,

Institute of Energy and Climate Research (IEK-3), 52425 Jülich,

Germany; d.stolten@fz-juelich.de

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Neuroscience and Medicine, Medical Imaging Department

(INM-4), www.fz-juelich.de/inm/inm-4/EN

Supervising scientist: Prof. Dr. N. J. Shah, Dr. J. Dammers

Research Project: Deep learning-based analysis strategies in functional neuroimaging

Research Field: Deep learning, neuroimaging, signal processing

Position: PhD Student X Sandwich PhD Student □

#### Research Area:

The relationship between electrophysiological activity and hemodynamics is typically referred to as neurovascular coupling. It describes the link between the neural activity that is accompanied by cerebral blood flow. In multimodal recordings, such as magneto- and electroencephalography (MEG, EEG) or functional magnetic resonance (fMRI) information about the underlying processes is recorded using different neuroimaging modalities. Tackling the aim of decoding the mechanisms underlying specific brain functions, the challenge lies in combining such complementary information as these different activation profiles act on different spatial and temporal scales.

In this project, we propose to develop a novel data analysis workflow for multimodal data integration, which is capable of bridging different scales between different neuroimaging modalities by utilizing novel machine learning strategies. The evaluation of the analysis workflow includes a simulation benchmark as well as real data analysis using existing data from multimodal recordings performed at Jülich.

### Specific Requirements:

Desirable: Experience with the methodology of deep learning as well as strong signal processing and programming skills.

Obligatory: Excellent educational records in the related field, programming skills in Python, EEG signal processing.

Desirable applicant's background: Computer Science, math or physics,

electrophysiology, neuroscience and related. Good knowledge of English language

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich, Jülich, Germany (near Cologne)

Earliest Start: October 2018

Language Requirement: Excellent command of English, written and spoken. A German

language course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. J. Dammers, Prof. Dr. N.J. Shah,

Forschungszentrum Jülich, Institute of Neuroscience and Medicine

(INM-4), 52425 Jülich, Germany; j.dammers@fz-juelich.de

Forschungszentrum Jülich GmbH - www.fz-juelich.de **Helmholtz Centre:** 

Institute of Neuroscience and Medicine, Medical Imaging Department Department/Institute:

(INM-3), www.fz-juelich.de/inm/inm-3/EN

Supervising scientists: Prof. Dr. K. Vogeley, Dr. J. Dammers

University for Registration: University of Cologne

Uncover the brain dynamics of time experience Research Project:

Neuroimaging, MEG/EEG data analysis, Psychology Research Field:

Sandwich PhD Student □ PhD Student X Position:

### Research Area:

The sense of time co-constitutes our subjective experience and embodied selfconsciousness. Time experience can be disturbed under psychopathological conditions and give rise to a variety of psychopathological symptoms. The project aims at uncovering the neural dynamics of the underlying network processing time experience, including the analysis of the causal relationship of brain regions being involved, both under conditions of mental health and psychiatric disturbances (depression, schizophrenia, autism). For this purpose, magnetoencephalography (MEG) provides excellent temporal resolution and allows to investigate slow and rapid interactions between functionally connected brain areas. The Institute of Neuroscience and Medicine at FZ Jülich provides a world-wide highly reputed research in neuroscience and a unique environment to support breakthrough discoveries. The project will be embedded in an interdisciplinary research consortium VIRTUALTIMES (EU, horizon 2020, 2019-2022). The successful applicant will participate in interdisciplinary research related to cognitive neuroscience and to the development and validation of new strategies in MEG data analysis.

## Specific Requirements:

Desirable: Experience with MEG or EEG data acquisition and analysis.

Obligatory: Excellent educational records in the related field, good programming and data processing skills, time series analysis.

Desirable applicant's background: Neuroscience, electrophysiology, physics,

neuroscience and related. Good knowledge of English language.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

October 2019 Earliest Start:

Language Requirement: Very good command of English, written and spoken. A German

language course will be offered parallel to the project.

Name and Address of Supervisors: Prof. Dr. Dr. K. Vogeley (INM-3), Dr. J. Dammers (INM-4),

Forschungszentrum Jülich, Institute of Neuroscience and Medicine

(INM-3), 52425 Jülich, Germany, j.dammers@fz-juelich.de

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH - www.fz-juelich.de

Department/Institute:

Institute of Neuroscience and Medicine, Structural and functional

organisation of the brain (INM-1)

http://www.fz-juelich.de/inm/inm-1/EN/Home/home\_node.html

Supervising scientist:

Prof. Dr. med. Dr. rer. pol. Svenja Caspers

Dr.-Ing, Jan Schreiber

University for Registration: Heinrich-Heine University Düsseldorf

Research Field:

Neuroscience

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

The Workgroup "Connectivity" at the INM-1 of the Research Center Jülich investigates structure and function of the normal aging brain and assesses factors that might contribute to the high interindividual variability seen in older adults. In this framework the planned research project aims at clarifying the processes involved in brain aging. The human brain changes with age and it has been shown that grey matter structural features can be used to compute a so called "BrainAGE Score". We are interested in the micro structural changes within grey and white matter as they occur during the aging process, particularly in connections via fiber bundles of the white matter. Diffusion weighted MRI allows for probing the white matter microstructure in vivo and provides qualitative maps representing features of the fiber bundle structure. The goal of this PhD project is to use methods of Machine Learning as well as Deep Learning to extract relevant features within these fiber bundles for capturing and predicting age related changes in the human brain based on large cohorts of thousands of in-vivo neuroimaging data.

## Specific Requirements:

The candidate should

- have a background in neuroscience, statistics, neuroinformatics or a closely related field
- be experienced in machine learning
- be experienced with UNIX-like operating systems and programming
- be fluent in spoken and written English

Knowledge on concepts of aging and structural neuroanatomy is desired.

Duration of stay:

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

September 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Dr. Svenja Caspers, Forschungszuentrum

Jülich, Institute of Neuroscience and Medicine (INM-1), 52425 Jülich,

Germany; s.caspers@fz-juelich.de

Helmholtz Centre: Forschungszentrum Jülich GmbH - www.fz-juelich.de

Institute of Neuroscience and Medicine, Structural and functional Department/Institute:

organisation of the brain (INM-1)

http://www.fz-juelich.de/inm/inm-1/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. med. Dr. rer. pol. Svenja Caspers

Dr. rer. medic. Christiane Jockwitz

University for Registration: Heinrich-Heine University Düsseldorf

Research Field: Neuroscience

Position: PhD Student X Joint PhD Student

### Research Area:

The Workgroup "Connectivity" at the INM-1 of the Research Center Jülich investigates structure and function of the normal aging brain and assesses factors that might contribute to the high interindividual variability seen in older adults. In this framework the planned research project aims at breaking through the long-lasting stereotype of differences between men and women in terms of cognitive abilities and brain structure and function. Men and women seem to partially differ in terms of cognitive performances, such as verbal versus spatial cognitive abilities. However, recent studies also showed that there is considerable overlap between the two sexes. In the planned project, we will investigate sex-specific cognitive processing strategies i.e. the way to solve a specific cognitive task, and relate this to the brain's architecture, i.e. brain structure and function using machine learning methods. Thereby, we aim at characterizing cognitive strategies based on multimodal brain imaging markers into different "cognitive processing strategy" groups rather than stratifying samples by sex.

### Specific Requirements:

The candidate should

- have a background in neuroscience, psychology, neuroinformatics or a closely related field
- be experienced with UNIX-like operating systems and programming
- be experienced in machine learning
- be fluent in spoken and written English

Knowledge on cognitive aging theories and functional neuroanatomy is desired.

**Duration of stay:** 

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start:

September 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Svenja Caspers, Forschungszentrum Jülich,

Institute of Neuroscience and Medicine (INM-1), 52425 Jülich, Germany

s.caspers@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Energy and Climate Research, Materials Synthesis and

Processing (IEK-1); http://www.fz-juelich.de/iek/iek-1/EN/Research/ElektrochemischeSpeicher/\_node.html

Supervising scientist: Prof. Dr. Olivier Guillon, Dr. Norbert H. Menzler, Dr. Mariya E. Ivanova

University for Registration: Rheinisch-Westfälische Technische Hochschule Aachen (RWTH)

Research Field: Proton conducting ceramic cells

Position: PhD Student □X Joint PhD Student □

### Research Area:

The main research topic of the applicant will be the development of proton conducting ceramic cell (PCCC), which can be then operated both as a fuel and an electrolysis cell. Proton conducting ceramics based on BaZrO<sub>3</sub>-BaCeO<sub>3</sub> solid solutions are viable choices for achieving the target performance of solid oxide cells operating at 400-500°C, while exhibiting reasonable stability and durability under steam conditions. Such materials display promising values of bulk proton conduction in the range of 10<sup>-2</sup> S/cm at low temperatures which suffice to achieve area specific resistance of electrolyte of 0.1  $\Omega \cdot \text{cm}^2$ . In any case, the significantly blocking nature of their grain boundaries restricts the overall electric performance of these materials. Therefore, the major task of the candidate will be to develop a specially designed anode supported electrolyte layer with thickness of 1-2 µm with preferable orientation of the crystal grains along the transport direction of charges. By that the transport pathways will be less impeded by the grain boundaries, while the overall performance will be largely dependent on material bulk (grain interior) properties. A part of the candidate's doctoral project will be also to develop the cell electrodes with tailored microstructure including deposition of thin electrode functional layers. The thermal and chemical compatibility of the components will be tested to ensure good cell integrity. Finally, cell performance will be tested in galvanic and electrolytic mode at 400-500°C.

### Specific Requirements:

The applicant should have master degree in material science, chemistry, physics or related area, with good performance in university and post-graduate period. Basic knowledge of inorganic material synthesis and processing, microstructure design and electrochemistry is necessary. The applicant should also have excellent English skills with German as a plus.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich GmbH, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Excellent command of English, written and spoken. A German language

course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. O. Guillon (o.guillon@fz-juelich.de), Dr. N. H.

Menzler (n.h.menzler@fz-juelich.de), Dr. M. E. Ivanova (m.ivanova@fz-juelich.de), Forschungszentrum Jülich GmbH, Institute of Energy and

Climate Research (IEK-1), 52425 Jülich, Germany

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Bio- and Geoscience, Agrosphere (IBG-3)

http://www.fz-juelich.de/ibg/ibg-3/EN/Home/home\_node.html

Supervising scientist: Dr. Anne E. Berns

University for Registration: University of Bonn

Research Field: Soil Science

Position: PhD Student X Joint PhD Student □

#### Research Area:

Magnesium and iron are both essential plant nutrients and are present in the environment in different stable isotopes. Several natural processes like plant nutrient uptake, nutrient translocation within plants or mineral precipitation discriminate against the lighter or heavier isotopes and create changes in the isotope ratios. The latter can hence be used to clarify pathways in nutrient cycling, provided the underlying mechanisms of the fractionation step are known.

Studies show that the isotope composition of several nutrient elements may vary between top- and subsoil due to such biogeochemical processes. The subsoil below the plough horizon is known to contain up to 80% of the overall nutient pool and is usually only mariginally accessed by the crop plants. Together with 7 partner institutions IBG-3 currently investigates how the whole subsoil volume can be made better accessible for plant nutrition through new subsoil management approaches and whether such procedures are sustainable. Using stable isotope ratios determined on a Multicollector-ICP-MS to trace the origin of nutrient uptake, the group is investigating how much nutrients crop plants acquire from the subsoil.

The planned CSC-project should focus on the nutrient pools and isotope ratios in water, soil and plant compartments from agricultural field sites in Germany having undergone different subsoil management practices. The aim of these investigations will be to identify pathways and main environmental parameters which influence the cycling of these two elements. The CSC-subproject can focus on one or both of these elements.

### Specific Requirements:

M.Sc. in environmental or natural sciences with a strong background and keen interest in chemistry, analytics and nutrient cycling. A meticulous and exact work style is mandatory. Hands-on experience in chemical or environmental laboratories is of advantage. Fluent knowledge in written and spoken English is a prerequisite (Cambridge Scale C1). The successful thesis will be graded by Prof. Amelung and will be defended at the Faculty of Agriculture of the University of Bonn.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Fluent in written and spoken English (Cambridge Scale C1)

Name and Address of the Supervisor: Dr. Anne E. Berns, Forschungszentrum Jülich, Institute

of Bio- and Geosciences (IBG-3), 52425 Juelich, Germany

a.berns@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

**Department/Institute:** Institute of Bio- and Geoscience, Agrosphere (IBG-3)

http://www.fz-juelich.de/ibg/ibg-3/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. Roland Bol (main supervisor),

Dr. Albert Tietema & Dr. Annemieke Kooijman (co-supervisors)

University for Registration: University of Amsterdam (The Netherlands)

**Research Project:** Quantification of nitrogen and phosphorus transformations in range of

forested and non-forested German and Dutch ecosystems.

Position: PhD Student X Sandwich PhD Student □

Research Area:

There is an increasing interest in soil N and P cycling of terrestrial ecosystems due to their important role as limiting nutrients for biota and the large effect of global change on N and P cycling. Changes in N and P cycling may in turn also affect regional food security and the environment. Improved knowledge on gross N and P soil transformation rates is therefore essential.

This proposed project will examine the underlying regulation of gross soil N and P transformations. The research will focus on the part clear-cut forest Wüstebach catchment, a small headwater catchment located in the Eifel National Park and part of the TERENO Lower Rhine Valley-Eifel field experimental observatory. We know that vegetation (e.g. tree and scrub type), soil type, hydrology, pH and N and P deposition all have significant, but poorly quantified, effects on gross N and P transformation rates.

We will additionally complement our research on the Wüstebach site, with that in other German Eiffel Tereno sites (grassland and arable observatories). This will be complimented with soils from Dutch research sites and ecosystems (e.g. heathlands, coastal and inland dunes, fens, arable lands) and other abiotic (e.g. climate, altitude) and biotic factor (e.g. soil fauna and microbial population).

### Specific Requirements:

Graduated in chemistry, biogeochemistry, agricultural or environmental sciences. A background in forestry, agriculture, ecology or soil science is beneficial. Experience with nitrogen and phosphorus cycling, (stable) isotope analyses, designing field & laboratory experiments, and data analysis skills are a plus. Good English language knowledge. Thesis is defended at the University of Amsterdam.

Duration of stay: 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Good knowledge of English, written and spoken. A German language course

will be offered parallel to the project.

Supervisor name & Address: Prof. Dr. Roland Bol, Forschungszentrum Jülich, Institute of Bio- and Geosciences (IBG-3), 52425 Juelich, Germany. Email: r.bol@fz-juelich.de

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH - www.fz-juelich.de

Department/Institute:

Peter Grünberg Institute, Electronic Properties (PGI-6)

http://www.fz-juelich.de/pgi/pgi-6/EN/Home/home node.html

Supervising scientist:

PD Dr. Daniel E. Bürgler

University for Registration: University of Cologne

Research Field:

Molecular Spintronics

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

Interest in magnetic properties of nanoscale structures is rapidly growing mainly driven by the advancing miniaturization in information technology. Understanding and control of individual electron spins opens a route towards nanospintronics and quantum computing, which could revolutionize information technology. One promising approach is to employ single molecules adsorbed on surfaces, which exhibit magnetic properties either intrinsically or due to the interaction/hybridization with the substrate. The offered project focuses on spin-polarized scanning tunnelling microscopy and spectroscopy (SP-STM/STS) investigations of individual or self-assembled molecules on well-defined metal surfaces in combination with complementary magnetotransport measurements of in-situ fabricated mesoscopic organics-based junctions. Most experiments will be conducted at low-temperature and in high magnetic fields. The project is part of a larger initiative on molecular spintronics that also comprises chemistry and theory groups performing adapted molecule synthesis and DFT calculations.

## Specific Requirements:

The project is highly competitive as we strive for (i) exploiting intrinsic single-molecule properties (e.g. chirality, hybridization with substrates, redox states, spin-crossover) in organic layers to derive novel device functionalities and (ii) bridging the gap in understanding between magnetotransport properties measured in mesoscopic organicsbased junctions and the microscopic structural, electronic, and magnetic properties of single adsorbed molecules studied by SP-STM and DFT calculations. Hence, we are searching for a highly-motivated PhD student, who wants to contribute to our cuttingedge research. Requirements are an above-average grade in Physics, good English skills, good knowledge of solid-state physics, possibly practical experience in surface science (preferably STM), good interpersonal communication skills, and interest in working with state-of-the-art instrumentation in an interdisciplinary and international environment. For information about the institute, our instrumentation, and research see <a href="http://www.fz-juelich.de/pgi/pgi-6/EN">http://www.fz-juelich.de/pgi/pgi-6/EN</a> and Nat. Commun. 4, 2425 (2013), SPIN 4, 1440007 (2014), Phys. Rev. B 95, 094409 (2017), New. J. Phys. 19, 053016 (2017).

**Duration of stay:** 

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

September 2019

Language Requirement: Good knowledge of English language, written and spoken. A German

language course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Daniel E. Bürgler, Peter Grünberg Institute (PGI-6),

Forschungszentrum, 52425 Jülich, Germany; d.buergler@fz-juelich.de

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute:

Institute of Complex Systems, Bioelectronics (ICS-8)

http://www.fz-juelich.de/ics/ics-8/EN/Home/ node.html

Supervising scientist: Prof. Dr. A. Offenhäusser, Dr. Yu. Mourzina

University for Registration: RWTH Aachen University

Research Field:

Key Technologies - Sensorics and bioinspired systems

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

Electrochemical (bio)sensors are prospective devices to achieve low detection limits, high selectivity, and spatio-temporal resolution for the quantification of (bio)chemical analytes due to catalytic reactions at electrodes and signal techniques. The Institute Complex Systems-8 amplifications of (Bioelectronics) performs research on functional coupling of biomolecules and biomimetic compounds with micro- and nanoelectronic signal transducers for the development of sensors and bioelectronics devices.

The proposed research is devoted to the development and study of properties of electrochemical sensors and multisensor systems with oxidoreductase enzymes, biomimetic electrocatalytic molecular macrocycles (porphyrinrelated compounds), and their nanostructures based on molecular assembly for detection and monitoring of reactive oxygen species and redox signaling in single cells, cellular systems, and tissues. Effective electron transfer between enzymes or biomimetic sensitive components and an electrode can be facilitated by nanomaterials. Chemically and electrochemically synthesized metal nanowires, nanoparticles, and carbon-based nanomaterials will be employed as nanoelectronic transducer building blocks. Based on the results of the studies, novel mediatoreless sensors and multisensor systems for the electrochemical detection of reactive oxygen species will be developed. The sensors will be employed in the studies of reactive oxygen species in normal and pathological conditions in the cell lines as well as cultured primary cardiac muscle cells, and stem cells.

At the institute, experience in nanotechnology, electrochemical methods, structural characterization, and cell culture is available.

#### Specific Requirements:

Master studies of Chemistry or equivalent. Good knowledge of English language. The successful thesis will be defended at RWTH Aachen University.

Duration of stay:

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

September 2019

Language Requirement: Very good knowledge of English, written and spoken. A German

language course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Y. Mourzina, Forschungszentrum Jülich, Institute of

Complex Systems (ICS-8), 52425 Jülich, Germany. E-mail:

v.mourzina@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Bio- and Geosciences, Agrosphere (IBG-3)

Dr. Carsten Montzka Supervising scientist: University for Registration: University of Bonn

Research Field: Soil moisture remote sensing and spatial scaling

PhD Student X Joint PhD Student □ Position:

#### Research Area:

Soil moisture (SM) is a key state variable for understanding hydrological processes involved in a broad variety of environmental applications. Many global-scale SM products are available, however, the spatial scale is often inappropriate for agricultural applications. To solve this problem, scaling methods need to be developed based on either sensor fusion or machine learning approaches. Validation with in situ networks is an important aspect.

#### Topic 1: SM upscaling by machine learning

Machine learning approaches such as random forest are able to predict variables based on a set of auxiliary variables. The candidate will use in situ SM data to generate regional high resolution SM maps using predictors such as soil properties, land cover, and elevation. Special focus will be laid on the uncertainty structure of the proposed product and on its ability to serve as a reference for satellite validation.

### Topic 2: SM downscaling by soil heterogeneity evaluation

The candidate will implement an approach predicting the soil moisture standard deviation as a function of the mean soil moisture. The main predictor is soil texture variability for the area. The approach is based on a closed-form expression using stochastic analysis of 1D unsaturated gravitational flow based on the Mualem-van Genuchten model and firstorder Taylor expansions. The scaling procedure makes use of auxiliary data such as backscatter and thermal inertia.

#### Topic 3: Hydrologic forecasting by machine learning

After obtaining high accuracy SM products, the candidate will investigate hydrologic coupling in order to conduct comprehensive hydrology forecasting. By using Recurrent Neural Networks (RNN) and specific analysis of the Long-Short Term Memory (LSTM) the ability of predicting extreme events will be evaluated. Especially meteorological, agricultural and hydrological drought events will be analysed by dividing remotely-sensed time series into long term and short term contributions to LSTM and their impact on vegetation and yield.

### **Specific Requirements:**

- University degree in either remote sensing, geosciences, computer science, physics, or applied mathematics
- Knowledge in the areas of microwave remote sensing, hydrology, numerical methods and knowledge of data fusion methods is a clear advantage
- Programming skills with Python, Fortran; Experience in machine learning methods
- Ability to work independently as well as collaboratively in an international, interdisciplinary team; very good communication and organizational skills

Duration of stay:

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

September 2019

Language Requirement: Very good command of the English language, written and spoken. A German language course will be offered parallel to the project.

## Name and Address of the Supervisor:

Dr. Carsten Montzka, Forschungszentrum Jülich, Institute of Bio- and Geosphere (IBG-3), 52425 Jülich, Germany, c.montzka@fz-juelich.de

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH - www.fz-juelich.de

Department/Institute:

Institute of Energy and Climate Research, Electrochemical Process

Engineering (IEK-3)

http://www.fz-juelich.de/iek/iek-3/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. Werner Lehnert / Dieter Froning

University for Registration:

RWTH Aachen

Research Field:

Water transport in porous structures with Lattice Boltzmann simulations

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

## Macroscopic impact of transport simulations on microstructures of thin lavers.

Multiphase transport of fluid in the microstructure of fuel cell and electrolyzer components are to be studied. The underlying materials have fine structures in the micrometer scale or below. Simulation of relevant domains in the mm scale requires their application on supercomputers. The underlying structures of the simulations are both real structures and artificial structures which are stochastically equivalent to real structures.

The research area addresses investigations on several effects on the macroscopic fluid transport. The effects cover

- Geometric characteristics of the microstructure,
- The nature of the boundary conditions of the transport simulations,
- Operating conditions of the simulations.

The effects shall be evaluated according to the foreseen application in the fuel cell and electrolysis area.

## Specific Requirements:

Foundations in gas kinetics; excellent grades in Mathematics; excellent programming skills; excellent knowledge in process engineering; very good understanding in inorganic chemistry; ability to work in a team / excellent team player

Duration of stay:

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

September 2019

Language Requirement: Very good knowledge of English language, written and spoken. A

German language course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. W. Lehnert, Forschungszentrum Jülich, Institute of Energy and Climate Research (IEK-3), 52425 Jülich, Germany,

w.lehnert@fz-juelich.de; Dieter Froning (d.froning@fz-juelich.de)

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH - www.fz-juelich.de

Department/Institute:

Institute of Energy and Climate Research, Electrochemical Process

Engineering (IEK-3)

http://www.fz-juelich.de/iek/iek-3/EN/Home/home\_node.html

Supervising scientist:

Prof. Dr. Werner Lehnert

University for Registration:

RWTH Aachen

Research Field:

Fundamental effects of fluid transport in microstructures of components

in electrochemical devices

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

### Electrochemical modelling with Pore Network simulations.

Transport of fluid - one and two phase flow - in the microstructure of fuel cell and electrolyzer components are to be studied. The underlying materials have fine structures in the micrometer and nanometer scale. Pore network models shall be built from both real structures and artificial structures which are stochastically equivalent to real structures.

The research area addresses investigations on several effects on the macroscopic fluid transport. The effects cover

- Geometric characteristics of the microstructure,
- Transfer of the results to real applications,
- Operating conditions of the simulations.

The effects shall be evaluated according to the foreseen application in the area of electrochemical devices, i.e. fuel cells and electrolyzers.

### Specific Requirements:

Excellent knowledge in process engineering; excellent grades in Mathematics; excellent programming skills; very good understanding in inorganic chemistry; ability to work in a team / excellent team player

Duration of stay:

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start:

September 2019

Language Requirement: Very good knowledge of English language, written and spoken. A German language course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. Werner Lehnert, Forschungszentrum Jülich,

Institute of Energy and Climate Research (IEK-3), 52425 Jülich, Germany, w.lehnert@fz-juelich.de, Dieter Froning (d.froning@fz-

juelich.de)

Helmholtz Centre:

Forschungszentrum Jülich GmbH - www.fz-juelich.de

Department/Institute:

Juelich Centre for Neutron Science (JCNS)

Quantum Materials and Collective Phenomena (JCNS-2/PGI-4)

http://www.fz-juelich.de/jcns/jcns-2/EN/Home/home\_node.html

Supervising scientist:

Priv.-Doz. Dr. Oleg Petracic, Prof. Dr. Thomas Brückel

University for Registration:

RWTH Aachen

Research Field:

Experimental Physics, Condensed Matter Physics, Materials Science

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

Electronic systems for future mobile or wearable devices will increasingly be multifunctional and flexible. Hence the fundamental understanding of the interplay between strain, magnetic anisotropy and magnetism in particular on flexible substrates needs to be established. This is a prerequisite for the design of e.g. strain-sensitive sensors for wearable devices, organic or printable electronics.

In this project two classes of systems will be fabricated, characterized and studied: a) FeOx nanoparticles spincoated onto flexible substrates (e.g. PET) and embedded with e.g. a Ti and Au layer.

b) Thin films of LSMO or Fe3O4 on top of flexible substrates.

Key methods to characterize the properties of the samples will be x-ray diffraction, X-ray reflectometry, polarized neutron reflectometry, magnetometry and ac susceptibility

1. P. Sheng, B. Wang, R. Li, J. Semicond. 39, 011006 (2018)

2. L.-M. Wang, O. Petracic, E. Kentzinger, U. Rücker, M. Schmitz, X.-K. Wei, M. Heggen,

Th. Brückel, Nanoscale 9, 12957 (2017)

3. S. R. Forrest, Nature 428, 911 (2004)

## **Specific Requirements:**

- · Completed studies in physics, material science or chemistry.
- Experience with and passion for experimental laboratory work.
- Solid experience with usual computer software for e.g. for analyzing and presenting data, writing scientific texts or presenting results, etc..
- Ideally prior experience in at least one of the following fields: condensed matter physics, magnetism, nanoparticles, thin films, neutron scattering, x-ray scattering, magnetometry

**Duration of stay:** 

4 years

Work Place:

Forschunsgzentrum Jülich GmbH, Jülich (near Cologne)

**Earliest Start:** 

October 2019

Language Requirement: Very good knowledge of English language, written and spoken. A
German language course will be offered parallel to the project.

Name and Address of the Supervisor: Priv. Doz. Dr. Oleg Petracic, Prof. Dr. Thomas Brückel,

Forschungszentrum Jülich GmbH, Quantum Materials and Collective

Phenomena, JCNS-2/PGI-4, 52425 Jülich, Germany

o.petracic@fz-juelich.de

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Energy and Climate Research, Materials Synthesis and

Processing (IEK-1); http://www.fz-juelich.de/iek/iek-1/EN/Research/ElektrochemischeSpeicher/\_node.html

Supervising scientist: Prof. Dr. Olivier Guillon, Dr. Frank Tietz, Dr. Qianli Ma

University for Registration: Rheinisch-Westfälische Technische Hochschule Aachen (RWTH)

Research Field: Solid state Sodium batteries

Position: PhD Student □X Joint PhD Student □

#### Research Area:

The main research topic of the applicant will be the development of all-solid-state-sodium batteries based on oxide-ceramic electrolyte materials. It is known that Li-ion batteries have governed the current worldwide rechargeable battery market due to their outstanding energy and power capability. However, the huge demands of battery for nowadays and future electrical vehicle and renewable energy applications have already rising the concerns of the availability of lithium and hence future cost. Unlike Li, sodium is one of the most abundant elements on Earth which exhibits similar chemical properties to Li, indicating that Na chemistry could be applied to a similar battery system. All-solid-state design was regarded as next generation batteries because of their non-leakage, nonvolatilization, non-flammability, separator-free design and wide application temperature change. This design has been attracting more and more research interests. In our institute, very fast Na+ ion conductors based on phosphate NASICON materials were developed with conductivity up to 5 mS cm<sup>-1</sup> at 25 °C. First battery cells with high performance were also developed with phosphate cathodes. The task of the current applicant is the development of oxide-based electrolyte materials for higher compatibility with the stateof-the-art cathode materials because they have higher energy capacity. Full cells will also be developed during his/her study.

### Specific Requirements:

The applicant should have master degree in material science, chemistry, physics or related area, with good performance in university and post-graduate period. Basic knowledge of inorganic material synthesis and processing, microstructure design and electrochemistry is necessary. The applicant should also have very good English skills with German as a plus.

Duration of stay: 4 years

Work Place: Forschungszentrum Juelich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Very good command of English, written and spoken. A German

language course will be offered parallel to the project.

Name and Address of the Supervisor: Prof. Dr. O. Guillon (o.guillon@fz-juelich.de), Dr. F.Tietz

(f.tietz@fz-juelich.de), Dr. Q. Ma (q.ma@fz-juelich.de),

Forschungszentrum Jülich GmbH, Institute of Energy and Climate

Research (IEK-1), 52425 Jülich, Germany

**Helmholtz Centre:** Forschungszentrum Jülich – www.fz-juelich.de

Department/Institute: Institute of Bio- and Geosciences, Agrosphere (IBG-3)

http://www.fz-

juelich.de/ibg/ibg3/EN/Home/home\_node.html;jsessionid=C403EE20D5

0017708B564C7188209DAB

Supervising scientists: Prof. Dr. Youri Rothfuss, Prof. Dr. Nicolas Brüggemann

University for Registration: University of Liège (BE)
Research Field: Earth and Environment

Position: PhD Student ☑ Sandwich PhD Student □

Research Project: High-frequency non-destructive isotopic partitioning of water and CO<sub>2</sub>

environmental fluxes

Research Area: Stable isotopic ecohydrology

Field-based quantitative observations of ecohydrological feedbacks of the terrestrial vegetation to the atmosphere are crucial for improving land-surface model parametrizations. This is especially true in the specific context of partitioning of net ecosystem water and CO<sub>2</sub> fluxes into their raw components (soil evaporation and respiration, plant transpiration and photosynthesis).

Stable isotopic analysis provides means for partitioning water and CO<sub>2</sub> fluxes, however is often limited by its low spatio-temporal representativeness. This is mainly due to the destructive sampling of soil and plant and off-line analysis in the laboratory which only allows for retrospective determination of the sources' contributions. The CSC fellowship PhD student will actively contribute to tackling these limitations by applying a newly-developed method for monitoring of the soil water and CO<sub>2</sub> isotopic compositions in the field. He/she will couple this method with on-line measurements of plant as well as ecosystem water and CO<sub>2</sub> fluxes using a combination of closed chamber systems and Eddy Covariance analysis. For this he/she will have access to low and high through-flow laser-based isotopic spectrometers embedded in a fully mobile system to be deployed at a series of experimental sites of the Rur catchment (North Rhine-Westphalia, Germany) differing in their land cover and use, and environmental conditions.

### Specific Requirements:

MSc in natural sciences (biosphere-atmosphere interactions, eco-hydrology and – physiology or related subjects) or engineering (environmental engineering, agricultural engineering) with sound technical skills. Very good knowledge of English language is required. Experience in stable isotopic analysis (e.g., IRMS) is welcome.

Duration of stay: 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Very good command of English, written and spoken. A German

language course will be offered parallel to the project.

Name and Address of the Supervisors: Forschungszentrum Jülich, Institute of Bio- and

Geosciences (IBG-3), 52425 Jülich, Germany

v.rothfuss@fz-juelich.de; n.brueggemann@fz-juelich.de

Forschungszentrum Jülich GmbH – www.fz-juelich.de **Heimholtz Centre:** 

Institute for Neuroscience and Medicine, Brain and Behaviour (INM-7) Department/Institute:

Supervising scientist: PD Dr. Oleksandr Popovych, Prof. Dr. Simon B. Eickhoff

University for Registration: Heinrich Heine University of Düsseldorf

Research Field: Computational Neuroscience

PhD Student X Joint PhD Student □ Position:

Research Area:

The human brain represents a highly complex network, which shows wellstructured spatio-temporal dynamics even at a resting state. Data obtained from a noninvasive neuroimaging (e.g. fMRI) allows to calculate the functional connectivity that captures the interactions between different brain regions as well as their time evolution. Using this information collected in large subject cohorts together with a detailed structural connectivity from anatomical measurements (e.g. dMRI), we can develop and validate sophisticated wholebrain neural mass mathematical dynamical models which can well reproduce activity and connectivity of the resting states networks revealed from the measured data.

These models can then be used to address mechanisms of brain dynamics. More specifically, a model-based investigation of the interdependence between brain activity and connectivity will be focused on how the corresponding model parameters and dynamics may be associated with healthy and diseased states or aging, which could be of clinical relevance. The model parameters and dynamics can further be utilized for a better the inter-individual variability (differences description of subjects/patients), structure-function relationships of the brain activity, as well as for an advance in data processing and analysis tools.

#### Specific Requirements:

- MSc or equivalent in a relevant field (Physics, Neuroscience, Applied Mathematics, Computer Science)
- Basic knowledge of non-linear dynamical systems/neuronal dynamics/ computational neuroscience
- Experience in numerical simulation of systems of differential equations and programming skills (C, C++, Python, MATLAB)
- Good written and oral communication skills in English

Duration of stay:

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

October 2019

Language Requirement: Very good command of English language. A German language course

will be offered in parallel to the project.

Name and Address of the Supervisor: PD Dr. Oleksandr Popovych, Forschungszentrum Jülich,

Institute for Neuroscience and Medicine (INM-7), 52425 Jülich,

Germany, o.popovych@fz-juelich.de

**Helmholtz Centre:** Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: : Institute for Neuroscience and Medicine, Brain and Behaviour (INM-7)

Supervising scientist: PD Dr. Susanne Weis, Dr. Robert Langner University for Registration: Heinrich Heine University of Düsseldorf

Neuroscience Research Field:

PhD Student X Joint PhD Student □ Position:

#### Research Area:

Sex differences in cognitive processing strategies have been well established, in particular with respect to the selectivity in allocating attentional resources. Given that the allocation of attention forms the basis for many other cognitive tasks (e.g. episodic and semantic memory, action control), a more comprehensive understanding of the neural basis of sex differences in attention has far-reaching implications, not only for healthy participants, but also for clinical conditions like ADHD or autism, where sex differences are reliably observed.

This PhD project will develop and conduct a large-scale, multi-modal brain imaging study to elucidate to what extent sex differences in different cognitive domains can be explained by differences in underlying attentional processes and their neural substrates. To disentangle the complexity of individual differences, the interaction of inter-individual (sex) and intra-individual (e.g. stress level, motivation, fatigue) variability in the allocation of attentional resources will also be taken into account. The envisaged multimodal imaging approach will integrate regional brain activation and morphology with measures of functional and structural connectivity. The integrative analysis of this very rich set of neuroimaging, behavioral, and self-report data will rely on classical statistical as well as recent machine-learning approaches to big data.

### Specific Requirements:

- MSc or equivalent in a relevant field (e.g. psychology, neuroscience, medicine)
- Basic written and oral communication skills in German, with a strong commitment to improving during the stay
- Knowledge in experimental design and/or statistical analyses
- Previous experience with behavioral and imaging data acquisition and analysis is a major advantage
- Programming experience (e.g., Python, MATLAB, Presentation) is a plus

Duration of stay:

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

**Earliest Start:** 

October 2019

Language Requirement: Very good command of English, written and spoken. A German

language course will be offered in parallel to the project.

Name and Address of the Supervisor: PD Dr. Susanne Weis, Forschungszentrum Jülich,

Institute for Neuroscience and Medicine (INM-7), 52425 Jülich,

Germany; s.weis@fz-juelich.de

Helmholtz Centre:

Forschungszentrum Jülich – www.fz-juelich.de

Department/Institute:

Institute for Neuroscience and Medicine, Brain and Behaviour (INM-7)

http://www.fz-juelich.de/inm/inm-7/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. Simon B. Eickhoff, Dr. Juergen Dukart

University for Registration: Heinrich-Heine University Düsseldorf

Research Field:

Digital biomarker technologies

Position:

PhD Student X

Joint PhD Student □

#### Research Area:

The primary focus of the PhD project will be on development and clinical integration (including own data collection) of a digital biomarker platform (primarily smartphone based assessments such as passive monitoring, ecological momentary assessments, patient reported outcomes, performance- and sensor-based tests) in specific clinical populations such as Parkinson's disease but also other potential neurological or psychiatric indications. The student will thereby closely work with me and other lab members in developing a clinical understanding of the relevant disease symptoms. The student will also work on development of an external database and appropriate pre-processing and analytical pipeline for handling of such data including conduct of synergistic analyses of the data with other biomarker and clinical modalities collected in those patients. exploration.

#### Specific Requirements:

- Master in Informatics, Engineering, Physics, Statistics, Mathematics, Computer Science or similar
- Solid programming skills in Matlab, Python, Java or similar necessary
- Experience in development of Android or IOS applications desired
- Experience with Machine Learning
- Solid knowledge of Statistics
- Strong interest in learning about Neuroscience, the brain and specific neurological or psychiatric diseases

Duration of stay:

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start:

September 2019

Language Requirement: Very good command of English, written and spoken. A German

language course will be offered parallel to the project.

Name and Address of the Supervisor: Juergen Dukart, Institute of Neuroscience and Medicine,

(INM-7), Forschungszentrum Jülich, 52425 Jülich, Germany;

s.eickhoff@fz-juelich.de

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute for Energy and Climate Research, Microstructure and

Properties of Materials (IEK-2)

http://www.fz-juelich.de/iek/iek-2/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. M. Krüger, Dr. J. Malzbender

University for Registration: RWTH Aachen

Research Field: Materials Science

Position: PhD Student X Sandwich PhD Student □

## Research Area:

Mechanical Behavior of Solid State Batteries. Batteries become increasingly important for stationary and in particular mobile applications. The use of solid-state batteries offers safer operation, higher performance in terms of energy storage, as well as high thermal and chemical stability. Furthermore, they are expected to possess enhanced ionic conductivity and mechanical stability that warrants a safer separation, and hence, potentially permits them to withstand long-term cycling operation. However, mechanical boundary conditions and operation under cyclic conditions might still induce micro-cracks, dendrite growth, structural and mechanical failure. Therefore, their mechanical reliability is important to warrant longterm reliability. In this project, aiming at a characterization of reliability and life-time relevant aspects, the mechanical behaviour of solid-state battery materials is studied on a micro-scale with correlation to the materials microstructural characteristics,, via a combination of advanced testing and non-destructive as well as post-operational characterization techniques in combination with advanced microstructural characterization techniques. Along with considerations of degradation effects, aim is the derivation of lifetime prediction models, where especially the relationships between long term behavior under different loading condition and microstructure are to be analyzed on the basis of supporting light-, scanning electron and tunneling electron microscopic investigations. The scientific work is focused on an extremely important subject with application importance in a strong interdisciplinary environment with the possibility to use up-to-date characterization technologies and access to modern light and electron microscopic methods.

### Specific Requirements:

A university degree (BEng., BSc., MSc) in one of the subject mechanical engineering, materials science, mineral science or applied physics and creativity, scientific interest and team working ability

**Duration of stay:** 48 months

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

Language Requirement: Very good command of English, written and spoken. A German

language course will be offered parallel to the project, additionally.

Name and Address of the Supervisor: Prof. Dr. M. Krüger, Forschungszentrum Jülich GmbH, IEK-2, 52425 Jülich, Germany; m.krueger@fz-juelich.de

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute for Energy and Climate Research, Microstructure and

Properties of Materials (IEK-2)

http://www.fz-juelich.de/iek/iek-2/EN/Home/home\_node.html

Supervising scientist: Prof. Dr. M. Krüger, Dr. J. Malzbender

University for Registration: RWTH Aachen

Research Field: Materials Science

Position: PhD Student X Sandwich PhD Student □

#### Research Area:

Advanced nano- and microscale mechanical characterization. Ceramic materials become increasingly important as functional materials for energy applications. Often these materials are exposed to mechanical loads at operation relevant elevated temperatures, requiring careful characterization of the mechanical properties. Although various methods exist to assess properties, materials development often requires characterization of specimens of limited volume, hence measurement of properties on nano- and microscale. In this project, aiming at a characterization of reliability and life-time relevant aspects, the mechanical properties of ceramic materials are studied by nano- and micro-indentation testing yielding elastic modulus, hardness and fracture toughness as a function of temperature. The novel indentation testing set-up available at the laboratory permit characterization of the properties in a temperature range -30°C up to 700°C. Loading as well as loading rate dependency of the properties are assessed to gain insight into deformation mechanisms as well as subcritical crack growth aspects. In addition, micro-pillar tests are carried out to separate properties of grain and grain boundary. The work is aided by complementary post-test characterization with advanced microstructural characterization techniques. Behavior under different loading condition and microstructure are to be analyzed on the basis of supporting light-, scanning electron and tunneling electron microscopic investigations. The scientific work is focused on an extremely important subject with application importance in a strong interdisciplinary environment with the possibility to use up-to-date characterization technologies and access to modern light and electron microscopic methods.

#### Specific Requirements:

A university degree (BEng., BSc., MSc) in one of the subject mechanical engineering, materials science, mineral science or applied physics and creativity, scientific interest and team working ability

**Duration of stay:** 48 months

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2019

**Language Requirement:** Very good command of English, written and spoken. A German language course will be offered parallel to the project, additionally.

language course will be offered parallel to the project, additionally.

Name and Address of the Supervisor: Prof. Dr. M. Krüger, Forschungszentrum Jülich GmbH, IEK-2, 52425 Jülich, Germany; m.krueger@fz-juelich.de

Helmholtz Centre: Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute: Institute of Bio- and Geosciences, Biotechnology (IBG-1)

http://www.fz-juelich.de/ibg/ibg-1/EN/Home/home\_node.html

Supervising scientist: Dr. Eric von Lieres (co-supervised by Dr. Marco Bocola)

University for Registration: Heinrich Heine University of Düsseldorf

Research Field: Computational Biology, Enzyme Structure-Activity Prediction and

Enzyme Desing

Position: PhD Student X Sandwich PhD Student □

Research Area:

Computational enzyme structure-activity prediction and enzyme design (3D-EnSAR) Computational enzyme design is a emerging field [Röthlisberger, Science] enabling selective biotransformations of pharmaceuticals and fine chemicals under mild conditions. Due to natural evolution, enzyme families have evolved, offering a broad diversity in terms of substrate specificity and stability and are more and more applied in industrial applications. However, natural enzymes often do not meet the required activity for the

desired non-natural substrate and are not stable under process conditions.

For development of an effective algorithm to correlate enzyme property with its sequence/structure, an extensive dataset with high-quality experimental results is necessary. Such dataset is now available from a directed evolution project of an experimental partner. The realm of computational enzyme design is still not reached yet, but the novel combination of available methods has the potential to reach this goal in the near future [Kiss, Angewandte Chemie].

## Specific Requirements:

Computational methods for prediction of hot spot regions and focused saturation mutagenesis libraries are needed to cope with the combinatorial complexity of protein sequence space. This is a particularly important and relevant application for the emerging tools from artificial intelligence and machine learning. Existing statistical algorithms for the analysis of directed evolution data in terms of protein sequence-activity relationship (ProSAR) [Fox, Nature Biotechnology] can help to analyze several thousand protein variants and identifying beneficial mutations for the next generation of a directed evolution experiment. Modern 3D-QSAR methods applied mostly in drug design [Seti, Int. J. Drug Design and Discovery) incorporate 3D-information of the protein and ligand structure as molecular descriptors (Comparative Molecular Field Analysis or Molecular Similarity Indices Analysis) and make use of advanced statistical methods (Genetic Algorithms, Simulated Annealing and Forward or Backward Feature Selection) to map molecular structure to inhibitor activity. These advanced algorithms have not been applied to predict enzymatic activity. Therefore strong interest in novel algorithm programming and protein 3D structure analysis is a prerequisite.

**Duration of stay:** 4 years

Work Place: Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start: September 2018

Language Requirement: Very good knowledge of English language, written and spoken. A

German language course will be offered parallel to the project.

Name and Address of the Supervisor: Dr. Eric von Lieres, Forschungszentrum Jülich, Institute of

Bio- and Geosciences (IBG-1), 52425 Jülich, Germany, e.von.lieres@fz-

juelich.de

**Helmholtz Centre:** 

Forschungszentrum Jülich GmbH – www.fz-juelich.de

Department/Institute:

Peter Grünberg Institute, Functional Nanostructures at Surfaces (PGI-3)

http://www.fz-juelich.de/pgi/pgi-

3/EN/Home/home\_node.html;jsessionid=C93223AB97961103F19A595F

949EB6DD

Supervising scientist: PD Dr. Ruslan Temirov

University for Registration: University of Cologne

Research Field:

Very-Low Temperature Scanning Probe Miscroscopy

Position:

PhD Student

Joint PhD Student □

Research Area:

Studies of artificial electronic systems engineered with individual molecules and atoms systems on surfaces by controlled manipulation with a very-low temperature scanning probe microscope operated in high magnetic field.

## Specific Requirements:

Master in physics with an average grade "good" or better.

Good communication skills

Experience with ultra-high vacuum

Experience in scanning probe microscopy is desirable Good programming skills (e.g. Matlab, Python, R, C++)

**Duration of stay:** 

4 years

Work Place:

Forschungszentrum Jülich, Germany (near Cologne)

Earliest Start:

September 2019

Language Requirement: Very good knowledge of English language, written and spoken. A

German language course will be offered parallel to the project.

Name and Address of the Supervisor: PD Dr. Ruslan Temirov, Forschungszentrum Jülich, Peter

Grünberg Institute (PGI-3), 52425 Jülich Germany;

r.temirov@fz-juelich.de