

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Development of a workflow and image processing pipeline for an integrated high-throughput plant phenotyping system for the simultaneous screening of root and shoot productivity traits.

Jülich's institute: Institute of Bio- and Geosciences 2 - Plant Sciences

Project leader: Dr. Fabio Fiorani, Dr. Kerstin Nagel

Web address: http://www.fz-juelich.de/ibg/ibg-2/EN/Home/home_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): Through this program we seek to establish partnerships with institutes in China that are developing non-invasive, imaging-based methods for the high-throughput analysis and screening of crop plants. In particular, we seek collaborations in the area of image processing from a diverse set of sensors ranging from RGB to spectral and fluorescence cameras. We are particularly interested in a collaboration with the Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, Wuhan, 430074, China. This institute has recently developed methodologies for the high-throughput analysis of rice shoot and seeds based on non-invasive imaging (Feng, H. et al 2013. A hyperspectral imaging system for an accurate prediction of the above-ground biomass of individual rice plants. *Review of Scientific Instruments*, 84(9), 095107. [<http://dx.doi.org/10.1063/1.4818918>]; Yang W., et al. 2014. Combining high-throughput phenotyping and genome-wide association studies to reveal natural genetic variation in rice, *Nature Communications*. DOI: 10.1038/ncomms6087; Yang W., et al. 2015. Genome-wide association study of rice (*Oryza sativa* L.) leaf traits with a high-throughput leaf scorer, *Journal of Experimental Botany*. doi:10.1093/jxb/erv100). We consider that a collaboration on the proposed project would be mutually beneficial and would deliver improved methods to the growing plant phenotyping community worldwide.

Required qualification of the postdoc:

- PhD in Biomedical Imaging and Processing or related field
- experience with implementation, integration in automated measurement routines and analysis of various sensors data and imaging modes (RGB, Near-Infrared, Fluorescence, Spectral) for the extraction of plant traits of target crop species (e.g., cereals). Experience with the C++ programming language, with the Labview software suite and with the ENVI software for the analysis of spectral data.
- additional skills in development of software middleware and data wrappers for automated storage and retrieval of data to relational databases is desirable.

¹ please add overleaf



PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

The Juelich Plant Phenotyping Center at the IBG2 Plant Sciences Institute, Forschungszentrum Juelich is leading national and international networks for the development of next generation phenotyping systems for the automated, non-invasive analysis of plant traits (root and shoot architecture and growth). To enhance crop water, nutrient and light use efficiency, it is crucial to develop new phenotyping infrastructure that enables the dynamic and simultaneous measurement of above- and below-ground plant traits at high-throughputs (i.e., hundreds of plants per day) to link phenotypic and genotypic data. To achieve this goal, we are developing a novel high-throughput platform that integrates shoot and root analysis based on our prior work (Nagel et al. 2012). GROWSCREEN-Rhizo is a novel phenotyping robot enabling simultaneous measurements of root and shoot growth for plants grown in soil-filled rhizotrons. *Functional Plant Biology* 39 (11), 891-904). The new platform with enhanced throughput will also include multiple sensors for the analysis of growth in 2- and 3-D, photosynthetic performance and spectral reflectance. The aims of a post-doctoral fellowship with the duration of two years are: a) develop a concept and implement automated imaging workflows for various sensor types as described above; b) develop a robust imaging processing pipeline for automated plant trait extraction; c) develop standardized data models and schemas for plant phenotypic data gathered with the new platform; d) validate the approaches for large scale experiments in selected crop models such as wheat and oilseed rape in collaboration with biologists, project leaders, and automation engineers at IBG2. The main expected output of the projects is high-throughput image processing for various sensor types. The results will be published in high impact factor journals targeting the plant biology community.

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PART A

Title of the project: Biotic and abiotic controls on bioavailability, sorption and leaching of nanoparticulate phosphorus

Jülich's institute: Institute for Bio- and Geosciences 3, Agrosphere

Project leader: Prof. Dr. Erwin Klumpp

Web address: www.fz-juelich.de/ibg/ibg-3/EN/

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): Excellence in soil science, especially soil chemistry, and soil biochemistry and soil management. Experience in international collaborative projects together e.g. with partners in Europe would be beneficial.

Required qualification of the postdoc:

- PhD in soil science / environmental science or a related field
- experience with environmental chemistry, soil colloids, and physicochemical and analytical methods. Some experience with phosphorus is beneficial.
- additional skills in proposal and paper writing

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
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- 2 letters of recommendation

PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years

¹ please add overleaf

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- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

The Agrosphere Institute conducts research to improve our understanding of biogeochemical processes in soils. One specific focus lies on the effect of climate and land use change on the formation of biogeochemical interfaces and colloids. Environmental nanoparticles and fine colloids (NP & FC) in soil effectively bind organic matter and nutrients like phosphorus. Phosphorus is the second most limiting nutrient for plant growth after nitrogen. The mobility of NP & FC contributes significantly to the nutrient cycling in the surface and subsurface environment. Soil properties, hydrodynamic parameters (e.g. intensive precipitation) and chemical dispersion parameters (pH, ionic strength, dissolved organic matter) affect the transport and release of NP & FC in soils. Ad-/desorption processes of phosphorus on colloids together with contemporary vegetation and associated microbial community strongly influence the bioavailability of this important nutrient. The goal of the project is to characterize and quantify the soil NP & FC and to understand their role for phosphorus cycling. One specific focus lies on the bioavailability of phosphorus co-transported by soil NP & FC. To investigate the composition as well as the nutrient content and speciation of NP & FC field flow fractionation (FFF) coupled e.g. to ICP-MS, ³¹P-NMR (off-line), and electron microscopy coupled to energy-dispersive X-ray spectroscopy will be used in combination with column experiments. The Agrosphere Institute has several long term field monitoring and observation facilities (TERENO) available for collecting soils for lab-based column studies or this can be done in-situ at these sites.

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PART A

Title of the project: Investigations of Mixed Cathode Materials for All-Solid-State Li-ion Batteries

Jülich's institute: Institute of Energy and Climate Research 1 - Materials Synthesis and Processing

Project leader: Prof. Dr. Olivier Guillon

Web address: http://www.fz-juelich.de/iek/iek-1/DE/Home/home_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:
(max. half page):

We are looking for a laboratory focusing on the issues of understanding i) the nano-scale transportation mechanism of mixed ionic conductors, ii) the effect of ion transport to the material surface, interface and crystal structure, iii) lithiation and delithiation process in oxide materials. Excellent advanced analytical facilities paired with expertise in materials science are required to fulfill the project's goals.

Required qualification of the postdoc:

- PhD in Physics, Chemistry, Materials Science or any relative field in ionic conductors and electrochemical storages.
- experience with material synthesis, Li-ion battery materials, electrochemical tests, TEM, ITIC, FIB/SEM, and AFM
- additional skills in PVD, XPS, XRD, Raman Spectroscopy, PEEM, XRD kelvin probe, force curve and electron holography.

PART B

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Description of the project: (max. 1 page)

In comparison to conventional lithium ion batteries using organic liquids as electrolytes, all-solid-state lithium ion batteries are expected to be much safer due to their chemical inertness. Among solid lithium ion conductors, as $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZ) oxide ceramic has the advantage of being stable against lithium metal combined with a wide electrochemical window, which makes it as one of the most promising candidates for high-voltage solid-state battery applications. Nevertheless, to increase the battery performance and reduce the interfacial resistances, it is necessary to optimize the contact area between electrolyte and cathode materials. One solution is to develop dense composites starting from a mixture of electrolyte and cathode ceramic powders. In order to rationalize the development of such new material compounds the ionic transfer between these two phases needs to be understood. Within the project, mixtures of LLZ and a reference cathode material (LiCoO_2) will be synthesized while grain size and volume content will be systematically varied. It has already been shown that these two materials do not seem to react with each other up to 1050°C . Their sintering behavior will be investigated, first pressure-less and then by Field Assisted Sintering Technique / Spark Plasma Sintering in order to attain full density and proper interfaces. Microstructures will be evaluated by FIB/SEM to evaluate the homogeneity and purity of the obtained composites. Electrochemical characterization will give insight into the performance of such materials. In order to understand the interfacial behavior between LLZ and LCO, thin film approach will also be followed, i.e., depositing LCO on LLZ ceramic pellet or depositing LLZ thin film on LCO. Preliminary tests in Jülich have shown that such coatings are possible. Selected samples shall be further investigated at the Chinese partner institute. In particular, high-resolution TEM will be interesting to reveal the transport mechanisms across the phase boundary between electrolyte and cathode. Possible local strains due to Li-ion insertion/de-insertion may modify the diffusion in the active material. The volume change may even lead to deleterious effects and degradation of the interface. In that regards, the determination of the cutting –off voltage (between 4.2 and 4.5 V) is an important issue for LCO cathode to avoid irreversible structural changes. These investigations are made possible by using a special sample holder,



which has been developed for the in-situ characterization of Li-ion battery materials.

The thin film approach is also helpful to clarify this issue. In addition, the transport behavior, formation of space charge layers, possible interfacial reaction and local strain will be investigated both in the dense ceramic composite and layer thin film samples using various techniques such as ITIC, IS, EIS, PEEM, Kelvin probe, C-AFM, force curve, electron holography, SIMS, XPS, XRD and Raman spectroscopy. The application of these techniques will be determined by the progress and scientific questions addressed within this post-doctoral project. Further developments directly deriving from this project can already be identified: strategies for improvement of electronic conductivity, use of other high-voltage materials to obtain a zero-strain cathode during charging/discharging, design of graded electrodes to reduce interface resistances.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Study of the structure, efficiency, and durability of membrane-electrode-assemblies for water electrolysis

Jülich's institute: Institute of Energy and Climate Research 3 - Electrochemical Process Engineering

Project leader: Dr. Marcelo Carmo

Web address: <http://www.fz-juelich.de/iek/iek-3>

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): Existing collaboration via a bachelor thesis with the School of Materials Science and Engineering, East China University of Science and Technology; further Chinese cooperation partners are welcome

Required qualification of the postdoc:

- PhD in Material science and/or electrochemistry
- experience with Electrochemical and physico-chemical characterization tools
- additional skills in Lab-scale synthesis; writing of research papers and proposals; presentations on international conferences

PART B

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Description of the project: (max. 1 page)

The modern society demands an increase in the electricity production and urge to obtain this energy from renewable power sources. Thus, the generation of electricity (surpassing the gigawatt range) from natural resources like the sun and wind has been viewed with great interest. However, this growing capacity of localized and stochastic production of electricity coming from renewables requires a storage system of equal magnitude. In this context, the energy storage in the form of hydrogen through water electrolysis is considered to be the best means by which to store energy coming from renewable but intermittent power sources. To date, many studies have concentrated on increasing the efficiency, durability, and at the same time reducing the costs of water electrolysis systems that use a polymer electrolyte membrane (PEMWE). Special focus is given to membrane electrode assembly (MEAs), since its materials, components, and nano-micro structure will affect performance and durability. In this work, the optimization of the metallic masses applied to cathodes and anodes, the quantity of polymeric ionomer used in these electrodes will be performed, in order to obtain a triple-phase boundary at the nano-microscopic level with maximum efficiency and durability. Using advanced methods and characterization tools such as X-ray diffraction spectroscopy (XRD), surface area analysis via BET, high resolution transmission electronic microscopy (TEM), we expected to develop a model to formulate and produce MEAs with a well optimized triple-phase boundary presenting maximum efficiency and durability. Additionally, studies and modifications of the support material will be performed. Titanium oxide (TiO₂) and tungsten carbide (WC) will be evaluated as catalyst support. Thermal and thermochemical treatments will be also applied to the support materials to enhance the physico-chemical properties of its structure. More importantly, the durability of the developed MEAs will be evaluated using single cells through long term experiments, according to the protocols considered to be the most appropriated when coupling water electrolysis to intermittent power sources.

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PART A

Title of the project: Development of silicon alloy based passivation layers for high efficiency silicon heterojunction solar cell

Jülich's institute: Institute of Energy and Climate Research 5 - Photovoltaics

Project leader: Dr. Kaining Ding

Web address: http://www.fz-juelich.de/iek/iek-5/DE/Home/home_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): The institute should be experienced in the studies on silicon thin-film related photovoltaic technologies. Knowhow in the fabrication of silicon heterojunction solar cell is welcome. A strong link to Chinese PV industry is preferential. The institute should be supported by "973" projects.

Required qualification of the postdoc:

- PhD in physics, material sciences, electrical engineering or a comparable discipline
- experience with deposition and analysis of silicon thin-film and its alloys as well as fabrication and characterization of silicon based solar cells
- additional skills in oral and written scientific English, software e.g. originlab and matlab

PART B

Documents to be provided by the postdoc:

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PART C

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Description of the project: (max. 1 page)

The saturation of silicon dangling bonds at the crystalline silicon (c-Si) surface is of major importance for c-Si solar cells. The next step towards a new generation of c-Si solar cell technology lies in the application of thin-films that not only passivates the c-Si surface but also forms the electronic junction. The successful silicon heterojunction solar cell concept using intrinsic amorphous silicon as passivation layer is one example. As a consequence of the successful Panasonic silicon heterojunction (SHJ) solar cell concept, research groups are encouraged to develop advanced alternative materials for SHJ solar cells. One possibility to improve the cell performance is to reduce the optical losses in the intrinsic layers by introducing more transparent amorphous silicon alloy materials. There are two silicon oxide composition regimes that provide high passivation quality, namely hydrogenated silicon-rich silicon oxide with O content less than 5 % (a-SiO_x:H) or near-stoichiometric silicon dioxide with H-incorporation (a-SiO₂:H). In addition, hydrogenated silicon-rich silicon carbide with C content less than 5 % (a-SiC_x:H) provides surface passivation comparable to a-SiO_x:H. Further advantage of silicon alloys are their higher chemical, thermal and mechanical stability as compared to silicon giving rise to more freedom for subsequent processes. Furthermore, the temperature coefficient seems to be beneficial when using silicon alloy providing better in-field performance as compared to SHJ solar cells with a-Si:H. However, the silicon oxide and carbide passivation layers feature higher band gap than a-Si:H and the impact of these layers on the electrical transport in the solar cell device, especially in conjunction with doped layers and transparent conductive oxide films, has to be taken into consideration carefully. This project makes comparative study on the device performance of plasma-enhanced chemical vapor deposited (PECVD) a-SiO_x:H and a-SiC_x:H as well as wet-chemically grown a-SiO₂:H on textured wafers with the focus on the trade-off between passivation quality (open circuit voltage) and electrical transport (fill factor). The solar energy conversion efficiency is to be optimized using silicon alloy passivation layer together with doped layers based on microcrystalline silicon alloy materials. This work includes the preparation of silicon oxide and carbide using PECVD and wet-chemistry silicon oxide as well as the fabrication and characterization of SHJ solar cells using these materials. The required infrastructure and preliminary works for this work are provided by IEK5.

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PART A

Title of the project: Large scale simulations of nuclear waste form materials.

Jülich's institute: Institute of Energy & Climate Research 6 - Nuclear Waste Management and Reactor Safety

Project leader: Dr. Piotr Kowalski

Web address: http://www.fz-juelich.de/iek/iek-6/DE/home/_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:
(max. half page):

We are looking for a partner in China to establish a collaboration on computational modeling of (nuclear) materials. Forschungszentrum Jülich as a leading European supercomputing center offers excellent access to the best supercomputing resources and related expertise on its utilization for scientific research and China becomes an emerging leader in that field, which is indicated by a number of the powerful supercomputing resources available across the country and an increasing number of scientific research emerging in the field of computational materials science. It would be therefore mutually beneficial to strengthen the collaboration on the academic level.

Required qualification of the postdoc:

- PhD in Physics, Chemistry, Computational Science, Materials Science, Geoscience, Mineralogy or related fields.
- Experience with simulations using molecular dynamics methods using *ab initio* or force field codes, fluency in supercomputing and basic programming skills.
- Knowledge of physics and chemistry of materials. Expertise on research on or modeling of nuclear materials would be appreciated but is not a necessity.

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
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¹ please add overleaf



PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

Radioactive waste as an unavoidable by-product of nuclear power generation and other applications of nuclear technology requires safe management strategies. In IEK-6 there exist an actively ongoing research program aimed into development of techniques for efficient separation, immobilization and disposal of radionuclides. With the continuously increasing power of supercomputing resources and performance of the simulation software it is now possible to simulate the properties of chemically complex materials using accurate methods of computational quantum chemistry and materials science. There are certain scientific questions which due to activity of the actinide-bearing samples or limitation of the experimental techniques could be addressed only by atomistic modeling. These relate to the materials properties and processes such as change in the structural, the mechanical and the thermodynamic properties of solid materials upon incorporation of actinides into their structures, the propagation of radiation damage cascades and the stability of radiation-induced defects. The information on these processes is essential for the assessment of the stability of the nuclear waste forms, including the ones planned for the permanent waste disposal. However, in order to make the simulation results reliable, the computational setup and models must be well calibrated and tested on the sets of available experimental data. Such a validation allows also for designing of more accurate simulations techniques. This for instance includes a better constraining of the interatomic interaction potentials (force fields) that are crucial for conducting reliable large-scale atomistic simulations using for instance molecular dynamics technique. The aim of the project is the design and testing of reliable computational methodologies and their subsequent applications to large scale simulations (involving millions of atoms) of kinetics-driven processes in materials that are of interest as potential nuclear waste host forms. The studies will include simulations of processes such as dissolution, diffusion and radiation damage and will be performed together with other group members and collaboration partners, among others with Prof. Julian Gale and Prof. Nigel Marks from Curtin University in Australia who are leading researchers in the field of development of codes for atomistic simulations (GULP code) and the atomistic simulations of nuclear materials. They will participate in design of a set of simple force fields with which the postdoctoral fellow will perform large scale simulations of the outlined properties of nuclear waste forms. The initial target materials will be borosilicate glasses and monazite- and pyrochlore- type ceramics investigated in IEK-6 and partner institutions. These computer simulations will be performed in parallel to the ongoing experimental work and the joint research is expected to deliver information that is crucial for the assessment of the stability of the nuclear waste forms. The project will be performed using the world class supercomputing resources available at Forschungszentrum Jülich and RWTH Aachen University and the interdisciplinary character of the proposed research will allow the postdoctoral fellow to gain the best experience in computational materials science and the nuclear engineering. The research will be performed in close collaboration with the experimental groups working in the IEK-6 as well as with the leading research groups in nuclear materials science and atomistic modeling simulations located in France (CEA, EDF), USA (ORNL) and Australia (Curtin U., ANSTO) and as such should lead to addition of China as a permanent partner to the existing collaboration net.

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PART A

Title of the project: How robust are trends in the Brewer–Dobson circulation derived from different re-analysis products?

Jülich's institute: Institute for Energy and Climate Research 7 - Stratosphere
(Institute Director: Prof. Dr. Martin Riese)

Project leader: Dr. Paul Konopka (p.konopka@fz-juelich.de)

Web address: www.fz-juelich.de/iek/iek-7/EN

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

The partner institute should focus on the research of the physical and chemical processes of the atmosphere. It would be desirable to establish connection to a world-class research institute or university that is strongly involved either in the Earth system science or in the Earth system modeling or in the Earth observation technology with a focus on global change issues.

Required qualification of the postdoc:

- PhD in Meteorology, Physics or Atmospheric Chemistry.
- experience with geophysical fluid dynamics and numerical methods applied in atmospheric dynamics and chemistry
- experience with developing and maintaining large scientific codes
- candidates must be able to work effectively in English
- good knowledge of high-level programming language such as Fortran-90, shell scripts, strong background in UNIX systems (and/or Linux)

PART B

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PART C

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Description of the project: (max. 1 page)

With 5500 staff members Forschungszentrum Jülich (FZJ) is the largest interdisciplinary research center in Germany focusing its research in the fields of health, environment and energy, and information technology. The upper troposphere and lower stratosphere (UTLS) is an atmospheric region, which is crucial for understanding climate change, because the Earth's radiation budget and surface temperatures sensitively depend on the trace gas composition in the UTLS. However, there is no scientific consensus regarding changes in the UTLS in a changing climate. In particular trends of water vapor, ozone and of the large-scale circulation itself, the so-called Brewer-Dobson circulation are not well quantified and the processes driving these changes are only poorly understood.

Meteorological analyses and reanalyses are best estimates of the true state of the atmosphere. As such, they are of eminent importance not only for initialization of weather forecast model runs, but for process analyses and detection and attribution of changes in the climate system. To understand trends of atmospheric trace gases like water vapor or ozone, Chemistry Transport Models (CTMs) which are driven by such a meteorological reanalysis are generally applied. The Chemical Lagrangian Model of the Stratosphere (CLaMS) provided by FZJ is a CTM that is particularly well suited for resolving strong tracer gradients like those in the vicinity of the tropopause. The current version of CLaMS is driven by ERA-Interim reanalysis product reproduces some features of the observed trends of water vapor and mean age over the last 35 years.

The main goal of this proposal is to extend such studies to another, widely accepted reanalysis products like the Modern-Era Retrospective Analysis for Research and Applications (MERRA), Japanese 25-yr Reanalysis and Japan Meteorological Agency Climate Data Assimilation System (JRA-25/JCDAS), and National Centers for Environmental Prediction/National Center for Atmospheric Research (NCEP/NCAR) Reanalysis. The analysis is expected to give new insights into long-term circulation trends, in particular in those which are independent on the applied reanalysis. Thus, it would be an important step towards better understanding of changes in transport processes in the UTLS region in a changing climate, and towards improving the representation of these processes in atmospheric models.

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PART A

Title of the project: Aerosol Ageing and Cloud Formation

Jülich's institute: IEK-8 (Troposphere)

Project leader: PD Dr. Thomas Mentel

Web address: <http://www.fz-juelich.de/iek/iek-8/EN/>

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): We are looking for a partner with strong interest in tropospheric aerosols and heterogeneous chemistry in context of air pollution and climate change. Since we are covering the clouds/climate aspect ourselves within the proposed project, it would add extra value if the partner in PR China could contribute to the air pollution aspects and cover the health aspects of tropospheric aerosols. We are looking for a partner who is active in experimental work with experience in laboratory studies and in field observations.

Required qualification of the postdoc:

- PhD in chemistry, physics, or environmental sciences
- experience with CCN measurements, heterogeneous chemistry, aerosol mass spectrometry
- additional skills in programming, data administration, working in teams

PART B

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PART C

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Description of the project: (max. 1 page)

Aerosols are important constituents of the atmosphere. They are either emitted directly or formed by gas-to-particle conversion during the (photo-)oxidation of trace gases. Atmospheric aerosol particles are undergoing chemical and morphological changes during their tropospheric lifetime of a few days. Tropospheric aerosols play an important role for climate as they affect the radiative balance of the Earth system. Most important, they determine formation, lifetime, and optical properties of clouds. They contribute to air pollution and can cause severe health problems (e.g. cardiovascular diseases). Despite their obvious importance, aerosols are the least understood component in the atmosphere and regional air quality models have difficulties to predict aerosol properties that are important for radiative balance, cloud formation, and health effects. The reasons are the diversity of aerosols sources, the ageing processes, and the medium long lifetime of aerosols, which causes overlapping transport and local processes. In cooperation with a partner from the People's Republic of China we want to exploit long term monitoring of aerosols, covering the four seasons of the year. We aim at measurements of particle size distributions and of the most important hygroscopic property: the ability to act as nuclei for cloud droplet activation (CCN activity). The monitoring will be operated on the Meteorological Tower of the Research Center in Jülich in three different heights: at the ground, at 50m, and outside the surface layer at 120m. Comparing observations at three different heights allows for separating local and regional effects. In addition we will perform in-situ chemical composition measurements by top of the art high resolution spectrometry at the meteorological tower. The projected novel and unique data set and will be used

- i) to relate the CCN-activity in 120m altitude to cloud base properties observed by the ground based remote sensing center JOYCE, located in the Research Center
- ii) to understand chemical processing of atmospheric particles
- iii) to optimize the chemical weather forecast of the regional model EURAD.

Especially the first requires longer monitoring (and statistical analysis as only in a convective, well a mixed atmosphere sub-cloud aerosol properties can be related to observations in 120m height.) The two topics i) and iii) will be supported by partners from University of Cologne and RIU (Rhenish Institute of Environmental Research). For topic ii) we will perform accompanying chemical simulation experiments in the laboratory and in our simulation chamber SAPHIR in order to understand ageing processes and their effect on droplet activation. One focus will be the coating of inorganic substrates by secondary organic components, especially mineral dust



Ministry of Human Resources
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components which are an important topic in China. As a novel tool we will implement high resolution FIGAERO-CIMS which measures gas-phase and particulate-phase composition by in-situ thermal desorption mass spectrometry.

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PART A

Title of the project: Development of and Application of Imaging Methodology in the Neurosciences

Jülich's institute: Institute of Neuroscience and Medicine 4 - Medical Imaging Physics

Project leader: Professor N. Jon Shah

Web address: http://www.fz-juelich.de/inm/inm-4/EN/Home/home_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): We are interested in collaborating with a strong partner with know-how in MRI, PET, hybrid MR-PET and MEG. We have cutting-edge hardware for neuroimaging and would like to collaborate to develop it further and use it for novel neuroscientific and clinical applications. Our partner will ideally have experience in one or more of the methodologies listed above and have experience in neuroscientific applications thereof.

Required qualification of the postdoc:

- PhD in physics, electrical engineering, or a neuroscience related subject
- experience with MRI, PET, and MEG
- additional skills in neurosciences or clinical brain imaging

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- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

The research and development activities of the Medical Imaging Physics division (INM-4) of the Institute of Neuroscience and Medicine concentrate on the development, experimental validation and the clinical implementation of novel brain imaging methods. The focus of our scientific activities is the development, experimental validation and the clinical implementation of novel brain imaging methods (MRI, PET, fMRI, MR-PET, MEG). The INM-4 built a worldwide unique platform for translational neurological research based on a hybrid, ultra-high MR-PET scanner for human research. Further, the Institute houses a 9.4T animal MR scanner, 3T and 4T MRI systems, a 3T MR-PET scanner, a human PET scanner, as well as an MEG system.

Our primary aim is the development and implementation of new imaging methods and technology for imaging the brain. In particular, the INM-4 has significant expertise in quantitative MR imaging, structural and functional imaging (including development of brain atlases), imaging of sodium, diffusion imaging and ultra-high field MR-PET.

To support these activities, the INM-4 is seeking qualified postdoctoral candidates for the development of methods for: (a) quantitative MRI; (b) imaging of sodium at 9.4T; (c) in vivo NMR spectroscopy; and (d) development of radiofrequency coils.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: High-throughput quantitative assessment of ligand/GPCR poses and potency via advanced molecular simulation

Jülich's institute: Institute for Advanced Simulation 5 - Computational Biomedicine, and Institute of Neuroscience and Medicine 9

Project leader: Prof. Paolo Carloni

Web address: <http://www.fz-juelich.de/ias/ias-5>

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page):

- Institutes focusing on the advancement of the state-of-the-art in computational science using high performance computing, with an interest in computational biology.
- Experimental institutes interested in the characterization of the mechanisms underlying GPCR/ligand interactions using high throughput techniques

Required qualification of the postdoc:

- PhD in computational biology, pharmacology, physics, applied mathematics, or in a related field.
- experience with biological systems, bioinformatics, classical MD simulations, statistical/soft matter physics and programming. Depending on the attitudes, skills of the selected candidate and the interests of the Chinese partner institute, the project can be more specifically oriented towards the pharmacological/biological applications or the methodological development.
- additional skills in : Fluency in English is a requirement.

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications

¹ please add overleaf

PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

Human G-protein coupled receptors (GPCR) are the largest membrane-bound protein family expressed in the genome (1). GPCRs participate in about the 80% (2) of cell signaling processes. They are of immense importance in pharmacology, being the targets of ca. 40% of the marketed drugs (3). Hence, determining structural molecular determinants of agonists/GPCRs complexes is crucial for pharmacology. The recent progress in GPCRs crystallography opened an unprecedented venue for receptor-ligand characterizations, allowing the use of structure-based drug design protocols for several members of the family. However, the lack of structural data for most (95%) GPCRs members calls upon computer-aided structural predictions. In this context, our group is developing and using a hybrid Molecular Mechanics/Coarse-Grained (MM/CG) approach (4-7) specifically tailored for GPCR / ligand complexes. Here, only the binding cavity is represented with full atomistic detail (MM region) while the rest is represented with a coarser resolution (CG region). See http://www.fz-juelich.de/ias/ias-5/EN/Research/1-NeuronFunctionandDysfunction/Methods/Receptors/_node.html for more details. The approach is much cheaper than all-atom MD simulations (8) and more accurate than using homology models and molecular docking (9, 10). We are currently implementing an adaptive resolution scheme (AdResS) (11),(12) to perform grand canonical ensemble simulations within the region of interest, which may lead to accurately predict not only binding poses (9, 13) but also ligands affinities. The employment of high performance computing will allow the use of this code for high-throughput quantitative predictions of poses and affinities for a variety of pharmaceutical targets.

The postdoc will work with us on implementing the code (background in physics or theoretical chemistry required) and/or using it for predicting the binding mode of pharmaceutically interesting ligands (background in pharmaceutical chemistry, biology), in close collaborations with Chinese groups interested in multiscale molecular simulations and/or pharmacological applications involving GPCR's.

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2. Sali A & Overington JP (1994) Protein Sci 3(9):1582-1596.
3. Overington JP, et al. (2006) Nat. Rev. Drug. Discov. 5(12):993-996.



4. Leguebe M, et al. (2012) PloS one 7(10):e47332.
5. Neri M, et al. (2005) Physical Review Letters 95(21):218102.
6. Neri M, et al. (2008) Biophysical Journal 94(1):71-78.
7. Neri M, et al. (2006) J. Phys.: Cond. Mat. 18(14):S347-S355.
8. Johnston JM et al. (2011) Current opinion in structural biology 21(4):552-558.
9. Marchiori A, et al. (2013) PloS one 8(5):e64675.
10. Giorgetti A, et al. (2005) Bioinformatics 21 Suppl 2:ii72-76.
11. Praprotnik M, et al. (2008) Annu. Rev. Phys. Chem. 59:545-571.
12. Junghans C et al. (2010) Comput Phys Commun 181(8):1449-1454.
13. Biarnes X, et al. (2010) PloS one 5(8):e12394.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Predicting structural ensembles of intrinsically disordered proteins involved in neurological disorders

Jülich's institute: Institute for Advanced Simulation 5 - Computational Biomedicine, and Institute of Neuroscience and Medicine 9

Project leader: Jun.-Prof. Dr. Giulia Rossetti

Web address: <http://www.fz-juelich.de/ias/ias-5>

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute: (max. half page): Institutes interested in the advancement of the state-of-the-art for treating IDPs, with application in human health. Experimental institutes interested in the characterization of the mechanisms underlying IDPs interactions with cellular partners as well as ligands.

Required qualification of the postdoc:

- PhD in chemistry, Biology, or Physics
- experience with molecular simulation of biomolecules. The successful candidate will work on improving directional statistics-based methods and/or will perform applications to drug/IDPs interactions, possibly within collaborations with theoretical or experimental groups in China.
- additional skills in ab-initio molecular dynamics. This request is optional.

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

¹ please add overleaf



PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

Intrinsically Disordered Proteins (IDPs) constitute a very important class of functional proteins with high abundance in nature (1-4). Indeed about one-third of eukaryotic proteins are predicted to be IDPs, playing crucial roles in signalling and regulation processes (1, 5-7). As a result, interfering with the function of disease-associated IDPs offers a highly attractive objective for drug development against diseases such as neurodegenerative disorders (8). Unfortunately, rational drug design targeting IDPs poses serious challenges: these proteins exist as dynamic, highly flexible structural ensembles that undergo conformational conversions on a wide range of timescales (9). They experience long-range conformational rearrangements, transient secondary and long-range tertiary structure (2, 3, 10). Computer-aided structural predictions need to address additional issues, from the accuracy of the force fields to sampling a very wide conformational space (11). Our group is currently facing these challenges by adopting apt computational protocols.

(see [http://www.fz-juelich.de/ias/ias-5/EN/Research/1-](http://www.fz-juelich.de/ias/ias-5/EN/Research/1-NeuronFunctionandDysfunction/Dysfunction/NeurodegenerativeDiseases/_node.html)

[NeuronFunctionandDysfunction/Dysfunction/NeurodegenerativeDiseases/_node.html](http://www.fz-juelich.de/ias/ias-5/EN/Research/1-NeuronFunctionandDysfunction/Dysfunction/NeurodegenerativeDiseases/_node.html))

On one hand, we are performing all-atom simulations in explicit solvent of those IDPs for which biophysical data are available. Here, analysis tools developed by us and based on directional statistics formalism (12) are able to quantify changes of IDP's flexibility and conformational transitions upon drug binding, allowing to compare the results with experimental data such as 2D NMR spectra (13). On the other hand, we adopt a powerful replica-exchange-based method, coupled with Monte Carlo simulations in implicit solvent, for IDPs whose experimental biophysical information is scanty. This method, developed at the Jülich supercomputing center (14), has already shown to lead to reliable structural predictions of an IDP (15).

We plan to share our expertise to model pharmacologically relevant IDPs with Chinese groups interested either in method/code development and/or in applications, especially to neurodegenerative disorders.

1. Dyson HJ, et al. (2005) *Nat. Rev. Mol. Cell Bio.* 6(3):197-208.
2. Tompa P (2002) *Trends Biochem. Sci.* 27(10):527-533.
3. Wright PE, et al. (1999) *J. Mol. Biol.* 293(2):321-331.
4. Uversky VN (2002) *Protein Sci* 11(4):739-756.
5. Babu MM, et al. (2011) *Curr. Opin. Struct. Biol.* 21(3):432-440.
6. Uversky VN, et al. (2005) *J. Mol. Recognit.* 18(5):343-384.
7. Smock RG, et al. (2009) *Science* 324(5924):198-203.
8. Uversky VN, et al. (2008) *Annu. Rev. Biophys.* 37(1):215-246.



9. Dunker AK, et al. (2001) *J. Mol. Graph. Model.* 19(1):26-59.
10. Wright PE, et al. (2009) *Curr. Opin. Struct. Biol.* 19(1):31-38.
11. Click TH, et al. (2010) *Int J Mol Sci* 11(12):5292-5309.
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13. Dibenedetto D, et al. (2013) *Biochemistry* 52(38):6672-6683.
14. Irback A, et al. (2005) *Biophys. J.* 88(3):1560-1569.
15. Cong X, et al. (2013) *J. Chem. Theory Comput.* 9(11):5158-5167.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Structure and Dynamics of Intrinsically Disordered Proteins: A Complementary View from Neutron Scattering and Single-Molecule Fluorescence Spectroscopy

Jülich's institute: Juelich Centre for Neutron Science 1 & Institute of Complex Systems 1

Project leader: Dr. A. Stadler

Web address: http://www.fz-juelich.de/ics/ics-1/DE/Forschung/Biologie/_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): We are looking for a partner with strong interest in protein internal dynamics and with experience in experimental work on proteins. As the fields of neutron scattering, FRET and computer simulation are covered by our groups an additional complementary experimental method like e.g. NMR would add extra value to the project in particular if it is related to the expression of intrinsically unfolded proteins.

Required qualification of the postdoc:

- PhD in physics, biophysics or physical chemistry with background in soft matter or biophysics
 - experience with advantageous knowledge in neutron or xray scattering
 - additional skills in programming skills advantageous (python)

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

¹ please add overleaf



PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

We are looking for a post-doctoral research scientist with a cooperative and structured working style to join our institute JCNS-1 & ICS-1. We would like to combine neutron scattering and single-molecule fluorescence spectroscopy to investigate the structure and dynamics of the intrinsically disordered myelin basic protein (MBP). MBP is a major component of the myelin sheath in the central nervous system. From a medical aspect MBP has significant importance as there are neurological disorders, e.g. multiple sclerosis, which are related to MBP misfolding and malfunction. In aqueous solution MBP is unstructured and is classified as intrinsically disordered. Lipid binding or specific solvent conditions induce partial folding of the protein. From a biophysical point of view MBP is an interesting system to study the basic physical properties of disordered or partially unfolded proteins in solution. In the research project we would like to study the protein in its intrinsically disordered state and in partially folded conformations. Small angle neutron scattering will be measured to investigate the structure of the protein. Protein dynamics on different time and length scales will be measured using neutron spin-echo spectroscopy and neutron backscattering spectroscopy. The PostDoc will perform the neutron scattering experiments and interpret the data using different theoretical models derived from polymer theory. The scientific question, which we would like to address, is whether and to which degree the structure and dynamics of an intrinsically disordered or partially folded protein can be described with concepts derived from polymer theory. Complementary information will be obtained from single-molecule fluorescence spectroscopy (FRET) measurements, which will be performed in collaboration with the institute ICS-5 of Prof. Jörg Fitter. An important component will be the inclusion of coarse-grained computer simulations, which will allow an atomistic interpretation of the neutron scattering and FRET data. The novel methodological aspect of the project is to combine neutron scattering and FRET, which will increase significantly the spatial and temporal resolution of the determined structures and dynamics of proteins in solution.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Observations meet simulations: Inverse Modelling of Volcanic Emissions in the Asian Monsoon Circulation based on satellite observations

Jülich's institute: Jülich Supercomputing Centre (JSC), Simulation Laboratory Climate Science (SLCS)

Project leader: Dr. Lars Hoffmann, Dr. Sabine Grießbach

Web address: www.fz-juelich.de/ias/jsc/slcs

Description of existing or sought Chinese collaboration partner institute:

We are looking for a partner who is interested to study the atmospheric composition and atmospheric processes by connecting atmospheric simulations with measurements. Having a strong background in satellite remote sensing of atmospheric trace gases (e.g. CFCs), clouds and aerosol (e.g. volcanic aerosol) we identified two possible research fields for collaboration:

We would like to use and offer our global satellite data products, which cover a time period of about 10 years, for the realisation of studies on challenging scientific topics, such as the Asian monsoon circulation. For collaborating scientists doing atmospheric simulations these data sets could provide valuable information for model initialisation and the validation of model runs.

On the other hand, the retrieval of information from satellite measurements is based on inverse modelling. In order to estimate and to reduce uncertainties of the retrieved data products it is always necessary to compare with measurement data. Hence, we would be interested in finding a partner institute that would contribute to retrieval data validation studies with measurements (e.g. in-situ, lidar).

Required qualification of the postdoc:

The candidate should either have

- a PhD in atmospheric sciences or physics
- experience with atmospheric transport modelling, remote sensing of the atmosphere, model validation

or

- a PhD in computational sciences or informatics
- experience with inverse modelling, parallel programming and a strong interest in atmospheric sciences

and

- additional skills in programming in C, visualisation of scientific data, preparation of scientific publications

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project:

The Asian monsoon is a large atmospheric circulation system extending from East Asia to north Africa developing each boreal summer. Its potential to distribute trace gases and aerosols over the entire northern hemisphere and its impact on troposphere-stratosphere exchange recently attracted great interest in climate science. The eruption of the Nabro volcano, Eritrea, in June 2011 injected a considerable amount of sulfur dioxide (SO₂) into the western tail of the Asian monsoon circulation. The SO₂ was oxidized to sulphate aerosol, which has long atmospheric lifetimes (several months to years) if injected into the upper troposphere and stratosphere and hence has an impact on the radiative budget. The Nabro event raised a scientific debate regarding the importance of the Asian monsoon circulation as an atmospheric transport pathway and transport barrier (Bourassa et al., 2012¹; Fromm et al., 2013²).

In contrast to the Nabro eruption that directly injected the volcanic material into the Asian monsoon circulation, where it was contained for a few weeks, the eruption of Sarychev volcano on the Kuril Islands in June 2009 can be considered as the opposite event. It injected the volcanic material into high latitudes outside of the Asian monsoon circulation and in the

1 Bourassa, A. E., Robock, A., Randel, W. J., Deshler, T., Rieger, L. A., Lloyd, N. D., Llewellyn, E. J. T., and Degenstein, D. A. (2012). Large volcanic aerosol load in the stratosphere linked to Asian monsoon transport. *Science*, 337(78):78–81. doi:10.1126/science.1219371.

2 Fromm, M., Nedoluha, G., and Charvat, Z. (2013). Comment on large volcanic aerosol load in the stratosphere linked to Asian monsoon transport. *Science*, 339(6120):647. doi:10.1126/science.1227817.

following weeks the volcanic aerosol was distributed over the entire northern hemisphere, but did not enter the Asian monsoon circulation.

Satellite instruments are well suited to observe trace gases and aerosols on a global scale. Together, the volcanic SO₂ and the sulphate aerosol provide excellent passive tracers to study atmospheric transport processes over a time frame of several months. The project partners in Jülich developed and published new detection algorithms for volcanic emissions for ESA and NASA satellite experiments (Griessbach et al., 20143, 20154; Hoffmann et al., 20145).

However, satellite observations are usually limited in temporal and spatial resolution due to their measurement principles and characteristics. Therefore atmospheric models are indispensable tools to study transport processes. In particular, Lagrangian particle dispersion models allow for transport and mixing studies of air masses based on the trajectories of individual air parcels. The SLCS recently developed the trajectory model MPTRAC that is designed for large-scale simulations on state-of-the-art supercomputers. The new model allows for efficient handling of trajectory calculations with up to 100 million air parcels. Recently, an inverse modelling concept to perform parameter estimations with MPTRAC was developed. With the inverse modelling concept and satellite data the time- and altitude-resolved volcanic emissions of the Nabro eruption were reconstructed.

Within the proposed project the inverse modelling concept shall be extended to the Sarychev eruption. In order to study the stability and permeability of the Asian monsoon transport barrier the observations and simulations of the two opposing volcanic eruptions shall be analysed.

3 S. Griessbach, L. Homann, R. Spang, and M. Riese. Volcanic ash detection with infrared limb sounding: MIPAS observations and radiative transfer simulations. *Atmos. Meas. Tech.*, 7(5):1487{1507, 2014. doi: 10.5194/amt-7-1487-214.

4 S. Griessbach, L. Homann, R. Spang, M. von Hobe, R. Müller, and M. Riese. Infrared limb emission measurements of aerosol in the troposphere and stratosphere. *Atmos. Meas. Tech. Discuss.*, 8(4):4379{4412, 2015. doi: 10.5194/amtd-8-4379-2015.

5 Hoffmann, L., Griessbach, S., and Meyer, C. I. (2014). Volcanic emissions from AIRS observations: detection methods, case study, and statistical analysis. In *Proceedings SPIE 9242, Remote Sensing of Clouds and the Atmosphere XIX; and Optics in Atmospheric Propagation and Adaptive Systems XVII*, 924214 (October 21, 2014) . doi:10.1117/12.2066326.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Identification of recombination centers and carrier dynamics in materials and nanostructures for solar cell applications by combining laser excitation with scanning tunneling microscopy

Jülich's institute: Peter Grünberg Institute, PGI-5

Project leader: Prof. Dr. R. E. Dunin-Borkowski, Dr. Ph. Ebert

Web address: http://www.fz-juelich.de/pgi/pgi-5/EN/Home/home_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute: (max. half page): The Chinese collaboration partner institute should be active in surface science of semiconductor nanostructures and/or quantum materials, preferably using scanning tunneling microscopy with laser excitation.

Required qualification of the postdoc:

- PhD in physics or materials science
- experience with surface science techniques and scanning tunneling microscopy and spectroscopy
- additional skills in semiconductor physics

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

PART C

Additional requirements to be fulfilled by the postdoc:

¹ please add overleaf

- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

Climate warming due to carbon-dioxide-releasing energy production and the inherent risks of atomic energy are the key driving forces for the development of carbon-dioxide-free and renewable energy production. At the same time, increasing demand for fossil fuels and limited oil availability are raising the costs of conventional electricity production, making the long term use of fossil fuels increasingly uneconomical. Therefore, solar energy is attracting considerable attention. However, at present the efficiency of solar cells is still relatively low and improvements are slow. Hence, it is of great interest to evaluate and develop technologies that can be used to increase the efficiency and reduce the economic cost of renewable solar energy production. This aim is not only a priority of the German federal government, but it is also of great importance for China as the largest electricity consumer and the largest producer of solar panels in the world.

In order to improve the efficiency of photovoltaic devices, a deep physical understanding of the atomic processes that are involved in the conversion of energy in materials is critical. At present, the lack of an atomic-scale understanding is often a major factor that is limiting progress in increasing the efficiency of solar cells, which is well below the thermodynamic limit. The efficiencies of solar cell devices are still limited primarily by losses associated with the excitation of electron-hole pairs and light absorption, thermalization of hot carriers and the unintentional recombination of electrons and holes within the solar cell before the carriers reach the electrodes. The latter two effects limit carrier collection efficiency and hence light-electrical energy conversion efficiency. In particular, defects in the active regions of solar cell devices may occur naturally in thermodynamic equilibrium. In addition, the drive towards using nanostructures also increases the surface to volume ratio and hence recombination at surfaces becomes relevant. For example, non-polar sidewall surfaces of nanowires may introduce recombination channels through surface defects. Hence, it is important to identify which defects are present on the outer surfaces of nanowires and in the bulk material and especially which of them act as recombination centers. The identification of individual recombination centers requires atomically-resolved direct imaging combined with simultaneous measurement of electronic and geometric properties under light excitation. This capability can be achieved using laser-excited scanning tunnelling microscopy, which combines optical excitation with atomic resolution characterization.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Characterization of group III nitride semiconductor interfaces using scanning tunneling microscopy

Jülich's institute: Peter Grünberg Institute, PGI-5

Project leader: Prof. Dr. R. E. Dunin-Borkowski, Dr. Ph. Ebert

Web address: http://www.fz-juelich.de/pgi/pgi-5/EN/Home/home_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:
(max. half page): The Chinese collaboration partner institute should be active in the field of semiconductor optoelectronics or surface science research and the physics of nanostructures and/or quantum materials.

Required qualification of the postdoc:

- PhD in Physics or Material Science
- experience with surface science techniques and STM
- additional skills in semiconductor physics

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years

¹ please add overleaf

- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

Group III nitride semiconductors have developed rapidly toward being the materials of choice for green to ultraviolet optoelectronics. Such optoelectronic devices are based primarily on heterostructures of different group III nitrides and/or differently doped layers, in which the exact atomic arrangement within the individual epitaxial layers in the nanostructures and at their interfaces sensitively influences their optoelectronic properties. Intense efforts have been invested in the optimization and improvement of the quality of the epitaxial growth. Although group III nitrides are now successfully applied in LEDs and lasers, rather little is still known about the atomic scale electronic properties of their interfaces. For further optimization of optoelectronic devices, a detailed knowledge and understanding of such physical mechanisms and properties is critical. In the proposed project, interfaces in III-N compound semiconductors will be characterized using cross-sectional scanning tunnelling microscopy and spectroscopy, as well as using complementary transmission electron microscopy techniques. The aim of the project will be to determine the local electronic properties of the materials with atomic resolution and to correlate these measurements with device properties.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Ultrasensitive detection of biomolecules with silicon nanowire field-effect transistors

Jülich's institute: Peter-Grünberg Institute 8 - Bioelectronics

Project leader: Prof. Dr. Andreas Offenhäusser

Web address: <http://www.fz-juelich.de/pgi/pgi-8/EN/>

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page):

We are looking for a partner with a focus on both fundamental and applied researches in information technology like SOI material, micro/nano sensors, RF and micro-wave integrated systems, and biochips. Since we are covering the nanotechnology aspect ourselves within the proposed project, it would add extra value if the partner in PR China could contribute to the molecular biology questions like biomolecular amplification strategies

Required qualification of the postdoc:

- PhD in Physics, Physical Chemistry, Bioscience, Biomedical or Electrical Engineering
- experience with silicon nanowire transistor, biosensing, molecular recognition
- additional skills in cleanroom technology, molecular biology, biotechnology

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

¹ please add overleaf

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

Thanks to the large surface-to-volume ration, electrical properties, and biocompatibility, SiNWs have recently drawn tremendous attention due to its ultrasensitivity and potential portable format. Up to now, a variety of SiNW devices configured as FETs have been employed for the ultrasensitive detection of biological and chemical species, including metal ions, DNA, microRNAs, proteins, small-molecules, virus particle, and cells. Moreover, SiNWs fabricated by top-down technique are amenable to large-scale integration and mass production, benefiting from mature silicon industry. For practical applications, label-free and ultrasensitive detections of biological relevant samples (serum, plasma et al.) are performed in physiologically relevant conditions. However, the specific detection of charged biomolecules requires to be performed in a very low-salt buffer solution to overcome Debye screening. To overcome this limitation, some methods have been investigated, such as sample dilution and high-frequency application. Within this project alternative routes will be developed based on biomolecular amplification strategies like hybridization chain reaction (HCR).

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Quantum transport in nanostructured topological insulators

Jülich's institute: Peter Grünberg Institut 9

Project leader: Prof. Dr. Thomas Schäpers

Web address: http://www.fz-juelich.de/pgi/pgi-9/DE/Home/home_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): The post-doc project is part of our research activities within the Virtual Institute for Topological Insulators (VITI). The virtual institute is formed by research groups at RWTH Aachen University, Würzburg University and Forschungszentrum Jülich. Furthermore, as an international partner the Shanghai Institute for Microsystem and Information Technology (SIMIT), member of CAS, is member of VITI. As mentioned in the detailed project description the goal of the virtual institute is to conduct research on topological insulators towards future spinelectronic and quantum information processing devices. In the past years VITI initiated a number of international collaborations, i.e. with the University of Southern California or the Russian Academy of Sciences in Chernogolovka, in order to broaden the material basis or to include characterization methods not being provided by the VITI partners. It is very well known in our research community, that at Chinese universities as well as at the Chinese Academy of Sciences (CAS), very competitive research on topological insulators is pursued. Therefore, we are very interested to establish new collaborations with partners in China or to further strengthen our ties with our partner at SIMIT. The envisioned post-doc projects would put us in the position to start a research activity with new partners, which will hopefully be extended in the future. The benefit for the Chinese partner would be to be integrated in a well-established and very lively research environment provided by VITI.

Required qualification of the postdoc:

- PhD in Physics or electrical engineering
- experience with cleanroom preparation, e.g. optical and/or electron beam lithography, wet and dry etching or evaporation. Furthermore, experience in transport experiments at low temperatures is advantageous.
- additional skills in computer aided design (CAD) would be advantageous, but not mandatory.

¹ please add overleaf



PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

Within the envisioned project electrical transport measurements shall be conducted on nanostructures based on topological insulators (TI). Topological insulators are a new state of matter, where the surface is conductive whereas the bulk is insulating. Compared to other materials with conductive surface states, these states are topologically protected, i.e. they cannot be removed by outer distortions. Since a few years the Peter Grünberg Institute 9 (PGI-9) conducts research on this novel material class. The research projects include the epitaxial growth of topological insulators, the nanostructuring in the Helmholtz-Nanoelectronic-Facility (HNF), and quantum transport investigations. The activities at PGI-9 are an integral part of the research performed within Virtual Institute for Topological Insulators (VITI). Within VITI research groups at RWTH Aachen University, Würzburg University, SIMIT in Shanghai, and Research Centre Jülich joined forces to establish the fabrication of high quality topological insulators, which might be integrated in future high performance spintronic devices or in circuits utilizing topological quantum computation. The post-doc candidate shall conduct research on nanostructured topological insulators. The aim of the research project is to find new routes for utilizing topological insulator nanostructures for device applications. By using nanostructured topological insulators where the phase-coherence length is smaller than the sample dimensions interference effects can be utilized for novel device functionalities. Furthermore, by employing superconducting electrodes, circuit concepts towards topological quantum computation can be assessed. The topological insulator layers grown by molecular beam epitaxy are provided from the



TI growth group at PGI-9. Regarding the epitaxial layers, mainly heterosystems, which were recently designed in Jülich, will be used. The epitaxial layers will be nanopatterned by means of dry etching. For some samples the device geometry will be directly defined by selective area growth. Subsequently, ohmic contacts as well as gate electrodes will be prepared. For a subset of samples superconducting electrodes will also be employed. The candidate will have the chance, to utilize the recently opened Helmholtz Nanoelectronic Facility for sample preparation. The transport experiments will be performed at the PGI-9 low temperature lab. Here, all equipment required to perform sensitive transport experiments is provided. From the transport experiments, information on the phase-coherent transport will be gained. As an example Aharonov-Bohm type conductance oscillations will be investigated, which is one of the interference effects, suitable for electron interference-based devices. For the nanopatterned structures equipped with superconducting electrodes, Andreev reflection and the Josephson supercurrent will be analysed.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Jiangmen Underground Neutrino Observatory (JUNO)

Jülich's institute: Central Institute for Engineering, Electronics and Analytics 2
- Electronic Systems

Project leader: Prof. Dr. Stefan van Waasen ; Christian Grewing

Web address: http://www.fz-juelich.de/portal/EN/AboutUs/organizational_structure/Institutes/CentrallInstituteEngineering/_node.html

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:

(max. half page): The research for the development of a verification setup and printed circuit boards (PCB) for the prototypes of the integrated circuit (IC), as well as to prepare the production tests for the ca 20000 IC that will be used in the detector is to be done in close cooperation with the Institute of High Energy Physics (IHEP) in Beijing, who have the lead in the JUNO project.

Required qualification of the postdoc:

- PhD in Electronics Science and Technology
- experience with application board design for particle detectors, design plug-in boards, including the schematic, PCB design and simulation
- additional skills in high speed digital signal design and practiced experience in high speed circuit design. Experienced in Free Programmable Gate Array (FPGA) design with verilog language. Skilled in using electronic measure instrument, such as oscilloscope, signal generator, etc. Good knowledge of the project requirements due to earlier experiences with particle detectors would be of advantage.

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications

¹ please add overleaf

PART C

Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

The Jiangmen Underground Neutrino Observatory (JUNO) is a multipurpose neutrino experiment designed to determine neutrino mass hierarchy and precisely measure oscillation parameters by detecting reactor neutrinos from the Yangjiang and Taishan Nuclear Power Plants, observe supernova neutrinos, study the atmospheric, solar neutrinos and geo-neutrinos, and perform exotic searches, with a 20-thousand-ton liquid scintillator detector of unprecedented 3% energy resolution (at 1 MeV) at 700-meter deep underground.

(http://english.ihep.cas.cn/rs/fs/juno0815/ATEjuno/201309/t20130912_109433.html).

The Electronic Systems Team of the Central Institute for Engineering, Electronics and Analytics (ZEA-2) is developing in cooperation with the III. Physics Institute of RWTH Aachen University the concept of new detector electronics for this project. These consist of an all new smart sensore approach, which includes the main receiver and digital signal processing in the detector photomultiplier tubes, so that the costs and power consumption can be reduced by minimizing the cables that are needed to build the detector. In the ZEA-2 Integrated Systems Team a new integrated circuitry (IC) is developed in a standard silicon CMOS technology, that combines the special needs of the detector with a concept that makes as far as possible use of standard components in order to reduce the costs and development risks. The development is done in cooperation with the electronics division of the IHEP, who are in charge of the overall electronics of the detector. Monthly conference calls and meetings 3 times per year are organized to make sure that the IC meets the requirement specification that is written as a joined work of IHEP, RWTH Aachen University and ZEA-2. For the development of a verification setup and the PCB for the prototypes of the IC, as well as to prepare the production tests for the ca 20000 integrated circuits that will be used in the detector an experienced postdoc is searched.

2015 Jülich – OCPC – Programme for the Involvement of Postdocs in Bilateral Collaboration Projects

PART A

Title of the project: Meson Decays with CLAS12

Jülich's institute: Nuclear Physics Institute 1 - Experimental Hadron Structure

Project leader: Prof. Jim Ritman

Web address: <http://www.fz-juelich.de/ikp/EN/Home/ExperimentelleHadronenstruktur.html>

Description of the project (max. 1 page)¹:

Description of existing or sought Chinese collaboration partner institute:
(max. half page):

We are looking for a partner with strong interest in hadron or particle physics. Since the hardware aspects are covered by our other partners within the proposed project, it would add extra value if the partner in PR China could contribute to the data analysis aspects. We are looking for a partner who is active in experimental work with experience in data analysis.

Required qualification of the postdoc:

- PhD in nuclear or particle physics
- experience with standard computing tools such as C++ and the ROOT package
- additional skills in : no requirements

PART B

Documents to be provided by the postdoc:

- detailed description of the interest in joining the project (motivation letter)
- curriculum vitae
- copies of degrees
- list of publications
- 2 letters of recommendation

PART C

¹ please add overleaf



Additional requirements to be fulfilled by the postdoc:

- max. age of 33 years
- PhD degree not older than 5 years
- very good command of the English language
- strong ability to work independently and in a team

Description of the project: (max. 1 page)

The CEBAF Large Acceptance Spectrometer (CLAS), located at the Thomas Jefferson National Laboratory located in Newport News, Virginia, United States of America, has been upgraded to operate with incoming photon beam energies from 6.5 GeV - 10.5 GeV. This upper photon beam energy is enough to produce the J/Ψ ($c\bar{c}$) near threshold as well as the lower photon beam energy is enough to produce light mesons containing u, d and s quarks. The physics interest of the Nuclear Physics Institute (IKP-1) at CLAS12 is how mesons decay via di-lepton (electron + positron) pairs which give insight into the structure and dynamics of the mesons through a line shape analysis measuring the transition form factor. Di-leptons from meson decays such as $J/\Psi \rightarrow e^+e^-$ or the recently measured $J/\Psi \rightarrow \pi^0 e^+e^-$ transition form factor performed at BESIII, can be cleanly identified in the CLAS12 detector by means of the High Threshold Cherenkov Counters (HTCC), Electromagnetic Calorimeter (EC) and Low Threshold Cherenkov Counters (LTCC) which give pion veto from electrons up to 10^7 for e^+e^- pairs while retaining large acceptance and millimeter vertex resolution, which is needed to reject external conversion background.

The goal of the project will be to perform simulations and write a proposal to the Programme Advisory Committee for a dedicated future experiment aimed at extraction of physics from meson decays involving di-lepton pairs.