Open PhD Projects

GRADUATE ACADEMY

FRIEDRICH-SCHILLER-UNIVERSITÄT JENA

PhD position (f/m/d) within the department of Mathematics

Reg. Nr. 348/2019

Application deadline: 30.11.2019

The Friedrich Schiller University Jena connects people and ideas, science and economy, institutions of higher education and external research organizations. Being rooted in the heart of Germany and having worldwide bonds, the university, covering all disciplines, characterizes the city of Jena as a future-oriented and cosmopolitan location together with its Partners.

Within the department of Mathematics, Faculty of Mathematics and Computer Science at the Friedrich-Schiller-Universität Jena we encourage applications for a

PhD position (f/m/d)

starting on February 1, 2020 or later.

The Chair of Numerical Analysis is devoted to the numerical approximation of partial differential equations and connected fields of mathematics. Among others, topics of research are adaptive finite elements, finite element exterior calculus, numerical homogenization, multiscale methods, nonlinear PDEs. The position gives the opportunity to work on a doctoral thesis on a modern topic of numerical Analysis.

Your responsibilities:

- Research in the field of computational partial differential equations
- Teaching for students in mathematics and other disciplines
- Work in research and teaching with the goal of a doctoral thesis
- Participation in the organizational work of the group

Our requirements:

- Master degree (or equivalent) in Mathematics
- Knowledge in numerical analysis is desirable

We offer:

- A responsible position within a highly motivated team in an internationally renowned research institution
- A multifaceted and complex research environment with an open atmosphere, state-of-the-art equipment and strong interdisciplinary collaborations
- A close collaboration of university and extra-university research institutions and their management boards
- Attractive staff benefits, for instance, contributions to the employee savings plan, season ticket loans for public transport, pension scheme (VBL)
- Remuneration in accordance with the Collective Agreement for the Public Sector of the Federal States (TV-L) depending on the personal qualifications up to salary scale 13

This fixed-term 75% position is limited to three years. In case of equal qualifications, applicants with disabilities will be favoured over the others.

Complete applications should include a CV, copies of certificates, publications (if applicable) and should be submitted by **30th November 2019** (preferably by e-mail with one pdf file) with reference to the ID 348/2019 to:

Prof. Dr. Dietmar Gallistl
Friedrich-Schiller-Universität Jena
Fakultät für Mathematik und Informatik
Institut für Mathematik
Lehrstuhl Numerische Mathematik
Ernst-Abbe-Platz 2
07743 Jena
dietmar.gallistl@uni-jena.de

For further information please also refer to: www.uni-jena.de/stellenmarkt_hinweis.html
For information on collecting personal data, please refer to:
www.uni-jena.de/Universität/Stellenmarkt/Datenschutzhinweis.html

Postdoctoral researcher (f/m/d) within the department of Mathematics

Reg. Nr. 349/2019

Application deadline: 30.11.2019

The Friedrich Schiller University Jena connects people and ideas, science and economy, institutions of higher education and external research organizations. Being rooted in the heart of Germany and having worldwide bonds, the university, covering all disciplines, characterizes the city of Jena as a future-oriented and cosmopolitan location together with its partners.

Within the department of Mathematics, Faculty of Mathematics and Computer Science at the Friedrich-Schiller-Universität Jena we encourage applications for a position as

Postdoctoral researcher (f/m/d)

starting on February 1, 2020 or later.

The Chair of Numerical Analysis is devoted to the numerical approximation of partial differential equations and connected fields of mathematics. Among others, topics of research are adaptive finite elements, finite element exterior calculus, numerical homogenization, multiscale methods, nonlinear PDEs. The position gives the opportunity to work on a doctoral thesis on a modern topic of numerical analysis.

Your responsibilities:

- Research in the field of computational partial differential equations
- Teaching responsibility for seminars, exercise clases, tutorials etc.
- Presenting your research on international conferences and publishing in international scientific journals
- Participation in the organizational work of the group
- Work in research and teaching with the goal of a habilitation in a modern field of the Numerics.

Our requirements:

- Doctoral degree (PhD or equivalent) in Mathematics
- Knowledge in the field of computational PDEs is desirable
- pedagogical suitability

We offer:

- A responsible position within a highly motivated team in an internationally renowned research institution
- A multifaceted and complex research environment with an open atmosphere, state-of-the-art equipment and strong interdisciplinary collaborations
- A close collaboration of university and extra-university research institutions and their management boards
- Attractive staff benefits, for instance, contributions to the employee savings plan, season ticket loans for public transport, pension scheme (VBL)

- Remuneration in accordance with the Collective Agreement for the Public Sector of the Federal States (TV-L) depending on the personal qualifications up to salary scale 13

This fixed-term 100% position is limited to three years. In case of equal qualifications, applicants with disabilities will be favoured over the others.

Complete applications should include a CV, copies of certificates, publications (if applicable) and should be submitted by **30th November 2019** (preferably by e-mail with one pdf file) with reference to the ID 349/2019 to:

Prof. Dr. Dietmar Gallistl
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For further information please also refer to: www.uni-jena.de/stellenmarkt_hinweis.html
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Stellenausschreibung
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FRIEDRICH-SCHILLER-UNIVERSITÄT JENA

Die Friedrich-Schiller-Universität Jena verbindet: Menschen und Ideen, Wissenschaft und Wirtschaft, Hochschulen und außeruniversitäre Forschung. Verwurzelt im Herzen Deutschlands und vernetzt in alle Welt, prägt die Volluniversität mit ihren Partnern eine lebendige und produktive Wissenschafts- und Wirtschaftsregion.

Am Institut für Informatik der Fakultät für Mathematik und Informatik der Friedrich-Schiller-Universität Jena ist ab sofort eine Stelle als

PhD Position in Causal Inference with Deep Learning

zu besetzen.

Friedrich Schiller University (FSU) in Jena together with the Max Planck Institute for Biogeochemistry (MPI BGC) is inviting applications for a PhD position in the field of machine learning. The position is hosted at FSU and jointly supervised by both institutions. We are looking for a highly motivated and creative scientist with strong interests in deep learning and dynamical systems. This position is focused on using deep learning capabilities to learn the complex causal models in multivariate dynamic systems, e.g. for videos analysis, analysis of the ecosystems and earth observations; the ultimate goal aims at enabling data-driven solutions for improved prediction and attribution of events and changes in these systems.

Scientific environment

This position is part of the Graduate School "Virtual Workshop for Digitization in the Sciences", a project funded by the Carl Zeiss Foundation. The graduate school consists of more than 10 PhD students from various disciplines, ranging from computer science, physics, bioinformatics to medicine, and 3 Postdocs. The successful candidate will join the Computer Vision Group of FSU – a young and vibrant, international team, actively publishing at major computer vision journals and conferences (e.g. PAMI, CVPR, ECCV, ICCV). We are currently developing several parallel research lines including biomedical image analysis, image understanding, and semantic segmentation with a focus on exploiting and extending deep learning for such areas. Developed methods are applied, for example, in video analysis, environmental systems, image understanding, and life-long learning. Research in this area also involves projects on fine-grained recognition, active learning and novelty detection, with applications such as activity recognition in video sequences as well as monitoring and event detection in biomedical applications. The Computer Vision Group has strong collaborations with the local research institutes, like the Max-Planck-Institute BGC and the DLR Institute for Data Science. For more details please visit http://www.inf-cv.uni-jena.de/en/research.html.

Requirements

- Master degree in computer science, machine learning, applied mathematics, statistics, or related disciplines.
- Strong programming skills in Python, MATLAB or C, C++.
- Interest in working with environmental data streams.
- Fluency in written and oral English. German is a plus.

We offer

- a salary (100% TV-L E13, actual pay depends on experience);
- three years contract with the possibility of extension for up to four years;
- a collaborative and internationally oriented research environment in the beautiful city of Jena. Located in the heart of Germany, Jena is a traditional and lively University town, and with its large percentage of students and researchers it is right to say: There is no University in Jena, Jena is the University.

Applications should include

- a motivation letter (to explain motivation, suitability and research interests);
- a full cv showing how the applicant's profile fits the requirements;
- a complete transcript of records to date;
- an electronic copy of the MSc thesis.

Please send your application by email to
Prof. Dr.-Ing. Joachim Denzler joachim.denzler@uni-jena.de.

Applications will be accepted until November 30th or until the position is filled. Successful candidates might start immediately, but are expected to start March 2020 at the latest.

As an equal opportunity and affirmative action employer, FSU further encourages applications from women. Applications of suitable disabled people are expressly desired. Information on the collection of personal data under Articles 13 and 14 General Data Protection Regulation (DS-GVO) can be found at https://www.lehramt-jena.de/datenschutzerklaerung/.

Applications with complete application documents (curriculum vitae in tabular form, certificates) should be sent by Email to:

Prof. Dr.-Ing. Joachim Denzler
Computer Vision Group
Institute for Informatics
Friedrich-Schiller-University Jena
Ernst-Abbe-Platz 2
D-07743 Jena

Phone : (+49)-3641-946420 or (+49)-3641-946301 (secretary)
Fax.: (+49)-3641-946302
Email: joachim.denzler@uni-jena.de
URL: http://www.inf-cv.uni-jena.de

Bitte beachten Sie auch unsere Bewerberhinweise unter: www.uni-jena.de/stellenmarkt_hinweis.html Bitte beachten Sie zudem die Informationen zur Erhebung personenbezogener Daten unter: www.uni-jena.de/Universität/Stellenmarkt/Datenschutzhinweis.html

Open PhD Positions in Computer Science

Computer Vision Group Jena

Institute for Computer Science, Faculty for Mathematics and Computer Science

Friedrich-Schiller-University Jena, Germany

https://www.inf-cv.uni-jena.de

The Computer Vision Group of Friedrich-Schiller-University Jena – a young and vibrant, international team, actively publishing at major computer vision journals and conferences (e.g., PAMI, CVPR, ECCV, ICCV) seeks for several PhD students for the following, potential PhD projects:

1. Continuous and Life-long Learning, including Active Learning and Novelty Detection
2. Deep Learning for Sensor Data Processing and Fusion for Autonomous Driving
3. Multivariate Spatiotemporal Signal Analysis using Deep Learning
4. Causal Inference using Deep Learning
5. Semantic Segmentation for Biomedical Applications

We are currently developing several parallel research lines, including biomedical image analysis, image understanding, and semantic segmentation, with a focus on exploiting and extending deep learning for such areas. Developed methods are applied, for example, in video analysis, environmental systems, image understanding, and life-long learning. Research in this area also involves projects on fine-grained recognition, active learning, and novelty detection, with applications such as activity recognition in video sequences as well as monitoring and event detection in biomedical applications. For more details, please visit http://www.inf-cv.uni-jena.de/en/research.html. The Computer Vision Group has strong collaborations with the local research institutes, like the Max-Planck-Institute BGC and the DLR Institute for Data Science. We are part of the Graduate School "Virtual Workshop for Digitization in the Sciences“, a project funded by the Carl Zeiss Foundation. The graduate school consists of more than 10 PhD students from various disciplines, ranging from computer science, physics, bioinformatics to medicine, and 3 Postdocs. Positions 3+4 will be part of a consortium of scientists from the US, Spain, and Germany supported by the EU (ERC Synergy Grant).

Requirements:

- Master degree in computer science, machine learning, applied mathematics, statistics, or related disciplines.
- Strong programming skills in Python, MATLAB or C, C++.
- Interest in working with environmental data streams.
- Fluency in written and oral English. German is a plus.

We offer

- a salary (100% TV-L E13, actual pay depends on experience);
- Three years contract with the possibility of extension for up to four years, for positions 3+4 up to five years
- a collaborative and internationally oriented research environment in the beautiful city of Jena. Located in the heart of Germany, Jena is a traditional and lively University town, and with its large percentage of students and researchers, it is right to say: There is no University in Jena, Jena is the University.

Applications should include

- a motivation letter (to explain motivation, suitability and research interests);
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Applications will be accepted until December 31th or until the positions are filled. Successful candidates might start immediately, but are expected to start March 2020 at the latest.

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PhD topics in nano & quantum optics

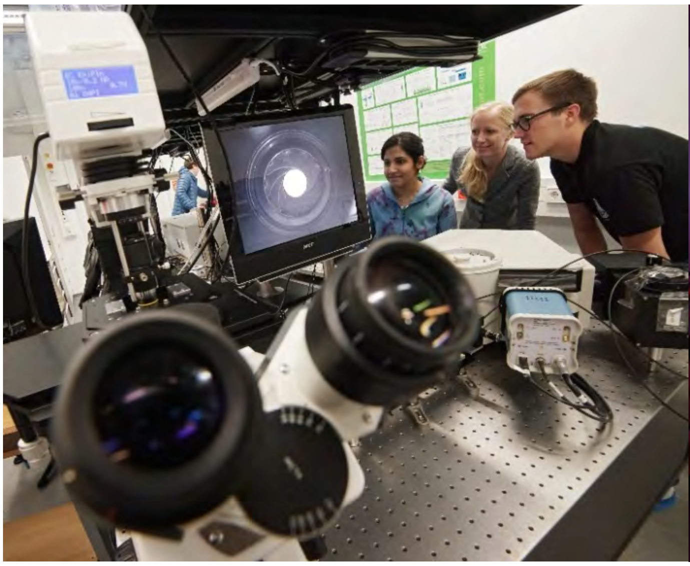
The research of the laboratory for nano & quantum optics at the Abbe Center of Photonics is part of the recently established Max Planck School of Photonics (www.maxplanckschools.de). The group's research targets the control of light at the single photon level and at the nanoscale using nanostructured materials and ultrafast nonlinear optical effects. The lab, which is a part of the Faculty of Physics and Astronomy of the Friedrich Schiller University Jena (Germany), covers a broad range of research fields in experiment and theory to study interaction of light with microstructured and nanostructured matter, employing advanced methods for nanofabrication, experimental characterization and numerical modelling.

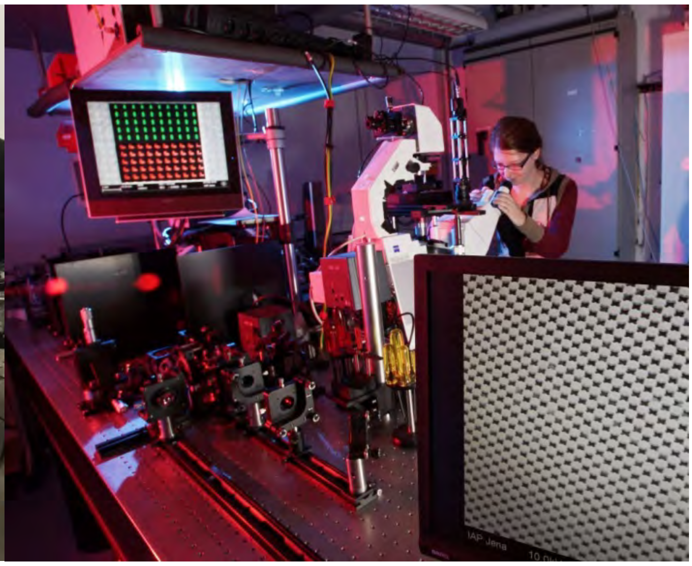
The laboratory is led by Prof. Dr. Thomas Pertsch, Jun.-Prof. Dr. Isabelle Staude, Dr. Frank Setzpfandt, and Dr. Falk Eilenberger. We are constantly looking for talented young scientists, who would like to contribute to cutting edge research projects on quantum photonics at the nano scale. Currently there are openings for PhD projects on several topics, which are also described in detailed project sheets:

- Sources for quantum states of light
- Quantum imaging and sensing
- Nanostructured photonic metamaterials
- Control of the optical nearfield by plasmonic nanostructures and SNOM investigation
- Ultrafast multidimensional, spatiotemporal pulse measurement techniques
- Interaction of light with 2D materials
- Ultrafast wavefront control with semiconductor metasurfaces

Besides these predefined topics, we are always open for candidates suggesting topics of their specific interest connected to our general research field. Details about the laboratory for nano & quantum optics can be found at www.iap.uni-jena.de/nano+quantum+optics. If you are interested in joining our lab, please contact:

Prof. Thomas PERTSCH: thomas.pertsch@uni-jena.de and www.acp.uni-jena.de/pertsch
Jun.-Prof. Isabelle STAUDE: isabelle.staude@uni-jena.de and www.iap.uni-jena.de/staude
Dr. Frank SETZPFANDT: frank.setzpfandt@uni-jena.de and www.iap.uni-jena.de/setzpfandt
Dr. Falk EILENBERGER: falk.eilenberger@uni-jena.de and www.iap.uni-jena.de/eilenberger





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Sources for quantum states of light

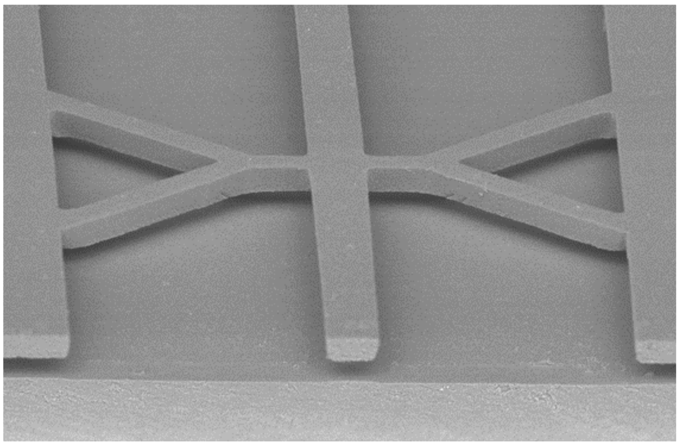
Quantum states of light with exactly a single or exactly a pair of entangled photons, are an important resource for applications of quantum optics. To fully use the potential of quantum optics for applications e.g. in computing, sensing, and cryptography, it is important to optimize the properties of the photons with respect to the targeted application. This means, their spectral, spatial, and polarization features have to be tailored with a wide range; their sources have to be integrated into accessible components and components.

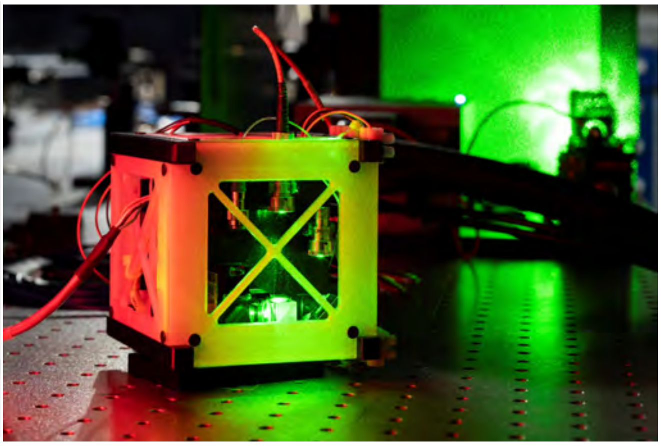
The most common mechanisms to generate quantum sates of light are spontaneous parametric down-conversion and defect state emission. While the former is a nonlinear optical process in which one photon is spontaneously split into a photon pair, the latter is a linear process, which can be observed in carefully crafted perturbations of two- and three-dimensional crystals. Both process, and thereby also the state of the generated photons, depend sensitively on the properties of the host material that is used for the generation and upon its nanostructure.

In our research, we investigate different platforms for the generation of photon pairs and single photons, ranging from bulk nonlinear crystals over waveguides all the way to nanostructured surfaces and two-dimensional materials. Furthermore, technologies to fabricate nanostructured photon-pair sources as well as experimental approaches for their characterization need to be developed and implemented. Depending on the specific topic, one or several of the following subjects will be covered.

Covered subjects

- Experimental and theoretical quantum optics
- Nonlinear optics
- Waveguides and nanostructured surfaces
- Numerical simulations
- Nanostructuring technology and systems integration





Contact for further information and application

https://www.iap.uni-jena.de/nano+quantum+optics

Dr. Frank SETZPFANDT (f.setzpfandt@uni-jena.de)

Dr. Tobias VOGL (tobias.vogl@uni-jena.de)

Quantum imaging and sensing

Entangled photon pairs enable new modalities for optical sensing and imaging. They can help to surpass classical noise limits, image through turbulent media, and image in spectral domains where no cameras are accessible. We are investigating several quantum imaging and sensing approaches, aiming to fundamentally understand, optimize, and implement them.

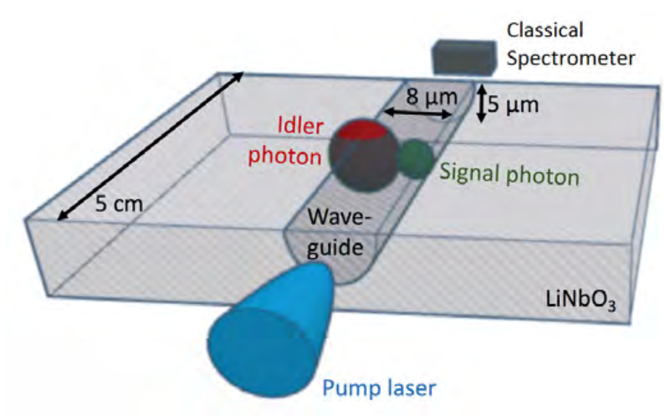
One example for studied imaging methods is quantum ghost imaging. Here, only one of the two photons of a photon pair is interacting with the sample and is afterwards detected with a single detector without spatial resolution. The second photon, which did not see the object, is spatially characterized using a single-photon sensitive camera. None of the individual detection events is able to generate an image, however, by correlating both measurements such image can be obtained. We are striving to implement quantum ghost imaging with high spatial resolution and in technically hardly accessible wavelength regions like the mid-infrared with the aim of applying it in real-world measurement scenarios.

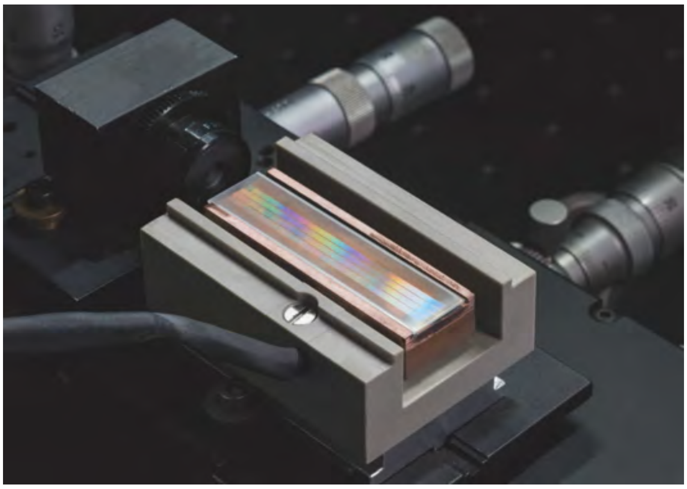
Another research topic is SPDC spectroscopy in waveguide platforms. Using the quantum interference of several sources of photon pairs, which characteristics depends on the properties of the sources and media between them, information about the optical properties of these media can be obtained by measuring only one of the two photons of a photon pair. Utilizing photon pair sources that generate pairs of different wavelength, e.g. in the mid-infrared and the visible, this enables the measurement of the spectral properties of analytes in the mid-infrared by simply characterizing the second photon in the visible. Our goal is to fundamentally understand this measurement principle and its properties, as well as to design, implement, and test suitable optical structures realizing it.

Depending on the specific topic, one or several of the following subjects will be covered.

Covered subjects

- Waveguide and nonlinear optics
- Quantum optics
- Optical Imaging
- Numerical simulations
- Correlation measurements





Contact for further information and application

Dr. Frank SETZPFANDT (f.setzpfandt@uni-jena.de)

Prof. Dr. Thomas PERTSCH (thomas.pertsch@uni-jena.de)

https://www.iap.uni-jena.de/nano+quantum+optics

Nanostructured photonic metamaterials

Photonic metamaterials represent a novel class of artificial matter consisting of periodically or randomly arranged unit cells, having a size smaller than the wavelength of light. Metamaterials promise to obtain complete control over all properties characterizing light propagation. By designing the metamaterials´ unit cells one can tailor light propagation in such media beyond the limits given by natural occurring materials. The envisioned achievements range from a dramatic enhancement of optical effects like polarization rotation by several orders of magnitude to the overall spatial and spectral shaping of light by appropriately designed and spatially distributed nanoparticles. Recent advances in fabrication technology have allowed for the realization of optical structures with sub-wavelength dimensions. Modern nanostructure technologies enable the creation of photonic nanomaterials in order to examine them experimentally.

Our group has a firm experience in the fabrication and characterization of photonic metamaterials. The student's projects range from the usage and optimization of available experimental setups for characterization, to the design and numerical optimization of novel photonic metamaterials and advanced investigations like the characterization of nonlinear optical properties or even quantum state control.

The candidate should ideally have high interest in new types of physics, basic lab and computational experience. Depending on the chosen task good experimental skills or advanced Matlab / Comsol knowledge is appreciated.

Covered subjects

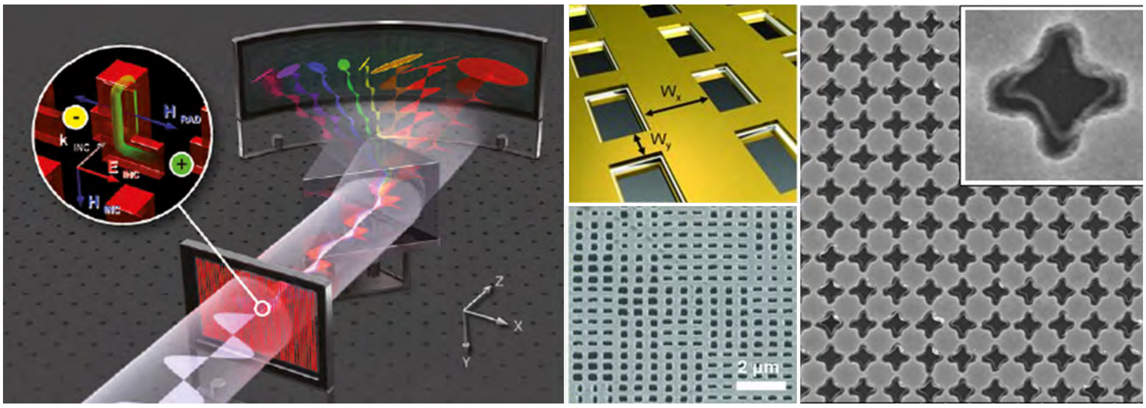
- structural characterization and nanofabrication (FIB, SEM, AFM, SNOM …)
- resonant excitation of plasmonic or dielectric eigenmodes in artificial structures with spectral & angular resolution
- spectral data processing and physical interpretation

Experimental activities

- characterization and optimization of existing experimental setups for the band structure measurement of highly dispersive nanomaterials
- computer controlled automation of an experimental procedure for parameter optimization and precise measurement procedures

Theoretical activities

- numerical modeling of single and periodic nanostructures based on rigorous solutions of Maxwell's equations on parallel cluster computers
- analytical modeling by simplified toy models and semi-analytical computer-supported calculations
- comparing experimental results to rigorous numerical simulations to extract basic physical phenomena



Contact for further information and application **www.iap.uni-jena.de/nano+quantum+optics**

Prof. Thomas PERTSCH (thomas.pertsch@uni-jena.de)

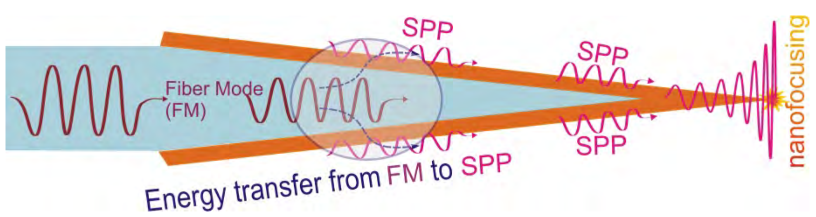
Control of the optical nearfield by plasmonic nanostructures and SNOM investigation

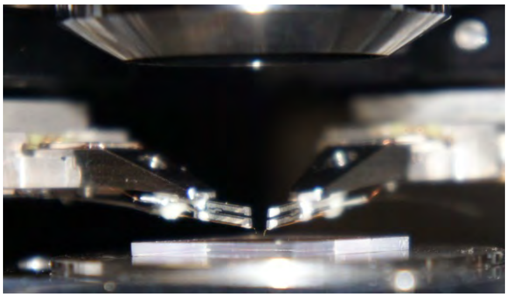
The emerging field of nano-plasmonics addresses the study of the interaction between electromagnetic waves and electron plasmas on metal surfaces and in metallic nanostructures, i.e. the hybrid states of plasmon-polaritons. It has received much attention in the last decade due to the high potential of new applications ranging from subwavelength photonic circuits to high-resolution microscopy. Plasmonic devices are capable of efficiently confining and enhancing optical fields, serving as a bridge between diffraction-limited optics and the nanoscale. One of the main research tools in nano-plasmonics to observe plasmon-polaritons beyond the optical diffraction limit is scanning near-field optical microscopy (SNOM) targeted to obtain ultimate topographic and optical resolution for nano-imaging. To break the diffraction limit, a plasmonic superfocusing SNOM (PS-SNOM) has been proposed in which a nano-sized plasmonic tip (metallic probe) scans the sample surface to form topography and optical image with extremely high spatial resolution. The principle of PS-SNOM is based on the excitation of localized modes of surface plasmon polaritons (SPP) at the metallic tip with far-field illumination, which generates a nano-sized spot of light at the apex of the nano-tip.

The goal is to develop and to operate different nearfield microscopy setups to address different purposes, such as plasmonic waves propagating on noble metal surfaces, locally excited plasmon-polariton eigenmodes in metal-dielectric nanomaterials and metamaterials, or chemically synthesized nanostructures such as semiconductor nanowires, and the generation of non-diffracting surface waves, so called plasmonic Airy beams. Another goal is the development of new SNOM techniques using two SNOM tips simultaneously on the same sample. Here, one tip is fed by an input signal exciting the probe at one local spot of the sample while the other tip collects the information on the field distribution from a different spot, disclosing the nearfield optical Green's function.

Covered subjects

- fundamentals of surface plasmon-polaritons at metal nanostructures
- theoretical modeling and numerical simulation of the spatio-temporal dynamics of light on the nano-scale below the diffraction limit based on rigorous solutions of Maxwell's equations
- design and realization of complex experimental setups for the control of scanning tips with nanometer precision and phase sensitive detection of scattered near fields
- experimental investigation of new functionalities of plasmonic nanostructures, as e.g. strong coupling of nano-antennas to quantum systems, as e.g. quantum dots for enhanced light-matter interaction





Left: Schematic for the excitation of a superfocusing surface plasmon-polariton at a metalized fiber tip by resonant coupling to a propagating fiber mode. Right: Two-tip nearfield scanning optical microscope for direct measurement of the optical nearfield Green's function of photonic nanostructures.

Contact for further information and application **www.iap.uni-jena.de/nano+quantum+optics**

Prof. Thomas PERTSCH (thomas.pertsch@uni-jena.de)

Ultrafast multidimensional, spatiotemporal pulse measurement techniques

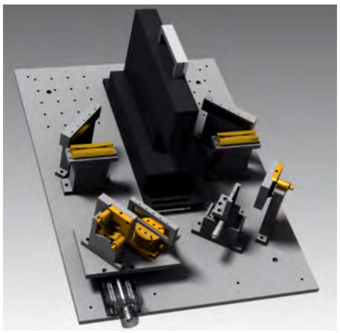
Ultrashort laser pulses give access to events, which are inherently inaccessible to electronics. They can resolve processes in physical, chemical or biological samples with femtosecond resolution. They are thus an ideal probe to study the motion of electrons in atomic scale systems, if the pulses can be measured precisely and reproducibly in space and time.

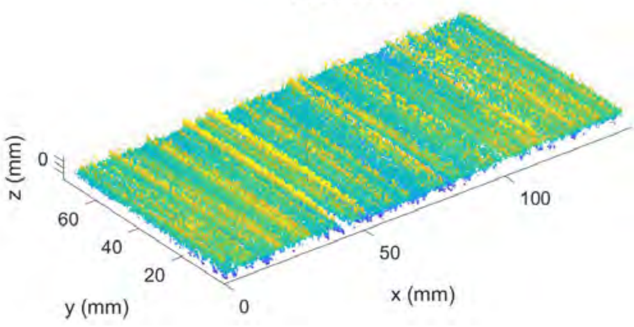
Our group is using ultrashort laser pulses to understand the complex physical systems in a multidimensional manner. We combine ultrashort pulses with electron microscopy to understand the motion of electrons in nanoplasmonic systems on a time-scale of femtoseconds down to the atomic level. We also combine ultrashort laser pulses with 3D-measurement techniques to visualize highly dynamic events in 3D. We develop techniques and devices to analyze spatiotemporally complex light fields with femtosecond and nanometer resolution.

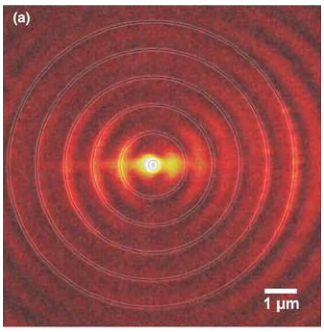
This field offers many opportunities for research projects: one opportunity would be the development of a real-time 3D-measurement fringe-projection based scheme with micrometer precision, which is capable to visualize highly dynamic effects, such as the propagation of high frequency phonons in crystalline materials. A second opportunity for projects is the understand of nonlinear light-matter interaction in atomic scale systems composed of metal nanocluster densely packed into dielectric matrices of various description. A third area are projects in real-time analysis of the dynamics of electrons in plasmonic nanoresonatores under the excitation of light and the ensuing interaction of light waves and matter waves in bound plasmons.

Covered subjects

- fundamentals of surface plasmon polaritons at metallic nanostructures down to the atomic scale
- theoretical modeling and numerical simulation of the spatio-temporal dynamics of light and electrons on the nano-scale below the diffraction limit based on rigorous solutions of Maxwell's equations coupled to materials models
- design and realization of complex experimental setups for spatiotemporal pulse reconstruction
- experimental investigation of the ultrafast dynamics of laser-excited solid state systems







Left: Schematic of a femtosecond pulse shaping device. Center: A planar surface measured with an ultrafast 3D-camera. Right: Measured electron wavepackets excited by a laser beam incident on a ring-type nanoantenna.

Contact for further information and application **www.iap.uni-jena.de/nano+quantum+optics**

Dr. Falk Eilenberger (falk.eilenberger@uni-jena.de)

Interaction of light with 2D materials

Two-dimensional semiconductors are the first class of atomic layer materials with a high degree of optical activity. Due to their unusual geometry, they exhibit extremely strong light-matter interaction. In comparison to bulk semiconductors they have superior linear and nonlinear coefficients, spin-valley coupling and strong fluorescence. They are a highly attractive platform for fundamental experiments related to effects induced by dimensionality and also suitable for applications, e.g. for sensing and nonlinear light converters.

We specialize on integrating two-dimensional semiconductors with optically resonant structures such as monolithic cavities, optical waveguides and nanoresonatores to further enhance and tailor their interaction with light. This gives access to experiments in fundamental physics of light-matter-interaction 2D-semiconductors, including experiments in strong coupling of exciton-polaritons, spin-valley coupling and defect-state-based single photon emitters. The integration with optical systems also allows for the development of highly novel sensing devices, new microscopic imaging modalities and new classes of highly nonlinear waveguides.

This field offers many possibilities for research projects. We offer projects in the fabrication of the materials themselves, their growth on and integration with micro- and nanooptical systems and the characterization of their properties. We also offer projects on fundamental questions on their light-matter interaction, such as their interaction with near-field active nanostructures and the ensuing photonic effects for sensing, imaging and quantum photonics.

Covered subjects

- fabrication, transfer, integration and growth of 2D-materials on photonics structures
- characterization and theoretical modelling of light-matter-interaction of 2D-materials with micro- and nanooptical systems
- design and realization of complex of experimental setups for 2D-materials-based applications in sensing, microscopy, nonlinear optics and quantum light sources

Left: A monolithic optical cavity loaded with 2D-materials. Right: Suspensions of 2D-materials for microscopy applications.

Contact for further information and application **www.iap.uni-jena.de/nano+quantum+optics**

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Ultrafast wavefront control with semiconductor metasurfaces

Photonic metasurfaces are two-dimensional arrangements of designed nanoscopic building blocks, which can convert an incident light field into an outgoing light field with tailored spectrum, polarization, and wavefront. While most metasurfaces realized so far are made of metallic nanoresonators, all-dielectric or semiconductor metasurfaces offer the advantage of low absorption losses. A flurry of optical functionalities has been demonstrated using all-dielectric metasurfaces in the last few years, including reflectors, magnetic mirrors, beam deflection, beam shaping, focusing and holographic imaging (see Fig. 1 (a)), clearly demonstrating their potential for flat wavefront shaping devices. While so far, dielectric/semiconductor metasurfaces have been mainly studied in the regime of continuous light waves, the goal of this PhD project is to study the ultrafast interaction of high-refractive-index semiconductor metasurfaces with femto-second laser pulses. The influence of the shape, size, arrangement, and material properties of the constituent semiconductor building blocks on the ultrafast optical response of the metasurface shall be experimentally investigated, opening the door to all-optical wavefront modulation on a picosecond time scale. This could eventually lead to the realization of spatial light modulators with switching times reduced by several orders of magnitude as compared to current liquid-crystal based solutions, as well as to completely new approaches for pulse shaping and spatiotemporal light-field synthesis.

Covered subjects

- building of an optical pump-probe measurement setup for ultrafast back-focal plane imaging
- design and numerical simulation of ultrafast photonic metasurfaces
- involvement in the development of dedicated nanofabrication procedures for ultrafast metasurfaces

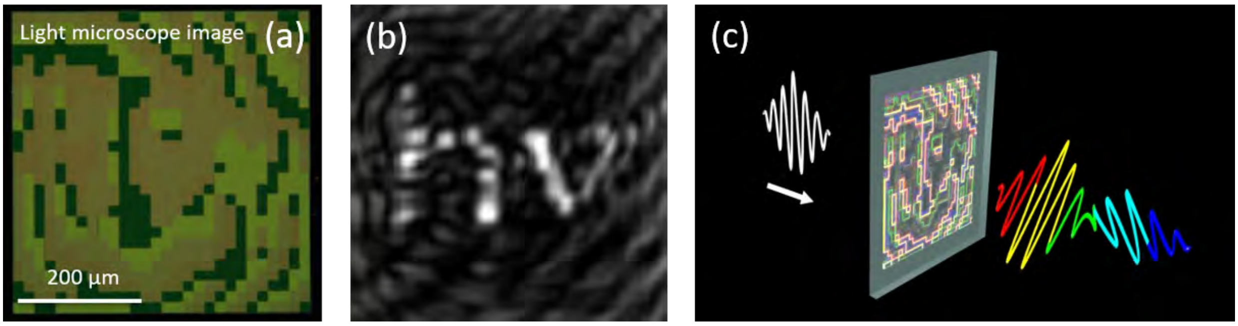

Fig. 1: (a) Light microscope image of a wavefront shaping semiconductor metasurface designed to interact with continuous light waves. (b) Image of the letters $h\nu$ produced behind the metasurface for illumination with an infrared laser. (c) An artist's impression of a photonic metasurface interacting with a femtosecond laser pulse

Contact for further information and application **www.iap.uni-jena.de/nano+quantum+optics**

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Jena, 14. November 2019

PhD-Workshop China am 23. und 24.11.2019 in Peking und am 26.11.2019 in Shanghai

We would like to offer four research projects for qualified PhD candidates from China, provided that they receive a fellowship from abroad to finance their position in our lab. Lab space and a limited amount of consumables could be provided from our side. Candidates should have basic knowledge, skills and strong interest in molecular biology.

Project 1: On the origin of ‘floral quartets’

Transcription factors including tetrameric complexes of MIKC-type MADS-domain proteins (‘floral quartets’) control the specification of floral organ identity during flower development; similar complexes (‘floral quartet-like complexes’, FQCs) control many other processes during plant development (Theißen et al., 2016). MIKC-type proteins originated in the stem group of streptophytes (land plants and charophyte green algae) (Nishiyama et al., 2018). They have very likely played important roles during the transition of plants to land and the diversification of land plants. In our project we will study the formation of FQCs of diverse representative land plants (charophytes, liverworts, mosses, hornworts, lycophytes, ferns, gymnosperms) to better understand the evolutionary origin of FQC formation and its role during the origin and evolution of land plants. Mostly well-established technology will be used during the course of the work, such as yeast two-hybrid assays (Y2H), electrophoretic mobility shift assays (EMSA) and systematic evolution of ligands by exponential enrichment (SELEX) (e.g., Melzer et al., 2009; Käppel et al., 2018). Moreover, transgenic technology employing model plants such as Arabidopsis will be used to test the conservation of gene function and protein-protein and protein-DNA interactions during land plant evolution.

Key words: land plant evolution, plant development, protein-protein interaction, transcription factor evolution, transition of plants to land

Key references from our lab:

Käppel, S., Melzer, R., Rümpler, F., Gafert, C., Theißen, G. (2018). The floral homeotic protein SEPALLATA3 recognizes target DNA sequences by shape readout involving a conserved arginine residue in the MADS-domain. *Plant J.* **95**, 341-357.

Melzer, R., Verelst, W., Theißen, G. (2009). The class E floral homeotic protein SEPALLATA3 is sufficient to loop DNA in ‘floral quartet’-like complexes *in vitro*. *Nucl. Acids Res.* **37**, 144-157.

Nishiyama, T., *et al*. (2018). The *Chara* genome: secondary complexity and implications for plant terrestrialization. *Cell* **174**, 448-464.

Theißen, G., Melzer, R., Rümpler, F. (2016). MADS-domain transcription factors and the floral quartet model of flower development: linking plant development and evolution. *Development* **143**, 3259-3271.

Project 2: Functional analysis of the enigmatic *OsMADS16*-miRNA5179 module in rice

A diversity of microRNAs (miRNAs) fine-tunes developmental processes in flowering plants often by regulating genes encoding transcription factors (Thieme et al., 2011). *DEFICIENS*-like genes encode transcription factors specifying the identity of several organs during flower development. In some taxa the activity of *DEFICIENS*-like genes is controlled by miRNA5179. This miRNA reveals an intriguing evolutionary dynamics. It originated early during flowering plant evolution, but was lost several times independently in diverse lineages. Evolution of miRNA5179 may have had important implications for biodiversity. For example, differences in the expression of *DEFICIENS*-like genes have been associated with the origin of three morphologically different perianth organs in orchids, one of the most species-rich groups of flowering plants (Mondragon-Palomino and Theißen, 2008). These differences in expression may have been brought about, at least in part, by regulation of the *DEFICIENS*-like genes by miR5179.
Despite frequent gene loss on the miRNA, both the miRNA5179 and its *DEFICIENS*-like target gene (*OsMADS16*) exist in the important monocot crop and model plant rice (*Oryza sativa*). This provides a unique opportunity to study the regulatory function of miRNA5179. A better understanding of the regulatory *OsMADS16*-miRNA5179 module may facilitate rice breeding to secure a stable harvest of one of the most important staple foods in the light of rapid climate change. During the course of this project the expression pattern of miRNA5179 during rice development will be determined employing e.g. *in-situ* hybridization and qRT-PCR. The miRNA expression pattern will be compared to that of the *OsMADS16* target. Moreover, the development of plants with the following genetic constitutions will be investigated in detail and compared: wild-type plants, *osmads16* knock-out plants, *miRNA5179* knock-out plants, and plants which express a miRNA5179-resistant version of *OsMADS16*. Our group has quite some experience with work on rice, not least due to a long-standing and fruitful cooperation with the research group of Prof. Zheng Meng at the IBCAS in Beijing (see, e.g. Liu et al., 2013; Schilling et al., 2015; Wu et al., 2017).

Key words: microRNAs, transcription factors, MADS-box genes, flower development, rice, biodiversity

Key references from our lab:

Liu, Y., Cui, S., Wu, F., Yan, S., Lin, X., Du, X., Chong, K., Schilling, S., Theißen, G., Meng. Z (2013). Functional conservation of MIKC*-type MADS box genes in *Arabidopsis* and rice pollen maturation. *Plant Cell* **25**, 1288-1303.

Mondragón-Palomino, M., Theißen, G. (2008). MADS about the evolution of orchid flowers. *Trends Plant Sci.* **13**, 51-59.

Schilling, S., Gramzow, L., Lobbes, D., Kirbis, A., Weilandt, L., Hoffmeier, A., Junker, A., Weigelt-Fischer, K., Klukas, C., Wu, F., Meng, Z., Altmann, T., Theißen, G. (2015). Non-canonical structure, function and phylogeny of the B_{sister} MADS-box gene *OsMADS30* of rice (*Oryza sativa*). *Plant J.* **84**, 1059-1072.

Thieme, C.J., Gramzow, L., Lobbes, D., Theißen, G. (2011). SplamiR – prediction of spliced miRNAs in plants. *Bioinformatics* **27**, 1215-1223.

Wu, F., Shi, X., Lin, X., Liu, Y., Chong, K., Theißen, G., Meng, Z. (2017). The ABCs of flower development: mutational analysis of *AP1*/*FUL*-like genes in rice provides evidence for a homeotic (A)-function in grasses. *Plant J.* **89**, 310-324.

Project 3: Genetic basis of fruit dimorphism in Aethionema

The genus Aethionema has an interesting phylogenetic position at the base of the model plant family Brassicaceae (crucifers) (Lenser et al., 2016). Moreover, some species, such as *Aethionema arabicum*, develop two types of fruits, dehiscent and indehiscent ones (Lenser et al., 2016, 2018). This fruit dimorphism is an interesting phenomenon from both an eco-physiological and developmental perspective. Our previous investigations revealed that fruit morph determination is a 'last-minute' decision happening in flowers after anthesis directly before the first morphotypical differences start to occur. Moreover, our data suggest that an accumulation balance of the plant hormones auxin and cytokinin in open flowers together with the transcript abundance of the *Ae. arabicum* ortholog of *BRANCHED1* (*BRC1*) may control fruit morph determination (Lenser et al., 2018). *BRC1* encodes a transcription factor known for its conserved function as a branching repressor. Based on these findings we hypothesize that the plastic control of fruit morph ratio in *Ae. arabicum* evolved through the modification of a preexisting network known to control primigenic dominance (meaning here, simply put, that early developing fruits suppress later developing ones) (Lenser et al., 2018). During the future course of this project we want to test our hypothesis using transgenic technology. Towards that goal we have recently established a transformation protocol for Aethionema. This protocol will be used to knock-out genes by CRISPR/Cas9 encoding putative key regulators of developmental transitions and growth habit in Aethionema, such as *FLOWERING LOCUS C* (*FLC*) and *BRC1*. Careful investigation of the phenotype of these plants under different growth conditions as well as of expression pattern of informative genes will help to understand better the link between plant growth habit (especially branching pattern), phytohormone activity and fruit dimorphism. Since primigenic dominance is of quite some importance during production of fruits such as cucumber and apple, insights provided by our project might well be of agronomic interest.

<u>Key words:</u> fruit development, transcription factors, CRISPR/Cas9, developmental transitions, crucifers, Brassicaceae,

<u>Key references from our lab:</u>

Lenser, T., Graeber, K., Cevik, Ö.S., Adigüzel, N., Dönmez, A.A., Grosche, C., Kettermann, M., Mayland-Quellhorst, S., Mérai, Z., Mohammadin, S., Nguyen, T.-P., Rümpler, F., Schulze, C., Sperber, K., Steinbrecher, T., Wiegand, N., Strnad, M., Mittelsten Scheid, O., Rensing, S.A., Schranz, M.E., Theißen, G., Mummenhoff, K., Leubner-Metzger, G. (2016). Developmental control and plasticity of fruit and seed dimorphism in *Aethionema arabicum*. *Plant Physiol.* **172**, 1691-1707.

Lenser, T., Tarkowská, D., Novák O., Wilhelmsson, P.K.I, Bennet, T. Rensing, S.A, Strnad, M., Theißen, G. (2018). When the BRANCHED network bears fruit: how carpic dominance causes fruit dimorphism in *Aethionema*. *Plant J.* **94**, 352-371.

FRIEDRICH-SCHILLER-UNIVERSITÄT JENA

Project 4: Developing an interaction model for MIKC-type MADS-domain transcription factors

Developmental processes are controlled by the dynamic interplay of transcription factors (TFs) and their target genes. Thereby TFs usually bind to DNA not as single proteins but as different homo- and heteromeric complexes. The set of target genes and thus the gene regulatory output highly depends on the composition if these complexes. MIKC-type MADS-domain TFs (MTFs) are a good case in point, as they control a variety of different plant developmental processes by forming DNA bound dimers and tetramers (Theißen et al., 2016). The protein-protein interactions that provide specificity are mainly mediated by the so called Keratin-like domain (K-domain) that is unique for MIKC-type proteins. In recent years much effort has been made to better understand the molecular mechanisms that mediate the specific protein-protein interactions of MIKC-type proteins (Puranik et al., 2014; Rümpler et al., 2018). However, so far relatively little is known about sequence features that determine whether two proteins can interact or not. Therefore during the course of the project we want to build up a large interaction database of all MIKC-type proteins from several model species including thale cress (*Arabidopsis thaliana*), snapdragon (*Antirrhinum majus*), petunia (*Petunia x hybrida*) and rice (*Oryza sativa*). We will use these interaction data to develop an algorithm that predicts interaction strength and specificity of MIKC-type proteins based on sequence information. In a complementary approach yeast two-hybrid (Y2H), Y3H, electrophoretic mobility shift assays (EMSAs) and in solution fluorescence resonance energy transfer (FRET) assays will be employed to independently determine dimerization and tetramerization capabilities of the examined proteins. The experimentally determined interaction data will be used as input to train a machine-learning model for predicting pairwise interactions. Similar approaches have already successfully been applied to transcription factor families with structurally similar protein-protein interaction interfaces such as basic-region leucine zippers (Potapov et al., 2015). Our interaction model will not only facilitate reliable prediction of MIKC-type protein interactions from species not examined in this study. It will also allow to trace back the evolutionary trajectories that shaped the structure of the present day MIKC-type protein-protein interaction networks and probably enable the design of artificial MIKC-type proteins with custom interaction capabilities.

Key words: coiled-coil interaction, gene regulatory network evolution, machine-learning model, protein-protein interaction prediction, transcription factor interactions

References:

Potapov, V., Kaplan, J. B., & Keating, A. E. (2015). Data-driven prediction and design of bZIP coiled-coil interactions. PLoS computational biology **11**, e1004046.

Puranik, S., Acajjaoui, S., Conn, S., Costa, L., Conn, V., Vial, A., Marcellin, R., Melzer, R., Brown, E., Hart, D. et al. (2014). Structural basis for the oligomerization of the MADS domain transcription factor SEPALLATA3 in Arabidopsis. Plant Cell **26**, 3603-3615.

Rümpler, F., Theißen, G., & Melzer, R. (2018). A conserved leucine zipper-like motif accounts for strong tetramerization capabilities of SEPALLATA-like MADS-domain transcription factors. Journal of experimental botany **69**, 1943-1954.

Theißen, G., Melzer, R., Rümpler, F. (2016). MADS-domain transcription factors and the floral quartet model of flower development: linking plant development and evolution. *Development* **143**, 3259-3271.

Host-specificity determinants of a smut fungus that discriminates between maize and sorghum

Project outline:

The aim of this project is to identify and functionally analyse factors important for host selection and host infection of the smut fungus *Sporisorium reilianum*. *S. reilianum* exists in two host-specific formae speciales. SRZ causes head smut disease of maize, whereas SRS causes disease on sorghum. We have identified genomic regions encoding factors putatively involved in host selection and host colonization. Putative factors shall be analysed by gene deletion and overexpression in *S. reilianum*, by identification of interaction partners by Y2H, co-immunoprecipitation /MSMS analysis, BiFC, enzyme assay, expression in Arabidopsis, bombardment of sorghum or maize, and similar experiments as required. The results will help in development of pathogen-resistant crop lines.

Required qualifications:

- Master's degree in Biology, Biotechnology, Biochemistry, Bioengineering, Microbiology, or equivalent, with excellent grades.
- Mandatory knowledge and practical education in plant-microbe-interaction, molecular biology, microscopy. Desired knowledge in biochemistry and bioinformatics.
- Scientific curiosity, motivation, creativity and perseverance.
- Team spirit, independent and cooperative work ethic.
- Very good communication skills in English. Knowledge of German is a plus.

Central Tasks

- Independent and strategic planning, managing and conducting of a research project
- Preparation, communication and discussion of written and oral research projects within and outside of the research group
- Participation in project development, manuscript writing and proposal preparation.
- Preparation of a PhD thesis.

For further information

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Keywords

Host-specificity, plant pathogenic fungus, genome comparison, molecular biology

Mitochondrial inheritance in smut fungi

Project outline:

Mitochondria supply the cell with energy, which is especially important in unicellular eukaryotes. In most eukaryotic systems, mitochondria are inherited from only one parent. We have observed mitochondrial recombination instead of uniparental mitochondrial inheritance during genetic crosses between different *formae speciales* of the smut fungus *Sporisorium reilianum*. The aim of this project is to elucidate the mechanism of mitochondrial inheritance in *S. reilianum*, identify important genes regulating mitochondrial recombination and inheritance, identify genomic regions that drive retention of mitochondrial genes, elucidate the impact of different mitotypes on cellular fitness and plant infection capacity.
This includes generation of gene deletion strains of S. reilianum, conducting precise genetic crosses between different strains, analysing genotype and mitotype, testing impact of mitotype on cell growth under different conditions, monitoring mitotype and fitness during plant infection. The results will help to understand the contribution of mitochondrial genes and their communication with genomic loci towards evolution of different formae speciales in fungi.

Required qualifications:

- Master's degree in Biology, Biotechnology, Biochemistry, Bioengineering, Microbiology, or equivalent, with excellent grades.
- Knowledge in plant-microbe-interaction, mandatory practical education in molecular biology and genetics of yeasts, microbiological techniques, microscopy. Desired knowledge in bioinformatics.
- Scientific curiosity, motivation, creativity and perseverance.
- Team spirit, independent and cooperative work ethic.
- Very good communication skills in English. Knowledge of German is a plus.

Central Tasks

- Independent and strategic planning, managing and conducting of a research project
- Preparation, communication and discussion of written and oral research projects within and outside of the research group
- Participation in project development, manuscript writing and proposal preparation.
- Preparation of a PhD thesis.

For further information

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Keywords

Mitochondrial inheritance, plant pathogenic fungus, genome sequencing, molecular biology, microbiology

Functional analysis of a cell-death inhibiting effector of *Sporisorium reilianum*

Project outline:

Sporisorium reiliaum is a dimorphic pathogen of maize and sorghum. In its haploid stage it grows yeast like and is amenable to molecular genetic modification. For plant infection, two strains of different mating type fuse to form a dikaryotic infectious filament. Leaf infection of sorghum and maize results in very little cell death. The fungus proliferates in the host plants without obvious damage to the plant. The disease becomes evident only at flowering time, when the spore-filled inflorescences appear. We have identified an effector protein of S. reilianum that putatively suppresses cell death. The aim of the project is to screen for additional cell-death suppressing effectors, prove cell death inhibiting function in the natural host system, and elucidate the mechanism of cell death suppression.
Putative factors shall be analysed in cell death suppression test systems, by gene deletion and overexpression in *S. reilianum*, by identification of interaction partners by Y2H, co-immunoprecipitation / MSMS analysis, and BiFC, by expression in the host plants via bombardment of sorghum or maize, and similar experiments as required. The results will help to understand how biotrophic fungi survive in their hosts and will contribute to the development of plant protection strategies.

Required qualifications:

- Master’s degree in Biology, Biotechnology, Biochemistry, Bioengineering, Microbiology, or equivalent, with excellent grades.
- Mandatory knowledge and practical education in plant-microbe-interaction, molecular biology, microscopy. Desired knowledge in biochemistry and bioinformatics.
- Scientific curiosity, motivation, creativity and perseverance.
- Team spirit, independent and cooperative work ethic.
- Very good communication skills in English. Knowledge of German is a plus.

Central Tasks

- Independent and strategic planning, managing and conducting of a research project
- Preparation, communication and discussion of written and oral research projects within and outside of the research group
- Participation in project development, manuscript writing and proposal preparation.
- Preparation of a PhD thesis.

For further information

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Keywords

Effector function, cell death suppression, plant pathogenic fungus, functional assay, molecular biology

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Project proposal for “PhD workshop China”

Title: Ancient organic carbon degradation in pristine groundwater

In subsurface environments, the absence of sunlight excludes the photosynthetic primary production of organic carbon that fuels food webs at the surface. Nevertheless, complex microbial communities are present in subsurface habitats and provide important ecosystem functions, such as the the provision of clean drinking water (Akob *et al.* 2011, Biogeosciences 8; Griebler *et al.* 2009, Freshwater Biol 54). In pristine groundwater, these essential microbial activities can be fueled by the surface input of plant-derived organic carbon as well as chemolithoautotrophic primary production (Cooper *et al.* 2016, Biogeochemistry 129; Emerson *et al.* 2016, Environ Microbiol 18; Hubalek *et al.* 2016, Isme J 10; Jewell *et al.* 2016, Isme J 10; Perrette *et al.* 2015, Org Geochem 88) . A further, much neglected source of organic carbon can be the sedimentary rock confining the aquifer, such as limestone and sandstone (Nowak *et al.* 2017, Hydrol Earth Syst Sc 21; Simkus *et al.* 2016, Geochim Cosmochim Ac 173). Organic carbon trapped during lithogenesis millions of years ago is still present in the present-day rock. This ancient organic carbon, containing a large fraction of hydrocarbons, is slowly released through rock weathering processes, which might be accelerated by the activity of microbes living in the rock matrix.

Taxonomic classification of the groundwater microbiome has revealed the presence of various organisms related to known hydrocarbon degraders, such as the genera *Thauera*, *Azoarcus* and *Dechloromonas*. Especially in anoxic groundwater, the microbiome was reported to show carbon isotope signatures hinting to the utilization of ancient organic carbon (Lazar *et al.* 2019, Sci Total Environ 679; Schwab *et al.* 2017, Biogeosciences 14; Schwab *et al.* 2019, Water Resour Res 55). However, evidence for an active degradation of rock-derived ancient organic carbon is still scarce.

Using the facilities of the Hainich Critical Zone Exploratory in central Germany, this project aims to understand the role of ancient organic carbon for the groundwater microbiome. Investigations will cover oxic as well as anoxic groundwater present in two aquifer assemblages with different biogeochemical properties. The project will take place in context of the Collaborative Research Centre AquaDiva. The following objectives will be addressed:

(1) To determine the metabolic potential for hydrocarbon degradation present in the groundwater microbiome.

(2) To determine the response of the groundwater microbiome to addition of ancient organic carbon and identify active hydrocarbon degraders.

(3) To isolate and characterize hydrocarbon-degrading microorganisms from the groundwater.

In order to address these objectives, the candidate will perform analyses of functional marker genes encoding key enzymes for hydrocarbon degradation using molecular approaches on gene and transcript level (amplicon sequencing, qPCR, analysis of metagenomics and -transcriptomics datasets). Stable isotope probing approaches in groundwater microcosms, including unspecific labeling with D_2O and ^{13}C reverse-stable isotope probing, will be conducted to identify microbes actively responding to powdered rock material and hydrocarbon model compounds (Schulte *et al.* 2019, Sci Total Environ 665; Taubert *et al.* 2018, Environ Microbiol 20). Metagenomics and metaproteomics will be used to characterize the physiology of the hydrocarbon degraders and to assist isolation approaches targeting these key organisms.

Key words: environmental microbiology, stable isotope probing, groundwater, ancient organic carbon, hydrocarbon degradation

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Group of “Molecular Biogeochemistry”at the

Max Planck Institute for Biogeochemistry, Jena, Germany

Head: apl. Prof. Dr. Gerd Gleixner

Webpage: https://www.bgc-jena.mpg.de/bgp/index.php/MolecularBiogeochemistry

Mission:

The research group explores key processes in the global biogeochemical cycles at the molecular level. Biomarkers and their isotopic content hold information on the regulation of the individual processes. The group is developing new tools and is applying existing techniques to investigate single key processes. Key topics of the group are:

- Understanding the origin, fate and stability of organic matter in the critical zone
- Understanding carbon flow in the plant-microbial-soil continuum
- Understanding the role of biodiversity in element cycling
- Understanding and reconstructing past climate and vegetation dynamics

The key questions in molecular biogeochemistry are: Who is there, what are they doing, and why? Proteomic and metabolomic approach bridges from the presence of organisms to their function in the environment. In order to explore the function of individual processes and how the microbial fluxes link to the overall functioning of ecosystems, additional information is drawn from the isotopic information of biomarkers. Compound specific isotopes (^{13}C, ^{14}C, ^{15}N, ^{18}O and ^{2}H) of biomarkers trace the flow of matter through the element cycles. The group of molecular biogeochemistry combines approaches using the natural abundance of stable isotopes, isotope labeling, and stable isotope probing (SIP) to quantify key processes in the environment.

Facilities of the Molecular Biogeochemistry Group:

- Gas Chromatography coupled to Flame Ionization Detector (GC-FID) and Mass Spectrometer (GC-MS)
- Gas Chromatography -Isotopic Ratio Mass Spectrometer (GC-IRMS) for C, N and H analysis
- High Performance Liquid Chromatography-Ultrahigh Resolution Mass Spectrometry (Orbitrap)
- High Performance Liquid Chromatography-Isotopic Ratio Mass Spectrometer (HPLC-IRMS)

Global drivers of molecular properties of dissolved organic matter

Keywords: dissolved organic matter, meta-analysis, multivariate statistics, mass spectrometry

The PhD project is offered by the working group "Molecular Biogeochemistry" at the Max Planck Institute for Biogeochemistry, Jena, Germany.

Dissolved organic matter (DOM) is a key component in the global carbon cycle and knowledge on its composition and reactivity is crucial to understand biogeochemical cycles (1, 2). DOM represents a snapshot of ecosystem activities and contains ecosystem-specific molecules (3, 4). Thus, DOM can be considered as ecosystem fingerprint (5) comprising information on ecosystem properties and processes (6). However, most DOM studies, in terrestrial systems investigate patterns on drivers of DOM on a local scale or at specific ecosystems.

This project aims at identifying global drivers of the molecular properties of DOM by conduction meta-analyses of already published studies on the one hand, and by analysing a large set of complex molecular data from ultra-high resolution MS on the other hand.

In order to address the project's aim the PhD candidate will i) gather published DOM data via literature and ii) analyze the molecular composition of a large number of DOM samples (already available data from the working group, plus data from potential collaborators). With this approach the project is able to identify drivers of molecular DOM properties on a global scale and to identify DOM compounds that reflect specific for ecosystems and are related to global drivers (3, 4)

Requirements:

- A Master's degree in Biostatistics, Biology, Geography, Ecology or Environmental Sciences
- Experience in processing and analyzing large data sets, in particular skills in univariate and multivariate statistics are mandatory.
- Background in soil science is of advantage.
- Very good oral and written communication skills in English.

1. Battin TJ*, et al.* (2009) The boundless carbon cycle. *Nature Geoscience* 2(9):598-600.
2. Roulet N & Moore TR (2006) Environmental chemistry - Browning the waters. *Nature* 444(7117):283-284.
3. Benk SA, Li Y, Roth V-N, & Gleixner G (2018) Lignin Dimers as Potential Markers for 14C-young Terrestrial Dissolved Organic Matter in the Critical Zone. *Frontiers in Earth Science* 6.
4. Roth V-N, Dittmar T, Gaupp R, & Gleixner G (2013) Latitude and pH driven trends in the molecular composition of DOM across a north south transect along the Yenisei River. *Geochimica et Cosmochimica Acta* 123(0):93 - 105.
5. Roth V-N, Dittmar T, Gaupp R, & Gleixner G (2014) Ecosystem-Specific Composition of Dissolved Organic Matter. *Vadose Zone Journal* 13(7).
6. Roth V-N*, et al.* (2019) Persistence of dissolved organic matter explained by molecular changes during its passage through soil. *Nature Geoscience* 12(9):755-761.

Identifying the microbial available soil organic matter and its processing

Keywords: dissolved organic matter, mass spectrometry, soil processes, microorganisms, stable isotopes

The PhD project is offered by the working group "Molecular Biogeochemistry" at the Max Planck Institute for Biogeochemistry, Jena, Germany.

The functioning of terrestrial ecosystems is dependent upon the energy supply by plants and the retention of soil nutrients and thereby the plant nutrients supply (1). These soil-plant-interactions are mostly mediated by small organic compounds that are found in the complex mixture of dissolved organic matter (DOM). Therefore, DOM plays a crucial role in a multitude of processes, such as microbial cycling (2) and distributing of nutrients and carbon that are central for ecosystem functions and services (3, 4). However, the role of DOM, its molecular composition and how DOM is affected by the microbial community is only partly understood.

This project will use a non-targeted ultra-high resolution mass spectrometric approach i) to study the molecular signatures of dissolved organic matter (DOM), ii) to better understand the functions of DOM in ecosystem processes and iii) to understand how DOM is affected by the soil microbial community. This project will take advantage of a long-term vegetation change experiment (C3 *vs.* C4 plants (5)) in order to combine natural labelling as a consequence of the vegetation change and contrast freely drainable soil water *vs.* soil extracts. This approach enables to differentiate between compounds found in soil micro-pores, which act as microbial hotspots and compounds found in freely drainable soil water. It will therefore further elucidate the microbial cycling of organic matter.

Requirements:

- A Master's degree in Chemistry, Environmental Chemistry or other chemistry related sciences.
- Experience in analytical chemistry, LC-MS, handling of big data sets.
- Experience in high resolution MS (FT-ICR-MS or Orbitrap).
- Very good oral and written communication skills in English.

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5. Mellado-Vázquez PG, Lange M, & Gleixner G (2019) Soil microbial communities and their carbon assimilation are affected by soil properties and season but not by plants differing in their photosynthetic pathways (C3 *vs.* C4). *Biogeochemistry* 142(2):175-187.

International Max Planck Research School for Global Biogeochemical Cycles (IMPRS-gBGC)

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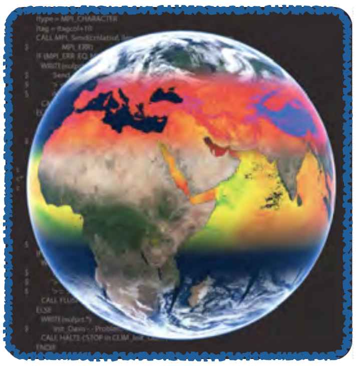

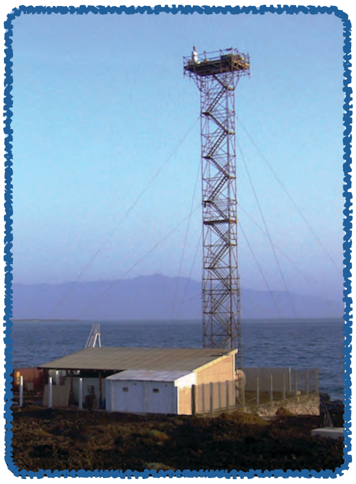

Open PhD project: Greenhouse Gas Budgets at the Amazon Tall Tower Observatory (ATTO)

Advisors

Jost Lavric, Susan Trumbore

Project description

The Amazon plays a large role in the global biogeochemical cycles of greenhouse gases (GHGs) – e.g., variations in carbon fluxes in tropical land areas are a major driver of interannual variations in the global atmospheric CO_2 growth rate. Other important GHGs, methane (CH_4) and nitrous oxide (N_2O) have large natural sources in the Amazon's wetlands and soils, as well as from biomass burning. Long-term continuous atmospheric observations of GHGs and other biogeochemical trace gases at the Amazon Tall Tower Observatory (ATTO project), located in a protected rain forest region in the central Amazon Basin, are already providing valuable data for regional estimates of GHG dynamics. The addition of new atmospheric concentration and stable isotopic composition gradient measurements from near surface up to 321 m a.g.l., will provide new insights into land-atmosphere exchange at spatial scales of meters and up to hundreds of kilometers. It will allow the attribution of fluxes to different source and sink processes, as well as provide information on atmospheric dynamics and mixing, including the location of the Intertropical Convergence Zone. In order to address the above research questions, the successful candidate will work with presently available data (CO_2/CH_4/CO data collected since 2012) and with data from the new CO_2, $^{13}CO_2$, CO, N_2O, CH_4, delta^{13}C-CO_2/CH_4 measurement systems (FTIR, CRDS) to be installed in late 2019/ early 2020, which s/he will also be responsible for.

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Working group & planned collaborations

The successful candidate will integrate the Tall Tower Atmospheric Gas Measurements group at the Max Planck Institute for Biogeochemistry (MPI-BGC). The candidate's work will be closely related to that of several other work groups of the ATTO project consortium; in particular, s/he will collaborate with colleagues from MPI-BGC, MPI-C and the University of Bremen (Germany), and INPA, INPE and EMBRAPA-Belem (Brazil).

Requirements

Applications to the IMPRS-gBGC are open to well-motivated and highly-qualified students from all countries. Prerequisites for this PhD project are:

- a Master's degree in atmospheric science, meteorology, bio(geo)chemistry or other disciplines related to environmental sciences
- Experience in scientific programming and handling of large data sets
- Knowledge on stable isotopes and land-atmosphere interactions are an advantage
- Hands-on experience with scientific measurement equipment
- Interest in occasional field work at remote locations
- Self-driven personality able to work both independently and in a team
- Excellent oral and written communication skills in English, knowledge of German and/or Portuguese is an asset
- Motivation to present results at scientific meetings and publish them in scientific journals

The Max Planck Society seeks to increase the number of women in those areas where they are underrepresented and therefore explicitly encourages women to apply. The Max Planck Society is committed to increasing the number of individuals with disabilities in its workforce and therefore encourages applications from such qualified individuals.

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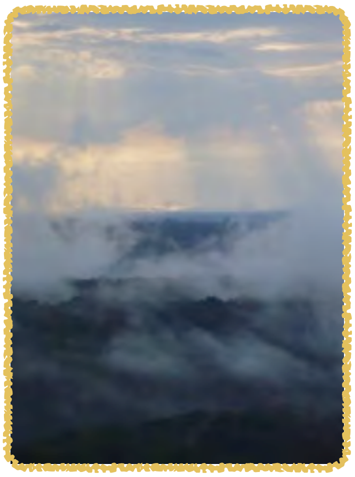
The heart of the Amazon Tall Tower Observatory is the 325 m-tall tower (Photo: RD, Nov 2016 / JL, Jan 2017)



ATTO with its infrastructure and surroundings is a unique natural laboratory that provides excellent opportunities for interdisciplinary research. (Photo: JL, Jan 2015)

Max Planck Institute for Biogeochemistry

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Open PhD project: Biotic and abiotic control on biofilm assembly

advisors: Juergen Popp, Gerd Gleixner, Lukas Wick

Environmental biofilms cover nearly all surfaces generating niches for synergistic and antagonistic interactions between microorganisms. The different gradients in such biofilms (nutrition, O_2, pH, etc.) form specific zones which are populated by various organisms. In such a community synergistic interactions like toleration, communication or complete cooperation but simultaneously antagonistic interaction like competition or killing can be found. Facing outside disturbances the biofilm community will be remodeled to adapt to the new conditions. [1] Such dynamic effects are not fully understood and corresponding interactions can be investigated with isotopic tracer experiments. This project will use modern analytic methods to evaluate the molecular and bacteriological changes of biofilms assemblies experiencing biotic and abiotic disturbances.

Raman spectroscopy is a phenotypic method thus analyzing all cell components without destruction. Due to the high spatial resolution Raman microscopy even can be applied to analyze single bacterial cells or monitor in vivo the development of eukaryotic cells in 2D over time. [2,3] Raman spectroscopic investigations of biofilms lead either to a sum spectrum of the entire biofilm or a 3D map of the biofilm revealing the distribution of bacteria, EPS and other components. The Raman spectroscopic analysis of planktonic and sessile bacteria already revealed distinct spectral differences due to the adaptation of the cells on the new conditions. [4] In addition, Raman spectroscopy can directly identify isotopic labeling of molecules with e.g. ^{2}H, ^{13}C, ^{15}N containing atoms even in organisms. [5,6]

Ultra-high resolution mass spectrometry (FT-MS) is able to identify multiple thousands individual molecules which resemble the bacteria interaction inside biofilms. [7] These molecules resemble the origin of molecules and ongoing metabolic processes. As so far the use of the isotopic information is not well established. [8] However, the use of such techniques will help to trace the flow of isotopic labels into individual molecules / organisms of the biofilm.

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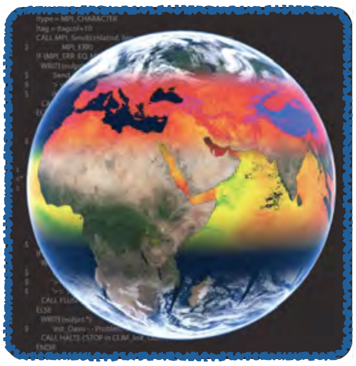

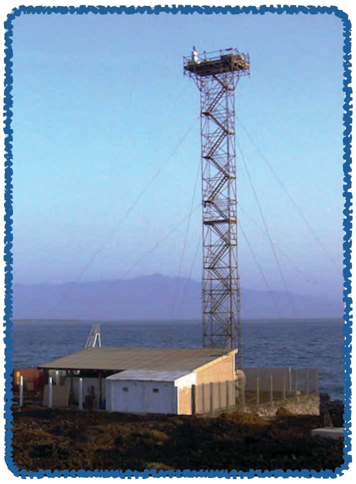

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In this project first defined biofilms from 3 to 5 species will be created and defined by means of Raman spectroscopy and ultra-high resolution mass spectrometry (FT-MS). The combination of Raman spectroscopy and FT-MS will allow an overall picture of the molecular situation inside biofilms. According to the type of interaction of different bacteria the resulting multispecies biofilm will most probably develop completely new characteristics. These undisturbed biofilms will be analyzed by means of different chemometric methods and will then be compared to biofilms which experience abiotic or biotic events. The second step of this projects is dedicated to the carbon/nitrogen turnover of biofilms. Such experiments might use isotope labeled or unlabeled small molecules. Raman spectroscopy and FT-MS will then be used to identify the likely endpoints of these labels/molecules. In a third step specific or non-specific phages will be introduced into the system. In both experiments it is expected that not only the abundance of the single bacteria will be effected but also the EPS composition and carbon/nitrogen flow to different parts of the community.

Overall, the PhD student will mainly focus on the spectroscopic and biological realisation of this new microbial Raman spectroscopic approach of this biofilm project. Thereby, the student can rely on the unique and rich expertise of the Leibniz Institute of Photonic Technology (IPHT) and the Institute of Physical Chemistry (IPC, Friedrich-Schiller University of Jena) in Raman based microbial analysis. The ultra-high resolution mass spectrometry (FT-MS) analysis will be performed at the Max Planck Institute of Biochemistry, Molecular Biogeochemistry. The phage project will be performed in cooperation with the CRC AquaDiva and the Working Group Bioavailability, UFZ Leipzig.

The Max Planck Society seeks to increase the number of women in those areas where they are underrepresented and therefore explicitly encourages women to apply. The Max Planck Society is committed to increasing the number of individuals with disabilities in its workforce and therefore encourages applications from such qualified individuals.

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- Improved understanding of biogeochemical processes with an emphasis on terrestrial ecosystems
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- Theory and model development for improving the representation of biogeochemical processes in comprehensive earth system models

Open PhD project: Cavity enhanced Raman spectroscopy for highly sensitive monitoring of biogenic gases

Advisors

Torsten Frosch, Juergen Popp, Susan Trumbore

Project description

The characterization of biogenic gases and their temporal fluctuations is important for the elucidation of environmental processes and the interactions with the biosphere. Currently there is a lack of miniaturized, field-portable, and robust sensors capable for simultaneous quantification of multiple components in complex biogenic gas mixtures. An innovative approach is Raman gas spectroscopy, a technique that is based on molecular vibrations and capable for the quantification of a whole variety of biogenic gases simultaneously in a broad concentration range (from ppm to pure compounds). Raman spectroscopy is a non-consumptive technique that can be applied for rapid online monitoring of gases.

In this project a new miniaturized and robust Raman gas sensing setup will be developed. The new device should potentially allow monitoring of reactive gases rapidly and with high spectral resolution. A novel optical cavity setup be developed and exploited for efficient light-analyte-interactions in order to achieve an improved analytical sensitivity. This novel gas sensing setup will allow precise online quantification of biogenic gases with low cross-sensitivities. Such spectrally highly resolved Raman gas sensing will help for detailed tracing of plant metabolites and thus enables a better investigation of resource flows in mesocosm experiments. Several interdisciplinary gas sensing experiments will be performed together with our collaboration partners.

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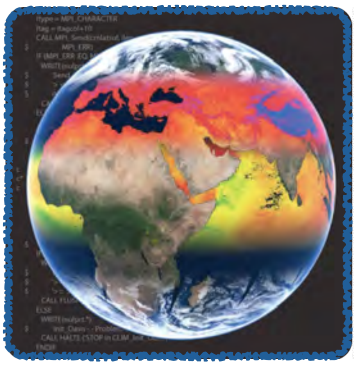

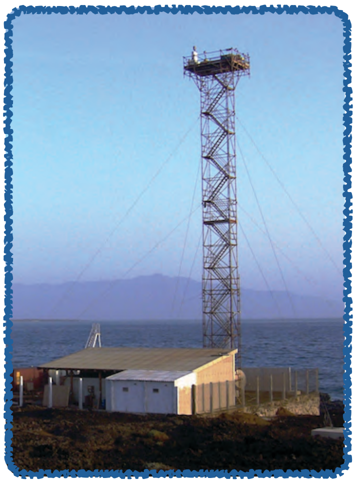

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Working group & planned collaborations

The work in the spectroscopic sensing group at the Institute of Physical Chemistry and the Leibniz Institute of Photonic Technology is focused on the development and application of enhanced Raman spectroscopic gas sensing techniques that enable new insights into complex biogeochemical processes.

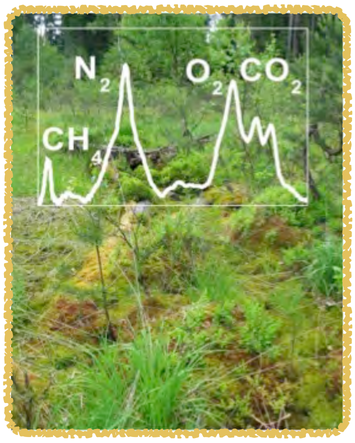
The interdisciplinary project is strongly connected to the collaborative research centre AquaDiva and includes several collaborations to groups at Max Planck and the Friedrich Schiller University.

Enhanced Raman multigas sensing – a novel tool for control and analysis of $^{13}CO_2$ labeling experiments in environmental Analytical Chemistry (2013), 85, 1295

Requirements

Applications to the IMPRS-gBGC are open to well-motivated and highly-qualified students from all countries. Prerequisites for this PhD project are:

- a Master's degree in physics, engineering, analytical or physical chemistry or related disciplines
- experimental and technical skills
- interest in the development and application of new instruments and setups
- interest in Raman Spectroscopy, optics, and gas sensing
- interest in environmental and biogeochemical sciences
- very good communication skills in English (both spoken and written)



Investigation of Gas Exchange Processes in Peat Bog Ecosystems by Means of Innovative Raman Gas Spectroscopy, Analytical Chemistry (2013), 85, 1295

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Open PhD project: Investigation of nitrogen fixation by means of Raman gas spectroscopy

Advisors

Torsten Frosch, Susan Trumbore

Project description

Biological N_2 fixation is a major input of bioavailable nitrogen, which represents the most frequent factor limiting the agricultural production throughout the world. Especially the symbiotic association between legumes and Rhizobium bacteria can provide substantial amounts of nitrogen (N) and reduce the need for industrial fertilizers. Despite its importance in the global N cycle, rates of biological nitrogen fixation have proven difficult to quantify. Currently there is a lack of miniaturized, field-portable, and robust sensors capable for simultaneous quantification of multiple components in complex biogenic gas mixtures. An innovative approach is Raman gas spectroscopy, a technique that is based on molecular vibrations and capable for the quantification of a whole variety of biogenic gases simultaneously in a broad concentration range (from ppm to pure compounds). Raman spectroscopy is a non-consumptive technique that can be applied for rapid online monitoring of gases.

In this project a new setup for Raman spectroscopic nitrogen gas sensing will be developed and applied for studying biological nitrogen fixation. The new device should potentially allow online monitoring of reactive gases rapidly, sensitively and with high spectral resolution. A novel optical cavity setup be developed and exploited for efficient light-analyte-interactions in order to achieve an improved analytical sensitivity. Several interdisciplinary gas sensing experiments will be performed together with our collaboration partners.

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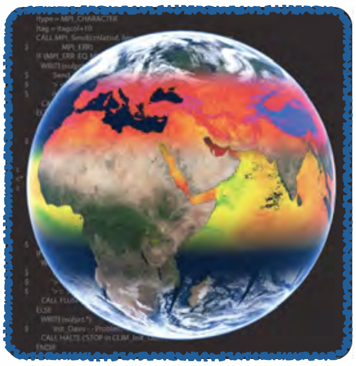

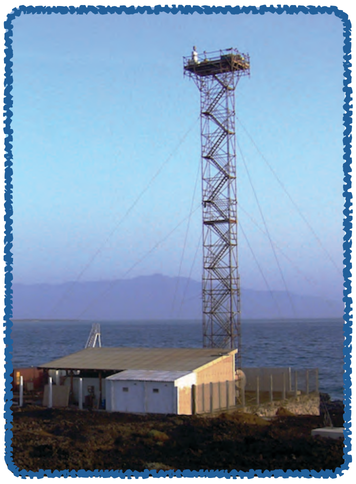

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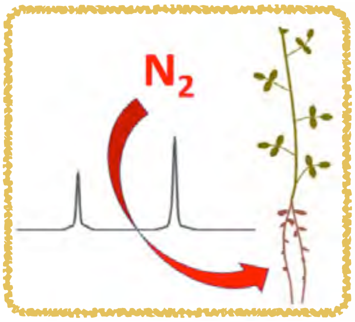

Direct Raman spectroscopic measurements of biological nitrogen (N_2) fixation under natural conditions Analytical Chemistry (2017); 89, 1117-1122

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PhD: Biosynthetic Pathway Analysis of A Microbial Natural Product

Key words: Natural Products, biosynthetic transformations, heterologous expression, genome mining, enzymes

Project title: Analysis of a unique PKS-hybrid pathway encoding for a highly bioactive natural product

We used various different culturing techniques to isolate termite-associated microbes and pursued the whole genome sequence of several key isolates. Subsequent chemical analysis of our isolates in axenic and co-cultures revealed several new natural product classes showing a diverse set of biological activities.

Within this PhD project, we aim to understand the key biosynthetic transformations underlying the formation of a newly identified unique PKS-hybrid-based natural product. The aim is to capture the biosynthetic pathway using a BAC library construct- Subsequent, key biosynthetic transformations should be investigated via knock-out studies and/or mutagenesis. Subsequently, key enzymes should be investigated *in situ*. These studies should enable the generation of a small natural library of biosynthetic intermediates and structural variants of the end product.

Project Start: Early summer 2019

Main topics and tasks:

- experience with PCR reactions, heterologous expression systems, protein purification, and/or mutasynthesis

Our requirements:

Your profile: A strong interest in conducting collaborative research on the topic outlined above is paramount. Candidates are expected to be interested in working at the boundaries of several research domains.

- Very good theoretical and practical skills in molecular biology, microbiology
- The candidate should embrace working in a young international research team and conducting research that covers multiple biological disciplines
- A Master degree or equivalent in Life Sciences, Molecular Biology, Microbiology.
- An integrative and cooperative personality with enthusiasm for actively participating in a lively community of the HKI, the JSMC (www.jsmc.uni-jena.de) and ILRS (www.ilrs.hki-jena.de) community
- Very good communication and writing skills (English)

We offer: A highly translational project with a promising career perspective. Highest standard laboratories with state-of-the-art instrumentation and the collaborative and constructive atmosphere at the HKI provide ideal conditions for the success of your project. We offer you great work opportunities in a dynamic research institute with high reputation. As a doctoral researcher you will be integrated into the structured training of our graduate schools and benefit from the extensive qualification program of the Graduate Academy of the Friedrich Schiller University. The successful candidate will be hosted in the Junior Research Group *Chemical Biology of Microbe-Host Interactions*.

For further information regarding the research topic: please contact: Dr. Christine Beemelmanns (christine.beemelmanns (at) leibniz-hki.de)

Topic: Organic Synthetic Chemistry – Natural Product Synthesis

Key words: Total synthesis, natural Products, drug discovery, organic chemistry

Project Start: Early summer 2019

Project Outline: Research into microbial sphingolipid signalling is an area of intensive scientific investigation. Only recently, sphingoid-like natural products have been isolated from marine bacteria, where they serve as essential multifunctional cellular compounds regulating fundamental inter and extracellular processes. The project aims for the total synthesis of novel sphingoid-like signalling molecules using state-of-the art organic-synthetic chemistry. All synthesized molecules will be used to understand principle (bio)chemical and small molecule-mediated communication mechanisms within microbe-host interactions.

Main topics and tasks:

- Synthesis of microbial sphingolipid-type signalling molecules and related core structures, using e.g. metal-organic reactions, enantioselective hydrogenation, enantioselective alkylation reaction,
- Development atom-economic synthetic approaches
- Derivatisation of natural products for comparative analysis
- Implementation of (additional) functionalities such as fluorescence or photo-reactive tags for target identification

Requirements:

- Very good theoretical and practical skills in Organic Synthesis
- Expertise in Analytical Chemistry (NMR, HRMS, IR, HPLC, LC-MS)
- The candidate should embrace working in a young international research team
- A Master degree (or equivalent) in chemistry or related natural and life sciences. Candidates about to obtain their degree are welcome to apply!
- An integrative and cooperative personality with enthusiasm for actively participating in a lively community of the HKI, the JSMC (www.jsmc.uni-jena.de) and ILRS (www.ilrs.hki-jena.de) Community
- To be able to perform team-oriented as well as independent work
- Very good communication and writing skills (English)

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For further information regarding the research topic: please contact: Dr. Christine Beemelmanns (christine.beemelmanns (at) leibniz-hki.de)

PhD: Genome-Mining based Natural Product Discovery

Key Words: Natural Products, genome mining, heterologous expression, enzymes, drug discovery

Project title: Application of **c**omparative genome analysis to identify unique secondary metabolite related biosynthetic gene clusters and their respective natural products

Within this project, we aim to identify and understand the role of natural products produced by microorganisms associated with fungus-growing termites. We have sequenced the genomes of selected new microbial species. Within this PhD project, the genomes should be evaluated for the genetic basis of symbiotic contributions, and with respect to new biochemical transformations and secondary metabolite production. These studies should guide subsequent natural product isolation efforts and/or heterologous expression of cryptic gene clusters in production hosts.

Project Start: Early summer 2019

Main topics and tasks:

- Able to perform comparative whole genome analysis
- experience with PCR reactions, heterologous expression systems, protein purification is advantageous

Our requirements:

Your profile: A strong interest in conducting collaborative research on the topic outlined above is paramount. Candidates are expected to be interested in working at the boundaries of several research domains.

- Very good theoretical and practical skills in bioinformatics and/or molecular biology
- The candidate should embrace working in a young international research team and conducting research that covers multiple biological disciplines
- A Master degree or equivalent in Life Sciences, Molecular Biology, Microbiology and/or Computational Biology, Bioinformatics.
- An integrative and cooperative personality with enthusiasm for actively participating in a lively community of the HKI, the JSMC (www.jsmc.uni-jena.de) and ILRS (www.ilrs.hki-jena.de) community
- Very good communication and writing skills (English)

We offer: A highly translational project with a promising career perspective. Highest standard laboratories with state-of-the-art instrumentation and the collaborative and constructive atmosphere at the HKI provide ideal conditions for the success of your project. We offer you great work opportunities in a dynamic research institute with high reputation. As a doctoral researcher you will be integrated into the structured training of our graduate schools and benefit from the extensive qualification program of the Graduate Academy of the Friedrich Schiller University. The successful candidate will be hosted in the Junior Research Group *Chemical Biology of Microbe-Host Interactions*.

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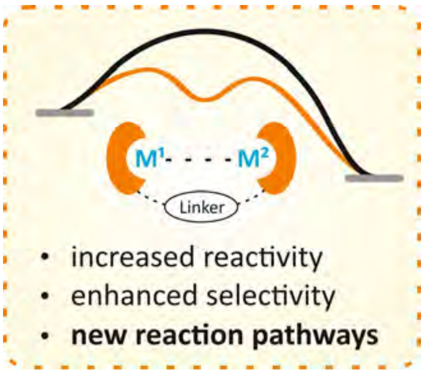
Join the Sustainable Catalysis Group of Prof. Dr. Robert Kretschmer

Catalysis belongs to the most ecologically and economically impacting technologies in today's society, enabling efficient access to complex molecular architectures relevant to various key disciplines such as energy conversion, environmental protection, human health care, and materials synthesis. As such, catalysis is of paramount importance, accounting (directly and indirectly) for about 20-30% of the world gross domestic product, and has been identified as the key technology to address the challenges the society is facing in 21st century. Although tremendous developments have taken place over the past century, many of the most useful catalysts still incorporate rare and thus expensive precious metals, such as iridium, palladium, platinum, rhodium, and ruthenium, whose supply is limited and dependent on geopolitical stability. In addition, these noble metals do not meet sustainable ecological needs. Catalysts based on main group elements or (eco)toxicologically unproblematic transition metals are interesting and promising alternatives. With regard to the composition of the earth's crust, the elements aluminium, calcium, magnesium and silicon are of particular interest, and the corresponding fields of research have become increasingly interesting in recent years.

Our research addresses this needs and focuses on the development of novel cooperative catalysts. On the one hand, we use binuclear metal(loid) compounds that enable reaction paths that are not accessible with the corresponding mononuclear counterparts. Furthermore, we are also developing new catalysts based on the concept of metal-ligand cooperativity, where so-called non-innocent ligands have a significant influence on reactivity and catalytic activity. We combine the areas of inorganic, organic, and computational chemistry to derive new catalysts, to understand their mode of action and to improve the activity and selectivity schemes.



Currently, we offer two PhD topics:

- **Homogeneous photocatalysis and solar energy storage using abundant and non-toxic transition metals**
- **Catalytic polymerization and depolymerization using catalysts based on main-group elements**

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Electrode-Electrolyte Interactions in Organic Batteries

Keywords:

- *Energy Storage*
- *Green Battery Materials*
- *Molecular Mechanism of Charge Storage*
- *Spectroscopy*
- *Electrochemistry*

Developing green materials for energy storage is a major task to address the looming energy crisis. A particularly interesting approach towards novel materials is the design of polymers as electrode materials as well as electrolytes for a novel generation of batteries. In order to investigate the molecular mechanism that lead to charging and discharging of all-organic batteries and characterize performance limiting processes such as self-discharge of the batteries, we will establish nonlinear spectroscopic tools to monitor the molecular interactions at the electrode surfaces of polymer batteries *in operando*.

To access the local structure and structural changes at the polymer-electrolyte interface *in operando* vibrational sum-frequency generation (VSFG) is used. The method as to allows to study IR-active vibrations selectively at surfaces and interfaces: A broad-band (femtosecond) mid-IR pulse is overlapped with a narrowband (picosecond) pulse in the visible, wave mixing yields a blue-shifted signal irradiated at the sum frequency. If the spectrum of the mid-IR pulse overlaps with a vibrational resonance of the sample, the signal generation becomes resonantly enhanced. Hence, vibrational spectra reflecting the IR active vibrational modes at surfaces and interfaces can be recorded combining the chemical specificity of vibrational spectroscopy with interfacial specificity.

This project will combine VSFG with electrochemical approaches to study for the first time changes in polymer electrode-electrolyte interfaces upon electrochemical trigger, i.e. application of a potential to initiate heterogeneous and homogeneous electron transfer processes at the interface. We will implement novel experimental schemes to introduce time-resolution down to the ms range in a chronoamperometric VSFG-spectroelectrochemical experiment. Thereby, we will be able to resolve structural changes and altered electrode-electrolyte interactions upon charging and (self) discharging of the electrodes in real time. Thus, the project will offer unprecedented mechanistic insights into the molecular structure changes and intermolecular interactions governing the performance of all organic batteries.

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Effect of mirror charges on the ultrafast dynamics of molecules at interfaces

Keywords:
- *Molecular Dynamics*
- *Nonlinear Optics*
- *Spectroscopy*
- *Photoinduced Charge Transfer*
- *Photoinduced Isomerization*

This project will experimentally investigate the influence of mirror charges on the structural dynamics of molecules deposited on surfaces of metallic nanostructures. For this purpose, femtosecond time-resolved vibrational sum frequency generation (tr-vsfg) will be used. This intrinsically surface sensitive method allows to detect changes in the IR-active vibrational modes after photo-excitation of molecules at interfaces with a time resolution of less than 100 fs.

The electronic excitation of molecules immobilized on metallic nanostructures now leads to the formation of mirror charges in the metal, since the electronic excitation in the molecule is associated with a change in electron density in the molecular structure. In order to investigate the effect of mirror charges on molecular dynamics, organic push-pull dyes, which on the one hand have a strong absorbance in the visible spectral range and on the other hand exhibit a strong and characteristic change in their electron density at the transition from the electronic ground state to the electronically excited state, are to be applied to metallic surfaces. In order to avoid a direct electronic interaction of the (photoexcited) molecules with the metal, a thin Al_2O_3 layer is applied by means of ALD. By varying this layer thickness from a few Å to several 10 nm, the distance between the charge distribution (in the molecule) and the mirror charge distribution in the metal is also varied. The effect of the thus varied Coulomb interaction between charge and mirror charge on the structural and electronic dynamics in the molecules can thus be investigated experimentally. As a further experimental parameter, the packing density of the photoactive molecules on the metallic surface is to be controlled by co-grafting optically inactive molecules. This method is known from the production of e.g. dye-sensitized solar cells and is suitable to reduce the electronic interaction between two optically active molecules at a molecule-solid interface. In this way, effects of intermolecular interactions on the excited state dynamics can be distinguished from effects caused by mirror charges in the metallic structures to which the molecules are applied.

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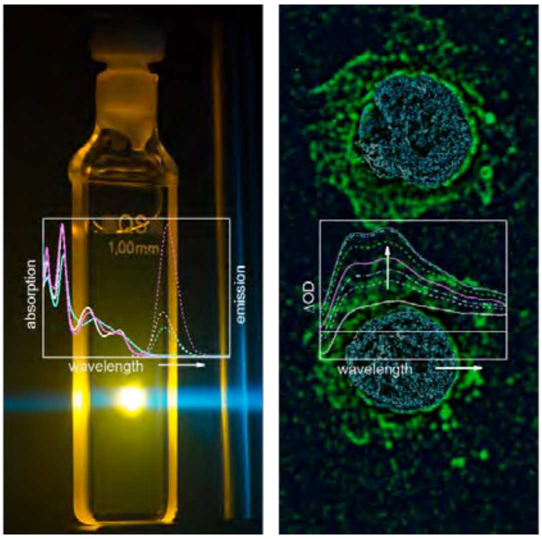
Deciphering the Mechanism of Cytotoxicity of Metal-Containing Drugs for Photodynamics Therapy

Keywords:

- *Photodynamic Therapy*
- *Tumor Treatment*
- *Ultrafast Spectroscopy*
- *Nonlinear Microscopy*

Developing novel drugs for therapy presents a challenging yet necessary task to improve our abilities for cancer treatment. Such matter becomes even more important facing the increasing lifespan in developed societies. An attractive rout to pursue is photodynamic therapy in which drugs are administered that are non-toxic when kept in the dark but become highly cytotoxic when exposed to light. As light is inherent to the function of these drugs, the response of the drug molecules to the external stimulus light must be taken into account when describing the molecular mechanism of drug activation.

In this project we will device novel experimental strategies to characterize the function determining photophysical and photochemical processes in metal-based drugs for photodynamic therapy. In particular, we will focus on Osmium(II)-complexes, which are ideally suited for photodynamic therapy as their absorption falls into the biological window, *i.e.* high penetration depths into tissue can be achieved. In order to determine the molecular processes, which determine and / or limit the function of these complexes as novel drugs, it is essential to study the complexes in their biological target environment, *i.e.* in human cells and tissue. This, however, is beyond the state of the art, which is essentially determined by spectroscopic investigations on the complexes in aqueous solution accompanied by cell toxicity assays.



To bridge this conceptual gap in the characterization of drugs for photodynamic therapy we will study the excited state processes of the Os-complexes embedded into human cells and tissue by ultrafast transient absorption microscopy, resonance Raman scattering microscopy and fluorescence lifetime microscopy. Thereby, the project will – for the first time – yield a holistic picture of the light-induced processes, which govern the function of the photodrugs once the complexes are within their biological target environment.

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Time-Resolved Cavity Ring-Down Spectroscopy

Keywords:

- *Molecular Dynamics*
- *Ultrafast Spectroscopy*
- *Cavity Ring-down Spectroscopy*
- *Two-dimensional Materials*
- *Photoinduced Charge Transfer*

Two dimensional materials such as graphene or self-assembled monolayers are currently on the spotlight of scientific research due to their versatility and their potential application in photovoltaics, water purification and artificial photosynthesis, between many others. Hence, there is a growing interest on learning about the nature of their electronic transitions and photoactivated charge transfer processes, in order to discover all their possible functionalities and assess their performance in diverse environments.

The aim of this project is to develop an optical setup that is able to perform time-resolved spectroscopy on single layers. The existing facilities to measure excited state absorption often cannot resolve signals from two-dimensional structures due to their extremely low optical density. This obstacle is here addressed by integrating the pump-probe technique to a cavity ring-down spectroscopy setup (crds), resulting in an increased sensitivity in transient absorption measurements while keeping a sub-picosecond time resolution.

Low-absorbing gold nanostructures measured with the home built time-resolved crds (tr-crds), using narrowband 800 nm sub-picosecond pulses, provide preliminary results with five times better sensitivity using 10^4 times less power at the sample, in comparison with data obtained in an equivalent non cavity-amplified setup (i.e. conventional transient absorption spectroscopy). The aspiration is not only to resolve further lower-absorbing samples, but also to make the system more versatile so the cavity can embrace different visible wavelengths for pump and probe, allowing the characterization of a much broader variety of two-dimensional materials.

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Wet-chemical deposition of semiconductor materials and transparent conductive oxides on textiles for energy applications

Keywords:

- *Smart Textiles*
- *Energy Generation*
- *Semiconductor*
- *Transparent Conductive Oxide (TCO)*
- *Wet Chemical Deposition*

Crystalline ZnO is a wide band semiconductor, which could be used for many optoelectronic applications like solar cells, UV detectors, LEDs or for thermoelectric applications. An additionally doping with Al results in Al:ZnO (AZO), which is a transparent conductive oxide (TCO) useable in photovoltaic or LED devices or as thermoelectric, piezoelectric or triboelectric material. At the *Leibniz Institute of Photonic Technology* (IPHT) we want to bring such applications into fabrics to enable *Smart Textiles*.

Typically ZnO and Al:ZnO thin film are prepared by physical vacuum deposition techniques like CVD, ALD or sputtering. The transfer of these processes to textiles is mostly limited due to the rough surfaces and the low vacuum and temperature stability of the textiles. The wet-chemical deposition directly on textiles offers new possibilities to prepare compact and homogenous thin films at textile compatible conditions.

The aim of the PhD project is to develop and optimize the wet-chemical deposition of ZnO films and to introduce an additionally doping with Al, Ga or In to enable TCOs like Al:ZnO. The layer properties like morphology, crystal quality, electrical conductivity, optical transparency have to be characterized. Chemical and physical modifications during the deposition could tune the layer properties. Also the pre-treatment of the textile substrate and the post-treatment, like annealing or passivation of the layers have to be investigated. All processes are limited to suitable conditions for textiles. Finally solar cells and thermoelectric devices can demonstrate the energy applications.

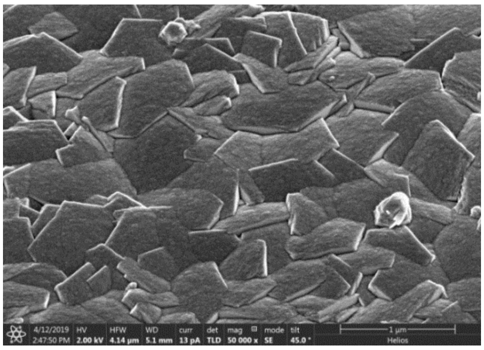

Figure: Wet-chemical ZnO thin film and thermoelectric generators with AZO layers on textiles.

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Artificial Photosythesis driving multi-electron redox processes

Multi-electron transfer reactions are still one of the great challenges in photoredox chemistry. Nonetheless, they are of great importance since single electron transfer steps often require more energy than concerted multi-electron transfers. Despite that, only a handful of systems exist, which are capable of transferring more than one electron at a time to a substrate. The approach taken so far was to combine several photosensitizer units to one catalytic centre in order to transfer one electron from each photosensitizer unit. This approach, however, requires simultaneous excitation of the photosensitizer units and thus high photon densities. Very recently we have developed a photosensitize and charge storage system based on a photoactive Cu(I) complex, which is able to store two electrons after photoexcitation. The stored electrons could be used in a subsequent dark reaction to reduce a model substrate. This approach allows to first collect the charges even under low light intensity conditions before they are used in a redox reaction.

The goal of the project is to the develop photosensitizer-storage-catalyst assemblies towards real world applications, such as carbon dioxide reduction into fuels. Starting with a catalytically active model system, the project will develop synthetic strategies for the covalent binding of the catalysts, such as manganese coordination compounds, to the Cu(I)-photosensitzer-storage unit and investigate the structural, photophysical and electrochemical properties as well as the catalytic behaviour. In a second step the knowledge gained from the first step will be used to custom-tailor these properties towards a selected redox transformation. The interdisciplinary project will make use of the combination of spectroscopic, electrochemical and chromatographic techniques to identify key structural features and find suitable synthesis pathways towards their realisation. This is a challenging project at the cross section of synthetic chemistry, electrochemistry and photophysics and is nested within our collaboration network comprising of experts from these fields as well as theoretical chemistry.

The successful applicant thus has a strong background in synthetic organic or inorganic chemistry and is highly motivated to advance her/his skills in the field of catalysis, electrochemistry and photophysics. We are an international team, thus fluent English in spoken and written is mandatory.

We offer an inspiring working atmosphere in an international team under direct supervision by our experienced scientific staff. Project benefits from state-of-the art synthetic labs and equipment as well as next door collaborations. The University of Jena has a long-standing research tradition and is ranked among the 500 top universities in the world, offering an inspiring research atmosphere. PhD students are part of the Jena Graduate Academy to further advance language, presentation and soft skill. The city of Jena is a prosperous, vibrant and ever-young city nested within the green hills along the valley of the river Saale and en-

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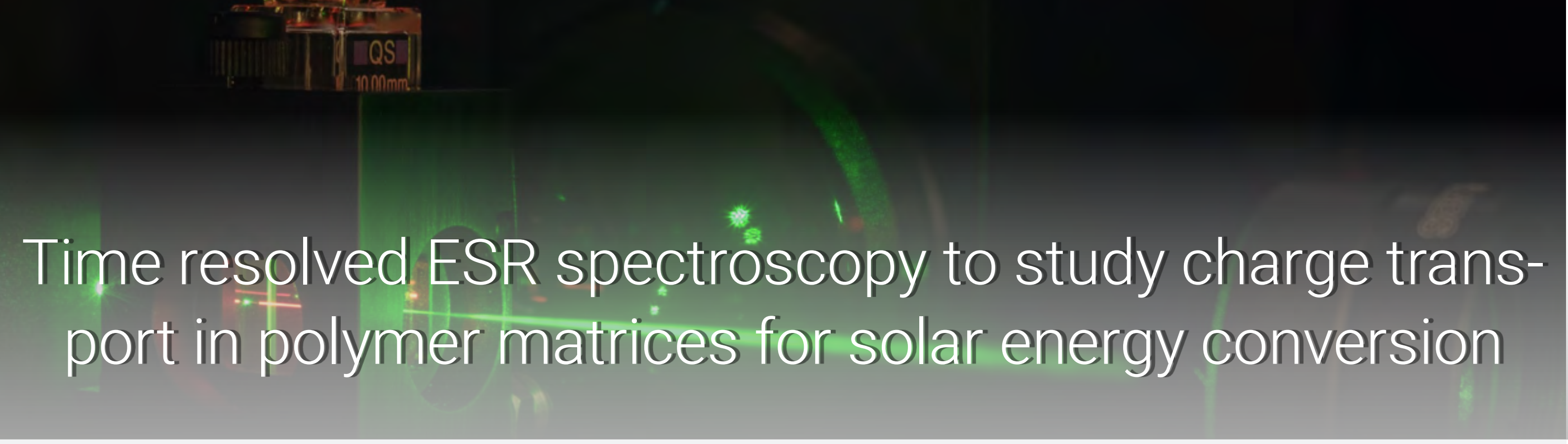

Time resolved ESR spectroscopy to study charge transport in polymer matrices for solar energy conversion

The efficient conversion of solar energy into storable fuels such as hydrogen is still a great scientific challenge. Despite tremendous efforts during the last decades, the number of reports on fully integrated systems still is comparatively low. While homogeneous systems are quite well understood the interfacing of the oxidation and reduction reaction imposes new challenges such as a charge carrier transport velocities, electron back transfer, or molecular rearrangements of and at the interface. In order to get detailed insights into such processes, the combination of spectroscopic and electrochemical techniques is necessary to study the system *in situ*.

A promising interfacing approach is the combination of a molecular photosensitizer and catalyst in a conductive polymer on an electrode surface. Here the photosensitizer drives the electron transfer via the polymer to the catalyst while being re-reduced through the electrode. And although this principle works well only little is known about the charge transfer processes.

The goal of the project is to study light-induced charge transfer processes of photosensitizer-catalyst assemblies in conductive polymers with time-resolved electron spin resonance spectroscopy (ESR-spectroscopy). To this end Fourier transform (FT)-ESR will be used in combination with electrochemical techniques as well as under irradiation with light to study charge transfer processes with time resolution down to 10 ns. In a first step the setup for these experiments needs to be developed. This setup relies on our experiences with other spectroelectrochemical techniques and will focus on the development of the FT-ESR techniques. In a second step the photosensitizer and catalyst will be studied independently as well as in the conductive polymer with the established techniques. This is a challenging project at the cross section of spectroscopy, electrochemistry and photophysics and is nested within our collaboration network comprising of experts from these fields as well as theoretical chemistry.

The successful applicant thus has a strong background in spectroscopy and preferably has already worked with ESR spectroscopy. The applicant is highly motivated to advance her/his skills in the field of catalysis, electrochemistry and photophysics. We are an international team, thus fluent English in spoken and written is mandatory.

We offer an inspiring working atmosphere in an international team under direct supervision by our experienced scientific staff. The project benefits from state-of-the art spectroscopy and electrochemistry labs and equipment as well as next door collaborations.

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Enhanced Generation of Multiple Excitons in Semiconductor Heteronanostructures

To secure a sufficient and sustainable energy supply for the growing world population solar energy is going to play a decisive role. Solar-driven catalytic approaches, e.g. splitting of water into hydrogen and oxygen, are potential sources of clean and renewable fuel. However, this reaction involving multiple charge transfer steps has been proven to be highly challenging and only the separate half reactions have been realized by now. Promising systems for light driven proton reduction combine colloidal semiconductor nanostructures as light harvesting unit with metal particles or molecular reaction centers for proton reduction. One critical step limiting efficiency in such systems is recombination of charges before sufficient charge is accumulated at the reaction center. By generating multiple excitations in the light harvesting unit quasi simultaneously and simultaneous transfer of multiple charge carriers, the recombination could be suppressed.

The goal of the proposed work is to investigate the generation of multiple excitons in colloidal semiconductor nanostructures and explore whether multi-electron reactions can be driven more efficiently via this process. Two strategies will be explored to generate multiple excitons:

1) Multiple exciton generation (MEG) upon excitation with radiation of energy of at least twice the band gap E_g generates several excitons from only one photon. If these excitations can be transferred into several charge carriers before relaxation to the band edge, this can lead to an increase in the efficiency of light-harvesting applications, since the energy of higher energy photons is not lost in large part in the form of heat, and the Shockley-Queisser limit can be overcome. MEG plays a significant role in macroscopic semiconductors only at very high photon energies (E >> 2Eg). Competing processes, i.e. charge carrier cooling and Auger recombination (AR) dominate in bulk materials. In colloidal semiconductor nanocrystals in the quantum confinement regime, however, an amplified MEG was observed at much lower photon energies near the threshold 2Eg. Especially segmented heterostructures of quasi-type II have been predicted by theory to show efficient MEG, which will be in the focus of the project.

2) Multiple excitons can also be generated by quasi simultaneous absorption of several photons. The high light intensities (high fields) necessary for this process are not achievable under ambient light conditions, but applying the concept of plasmonic field enhancement absorption of light and hence generation of multiple excitons can be enhanced. For this purpose, we will couple the colloidal semiconductor nanostructures with Au or Ag with a localized surface plasmon resonance (LSPR) band in resonance with the excitonic transitions of the semiconductor nanoparticle. The metal particles will be isolated from the semiconductor to prevent energy and charge transfer by an insulating shell, e.g. a SiO_2 or Al_2O_3.

For both approaches the factors which determine the efficiency of the MEG process and the dynamics of with charge transfer to acceptors competing AR will be studied. The dynamics of multiple excitons in semiconductor heterostructures of quasi type II and the relation between structural parameters and the efficiency of MEG will be investigated by means of time-resolved spectroscopic methods, i.e. photoluminescence and transient absorption spectroscopy. One of the initial challenges will be to study the interactions between the excitons localized in different parts of the heterostructures by developing a pump-pump-probe scheme with variation in intensity of pump for different areas of the structure. Spectral signatures identified as indicators for the generation of multiple excitons will be used to evaluate the generation of multiple excitons via plasmon enhanced absorption. Promising structures will be finally coupled with model reaction centers for hydrogen generation and the enhancement of catalyst performance will be evaluated.

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PhD Project: Fiber spectroscopic gas sensing

Keywords: Optical spectroscopy, Photonics, Raman spectroscopy, fiber sensing, gas sensing, environmental monitoring, medical technology

The research group “fiber spectroscopic sensing” from Torsten Frosch at the Leibniz Institute of Photonic Technology in Jena offers a topic for a PhD position for:

Fiber spectroscopic gas sensing

In this project, novel fiber optical setups for Raman spectroscopy will be developed and applied for sensitive analysis of biogenic gases. Different micro-structured optical fibers, optical cavities, and spectroscopic systems will be designed, built up, and evaluated for sensitivity, selectivity, versatility, and robustness. A main aim of Raman gas sensing is monitoring of climate relevant processes to contribute to a better understanding on a local scale and element budgets.

Your Qualification:

- Master degree in physics, photonics, engineering, physical chemistry, analytical chemistry, or related discipline.

Experiences and Interests:

- Experimental and technical skills and interest in developing optical setups
- Knowledge in Raman spectroscopy, analytical techniques, and gas sensing would be helpful
- Interest in interdisciplinary work
- Scientific ambition and high motivation

We offer:

- Excellent scientific environment with attractive interdisciplinary collaborations
- Excellent instrumentation and equipment
- Young, dynamic, interdisciplinary team
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Quantum Chemistry and Dynamics of Photophysical and Photochemical Processes in Photocatalytic Molecular H_2 Generation

Photocatalytic water-splitting is of tremendous importance as it offers the opportunity to contribute to our future sustainable supply of renewable energy. In the last years, promising molecular photocatalysts have been synthesized. Intermolecular homogeneous photocatalysts for proton reduction are often based on a design combining a photosensitizer (electron donor), an intramolecular bridge (electron accumulator), and the catalytically active center (electron acceptor). However, significant obstacles need to be overcome for practical applications due to our limited knowledge – our current understanding is mainly limited to the first electron transfer, while the generation of molecular H_2 necessitates the involvement of two electrons. Thus, it is of uttermost importance to investigate the photophysical and photochemical processes following light absorption, which ultimately determine the functionality and efficiency of these molecular photocatalysts.

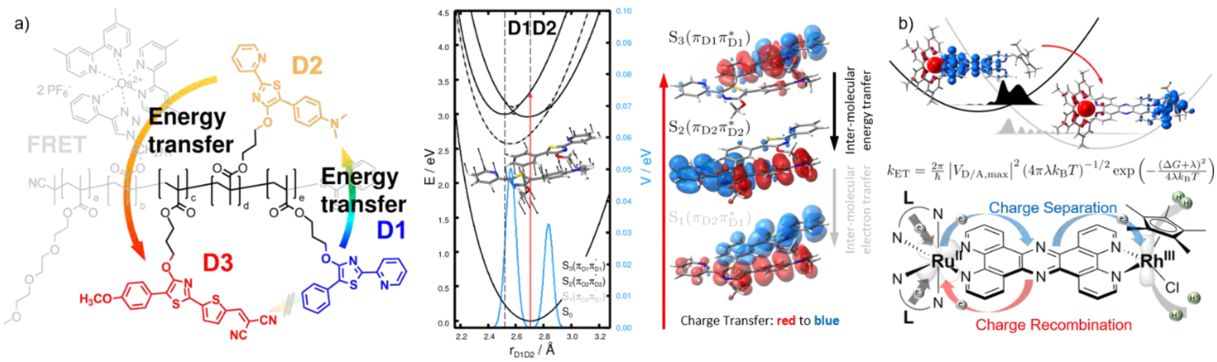

Figure 1: Computationally investigated, a), photo-induced energy transfer dynamics in a hierarchical light-harvesting antenna[1] and, b), competitive light-driven electron transfer processes leading to charge separation vs. charge recombination in hydrogen-evolving photocatalysts. [1,2]

This PhD project aims at investigating light-induced processes in molecular catalysts from a theoretical point of view. Quantum chemical and dynamical approaches will be employed to investigate the fundamental mechanisms of charge and energy transfer as well as photocatalytic activity of transition metal complexes, with a focus on Ru(II) or Cu(I) photocenters. The theoretical studies will be performed in close collaboration with our long-term experimental colleagues from physical chemistry who employ spectroscopic techniques to elucidate the light-induced processes of such photocatalysts.

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Quantum Chemical and Dynamical Investigation of the Photochemistry of Photoactive Drugs

Modern research on the photophysics and –chemistry of transition metal complexes involves the investigation of these systems as photoactive drugs, as several of these complexes feature anti-tumor or anti-inflammatory activity. On the molecular scale, these transition metal complexes possess weakly bounding ligands, such as e.g. NO or CO ligands, which are released upon light irradiation. NO and CO thereby serve as anti-inflammatory agent. Other photo agents are designed to coordinate to the DNA and form adducts, which inflicts a high toxicity of the tumor cell, which is known as photo dynamic therapy.

For the design and possible application of novel transition metal-based photoactive drugs, it is important to understand their photophysics on a molecular scale. It is thus necessary to investigate the excited state structure and the electronic structure of the complex leading to ligand dissociation (NO or CO). In particular, it is of vital importance to investigate how does the particular local environment influence the structure and dynamics.

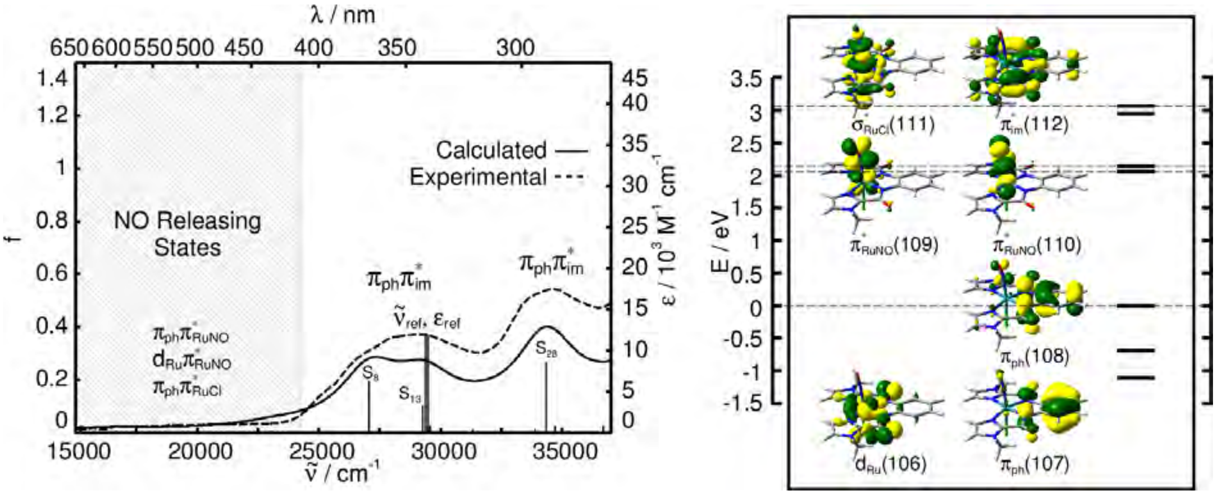

Figure 1: Results of quantum chemical calculations on a Ru(II) complex leading to photo-induced release of NO.

This PhD project aims at investigating the excited state structure and dynamics of a specific class of Ru(II)/Mn(I)-based photoactive drugs as a function of their (biological) environment using quantum chemical methods. This requires taking the local environment explicitly into account using a QM/MM approach (Nobel prize 2015) rather than using the more common continuum model for the environment. The theoretical investigations will be performed in close collaboration with our long-term experimental colleagues from physical chemistry who employ spectroscopic techniques to investigate the light-induced processes of these photo-active drugs.

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Quantum Dynamical Modelling of Photoelectron-Circular Dichroism

Chirality plays a key role in the functionality of biological, chemical, pharmaceutical and physical systems. The molecules constituting the basis of life, such as amino acids and sugars, are chiral. Chiral molecules are such molecules, which cannot be superimposed with their mirror image, thus containing at least one atom (in most cases a carbon atom) where all chemical bonds connect to different atoms or fragments: the chemical surrounding of such a chiral center is asymmetric. Chiral media are optically active - they rotate the polarization plane of linear polarized light propagating through the medium and feature a small difference in the absorption of left- and right-circularly polarized light (circular dichroism, CD), which enables a spectroscopic characterization of chiral molecules. The difference in absorption, however, is very small. Another method spectroscopically characterizing chiral systems is photoelectron circular dichroism (PECD) and multi-photon PECD, a relatively new method with high sensitivity of two till three orders of magnitudes higher than that of circular dichroism.

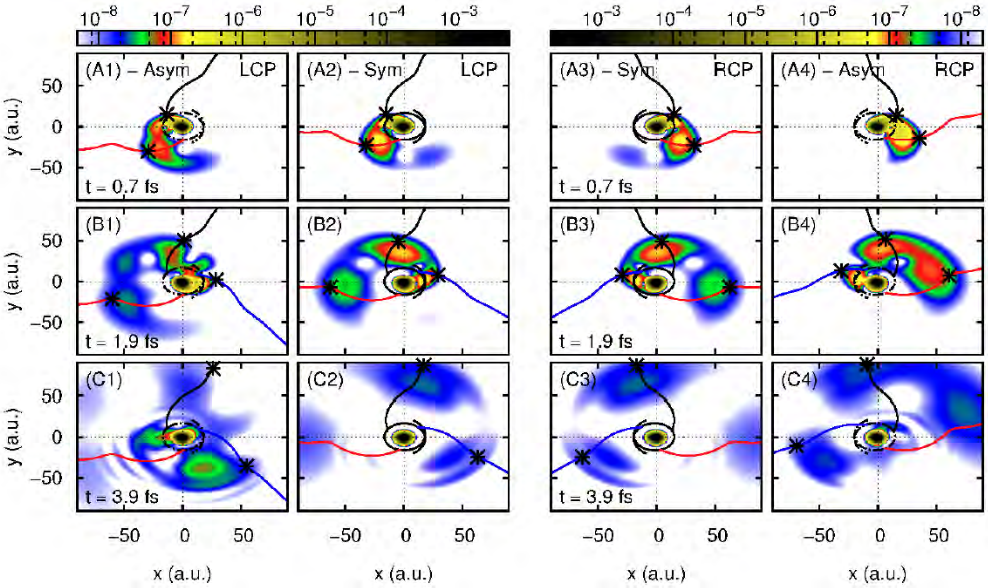

Figure 1 Snapshots of the electron density, comparing asymmetric and symmetric potentials. Left panels: ionization with left-circularly polarized pulses; right panels: corresponding ionization dynamics with right circularly polarized fields. The difference gives rise to the PECD effect.

Together with our experimental collaborators from Oldenburg (Germany) and Vienna (Austria), we aim at extracting the basic molecular properties leading to the asymmetric response, and thus to PECD, by directly comparing chiral and non-chiral molecules. In this PhD project, we will employ the real-time real-space time-dependent density functional theory (RT-TDDFT) to simulate small molecules, which are experimentally examined by our collaboration partners. We will focus on small, chiral molecules such as oxiranes, to allow a full quantum chemically description. Special attention will be paid to investigate (i) the possibility of transient chirality, thus involving not only the electronic dynamics but also vibrational dynamics and (ii) the influence of asymmetric laser fields on these systems.

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Improved Implementation and Parallelization of MACGIC-iQUAPI

Despite the immense growth of computational resources in the last decades, the dynamics of dissipative quantum systems still presents a challenge for systems of biological relevance that typically include dozens of coupled exciton and charge transfer states. Moreover, the 'sluggish' protein environment imposes non-Markovian system-bath memory times of substantial length. A promising approach to solve the dynamics of extended quantum systems in a numerical exact fashion is the recently developed MACGIC-iQUAPI method [1]. It is based on the quasi-adiabatic propagator path integral method (QUAPI) but extends its applicability to systems with many states coupled to environments with long correlation times by mask-assisted coarse graining of Feynman-Vernon influence coefficients (MACGIC).

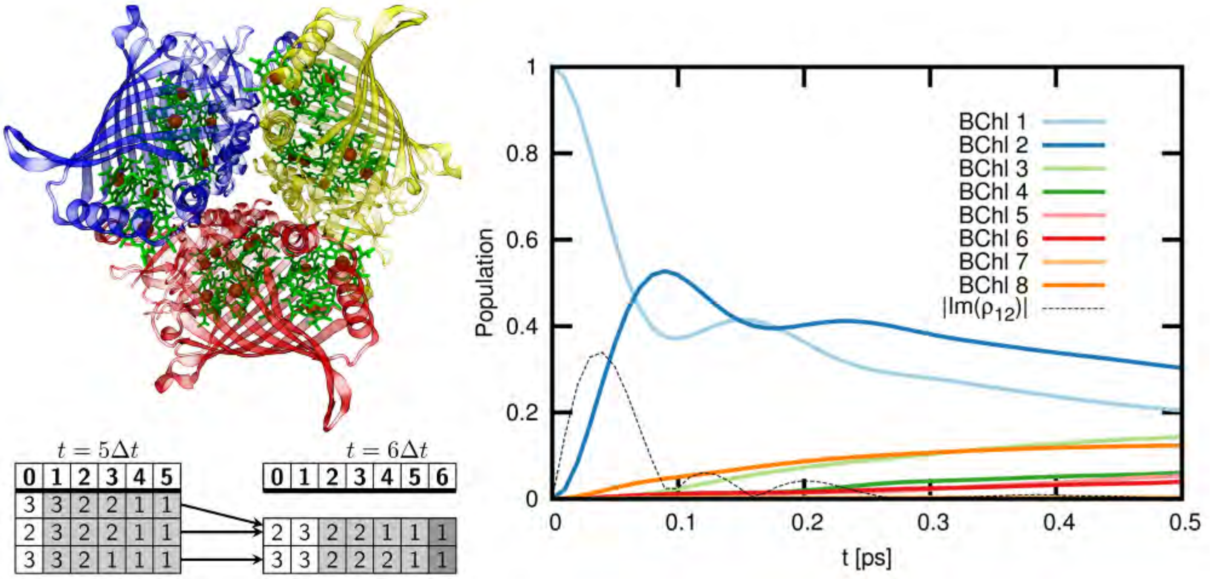

Figure 1 Simplified Scheme of path-merging in QUAPI applied to simulate the exciton dynamics of the Fenna-Matthews-Olson complex.

The aim of this PhD project is twofold. The first goal is to improve the numerical efficiency of MACGIC-iQUAPI. A task will be inter-node parallelization on modern HPC hardware as well as methodological improvements of the mask selection procedure using machine-learning algorithms. Therefore, a strong background in programming of the applicant is mandatory. The second goal is the application of MACGIC-iQUAPI to numerous model systems including complex shaped spectral densities and comparison to various approximate and exact established methods such as Marcus, Förster and Redfield theory or hierarchical equations of motion. The project will be conducted in close collaboration with our partners from Berlin.

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PhD-Workshop China 2019

Lieber Herr Dr. Schwarzkopf,

ich darf mich auf Ihre Email beziehen und Ihnen mitteilen, dass ich großes Interesse habe, CSC-Stipendiatinnen und -Stipendiaten in meiner Gruppe aufzunehmen. Wie ich Ihnen schon mitgeteilt habe, arbeitet derzeit eine CSC-Stipendiatin schon bei mir als Doktorandin und ich bin mit Ihrer Leistungen sehr zufrieden.

Ich darf kurz unsere Themen vorstellen:

Research Interests:

1. Bioinorganic/Bioorganometallic chemistry: [FeFe]-hydrogenases mimics and light driven organometallic reactions (hydrogen production)
2. Metal complexes for anticancer therapy.
3. Coordination chemistry with reactive chalcogen-containing ligands.
4. Prebiotic chemistry, Synthetic Cells.

ad 1. Bioinorganic/Bioorganometallic chemistry: [FeFe]-hydrogenases mimics and light driven organometallic reactions (hydrogen production):

Here we are dealing with the synthesis of [FeFe]-hydrogenase model complexes, which are mimicking the structure and the functions of these enzymes. Hydrogen is considered one of the best environmentally benign alternatives “Green Alternatives” compared to the presently used fossil fuel due to its high energy density and its clean cold combustion product in fuel cells. In fact, the nature has high ability to catalyse the reversible process of proton reduction with high catalytic efficiency (ca. 10^4 turnover per s) and this occurs through enzymes known as [FeFe]-hydrogenases. The active site of the latter contains an organometallic cluster, the so called H cluster, which consists of an [Fe4S4] cluster attached through a cysteinyl residue to a butterfly [Fe2S2] sub-cluster. This sub-cluster contains a bridging azadithiolato ligand (adt = $[SCH_2NHCH_2S]$) as well as biologically unusual CO and CN^- ligands. Over the past few decades, numerous synthetic models which mimic the H cluster with the general formula $[Fe_2(CO)_6\{\mu\text{-}(SCH_2)_2E\}]$, in which the central atom/group E is NR, CR_2, O, S, Se, SiR_2, Ge, Sn or PhP=O have been reported in order to provide a better understanding of the structure and function of the active site of the enzyme-mimic models. Moreover, these models have been extended to diiron complexes containing diselenato and ditellurato ligands (Fig. 1).

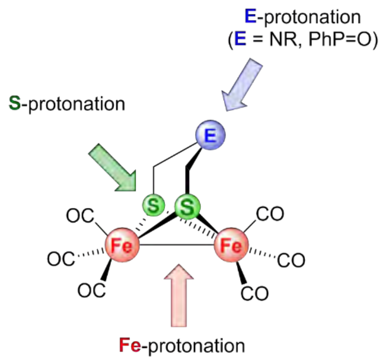

Figure 1. Possible sites for protonation in $[Fe_2(CO)_6\{\mu\text{-}(SCH_2)_2E\}]$ complexes.

Photo(electro)catalytic water cleavage represents an innovative and one of the most direct approaches to store solar energy in chemical bonds, *i.e.*, to convert light into a storable fuel. The yet unsolved problems of water cleavage comprise for example the missing absorption of water in the visible regime of the solar spectrum and the high energy content of the breakable bonds. Most molecular systems so far developed for photocatalytic water cleavage contain complicated catalytic transition and noble metal complexes. In this respect, noble metal free molecular photocatalysts, which can be driven by visible light, are highly desirable for full water cleavage or at least one half-reaction, such as hydrogen or oxygen evolution.

A typical photocatalyst for H_2 evolution consists of a photosensitizer and a $[Fe_2S_2]$ subunit mimic as the catalyst as well as the sacrificial electron donor. The photosensitizer harvests light to generate an excited state interacting with the $[Fe_2S_2]$ moiety, which will be reduced twice by electrons to $[Fe^0Fe^0]$-hydrogenase species delivered by the sacrificial electron donor followed by double protonation with final H_2 release (HER).

In order to use solar energy efficiently for water cleavage or one of the half-reactions as a long term goal, sensitizers which absorb in the visible region of the sun light should be developed and implemented to the photocatalytic system. We will address this problem by providing a viable synthetic pathway towards noble metal-free $[Fe_2S_2]$ hydrogenase subunit mimics comprising covalently linked photosensitizers based on oligothiophenes which strongly absorb in the visible and shall be directly embedded into the bridging dithiolate unit of the central iron subunit. Oligothiophenes are ideal candidates as sensitizers, because a wide variation of the molecular structure is possible, which is important in order to adjust absorption and additionally the redox levels, which decisively influence electron transfer (Fig. 2)

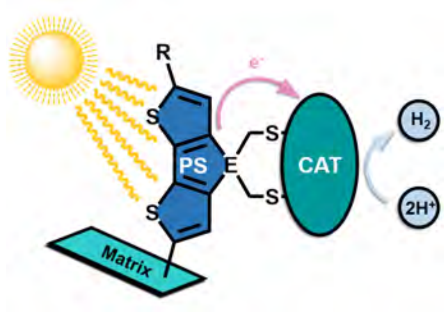

Figure 2. Molecularly defined PS-CAT dyads for HER

ad 2. Platin(IV) prodrugs with sulfur containg ligands: Antitumor active compounds

Pt(IV) prodrugs are an interesting alternative to their Pt(II) homologs. In contrast to the square-planar Pt(II) compopunds, Pt(IV) complexes exhibit octahedral structures. The low spin d^6 Pt(IV) centre is coordinatively saturated and thus more resistant to ligand substitution as compared to the four-coordinate Pt(II) core. This is advantageous as it limits the interactions of the Pt(IV) prodrug with biomolecules prior to reaching its desired target, thus reducing unwanted side reactions and associated side-effects. In addition, only upon entry into the more reducing environment of tumor cells will the prodrug be activated *via* a 2-electron reduction in the presence of reducing agents, resulting in the formation of their Pt(II) cytotoxic species to bind DNA and with concomitant release of their axial ligands. Moreover, the presence of two axial ligands provides a means to further enhance the biological profile of the resulting Pt(IV) prodrug – e.g. the prodrug can be fine-tuned to increase cellular uptake or improve tumor cell targeting or indeed further enhance its cytotoxicity by incorporating additional moieties which in their own right have anti-proliferative properties which will support and potentiate the activity of the Pt(II) drug. These bifunctional (concept of dual action) Pt(IV) derivatives, where one or two synergistic drug molecules are conjugated to the octahedral Pt(IV) complexes in the axial positions, represent an efficient tool to realize such a combination therapy.

In a doctoral thesis we will combine Pt(IV) prodrugs with sulfur ligands to isolate these above mentioned bifunctional Pt(IV) systems. Some sulfur ligands are naturally occurring compound, which are essential for energy production in cells. There is some evidence for the protective effect of sulfur ligands in cases such as rheumatoid arthritis, lyme disease, diabetes mellitus, and vascular and neurodegenerative diseases andage-related conditions in which free radicals are involved.

ad 3. Coordination and organometallic chemistry of these reactive thioketones

In recent years, aromatic and cycloaliphatic thioketones were shown as useful reagents for the preparation of sulfur heterocycles with variable ring-size as well as diverse metal complexes, *e.g.* three-membered platinathiiranes. The (3+2)- and (4+2)-cycloadditions with thioketones are of special importance. It has been demonstrated, that they react as ‘superdipolarophilic’ agents with such 1,3-dipoles as diazomethanes, thiocarbonyl *S*-methanides, nitrones, and nitrile imines. Moreover, reactions of hetaryl thioketones with diazomethanes and thiocarbonyl *S*-methanides were shown to occur *via* non-classical, step-wise diradical mechanisms. In the case of (4+2)-cycloadditions (thia-Diels-Alder reactions) aryl and hetaryl thioketones can be used either as heterodienophiles yielding 2*H*-thiapyrane derivatives or as heterodienes (thia-buta-1,3-dienes) forming polycyclic sulfur heterocycles, respectively. Thia-Diels-Alder reactions with aryl and hetaryl thioketones and in situ generated trienamines were also described. In this project the coordination and organometallic chemistry of these reactive thioketones will be investigated.

ad 4. Prebiotic chemistry: The “Iron-Sulfur-World”

According to Wächtershäuser’s “Iron-Sulfur-World” one major requirement for the development of life on the prebiotic Earth is compartmentalization. Vesicles spontaneously formed from amphiphilic components containing a specific set of molecules including sulfide minerals may have led to the first autotrophic prebiotic units. The iron sulfide minerals may have been formed by geological conversions in the environment of deep-sea volcanos (hydrothermal vents), which can be observed even today. Wächtershäuser postulated the evolution of chemical pathways as fundamentals of the origin of life on earth. In contrast to the classical Miller-Urey experiment, depending on external energy sources, the “Iron-Sulfur-World” is based on the catalytic and energy reproducing redox system $FeS + H_2S \rightarrow FeS_2 + H_2$. The energy release out of this redox reaction ($\Delta_R G°$ = -38 kJ / mol, pH 0) could be the cause for the subsequent synthesis of complex organic molecules and the precondition for the development of more complex units similar to cells known today.

CSC PhD thesis project (Life Science or Information Technology, full programme): Applying machine learning techniques to derive treatment rules from clinical data

Keywords: machine learning, decision trees, propensity scoring, theranostics, treatment suggestion, clinical data

Scope: Community acquired pneumonia (CAP) is a severe health burden. If not treated early and appropriate, CAP is often followed by severe clinical complications and even sepsis,. Besides this, clinical data is collected by technicians/study nurses guided by experts and physicians leading to valuable data base resources. However, often these experts lack profound machine learning background making it necessary to join forces with bioinformaticians and data scientists.

We are collaborating with physicians from the Institute of Infectious Diseases and Infection Control at our clinical center. We have access to the database CAPNETZ (*1*) containing all aspects for treatment of CAP including comorbidities, risk factors, clinical check-up results, historical and clinical therapeutic management, pathogen spectrum and resistance, follow-up. In the meanwhile, the database contains data from about 12,000 patients from 5 countries with comparable standards of health care (Germany, Switzerland, The Netherlands, Austria, and Denmark). As a perspective, we will also use data from other competence networks such as from the CAP North network. Until now, we were already very successful in finding a decision rule for macrolide treatment (*2*). Macrolides are a very effective antibiotics group. However, they have also a lot of side effects. Hence, intelligent sub group partitioning of patients is mandatory addressing this tradeoff.

In the planned project we will develop means to find more complex rules for the same task based on e.g. random forests, Support Vector Machines, neural networks. Furthermore, we want to systematically broaden the application of more antibiotics groups, such as fluoroquinolones, in combination with beta lactams and macrolides.

Your profile: If you are interested in clinical data analysis, in systematically detecting functional patterns in complex data and machine learning, have a degree in bioinformatics, biology, the medical sciences, bioengineering, data science or related subjects, and you have a good working knowledge in English, we are looking forward to your application.

Jena University Hospital: Being the largest employer in the region, our around 5,000 employees working in 26 departments and clinics provide ambulatory care for around 280,000 patients and inpatient treatment for more than 55,000 patients each year. In addition, 2,300 students of medicine and dentistry are trained, and in 25 institutes, scientists from more than 25 nations do research to advance medicine. PhD students at Jena University Hospital can benefit from a wide range of offers that encourage individual health promotion at work.

The group: We are a team of a couple of PhD-students, several postdocs, varying undergraduates and the group leader. We can host you as a PhD student holding a CSC grant or other grant. Please apply for this project via email to Prof. Dr. Rainer Koenig: rainer.koenig@uni-jena.de. In case of equal qualification, persons with disabilities will be given priority.

Prof. Dr. Rainer König, Jena University Hospital, Germany

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CSC PhD thesis project (Life Science, full programme): Reprogramming of macrophages employing gene regulatory networks

Keywords: bioinformatics, immune system, macrophages, reprogramming, machine learning

Scope: Immune cells, and in particular macrophages get activated into different kinds of polarizations. This can cause fatal dysfunction in a large range of diseases such the inflammatory overflow after systemic infection leading to sepsis or, in turn induce tolerance after the acute phase of sepsis and of macrophages in the tumor micro environment. The transcriptional regulation on macrophage function, and particular its involvement in metabolism is central for these pathomechanisms but incompletely understood.

Method: We investigate transcriptomics, protein/cytokine and metabolomics data to develop gene regulatory and metabolic networks. We want to identify the central regulators of the metabolic switch during their polarization. We aim to manipulate the cells and to reprogram them into the opposing polarization state. We employ constraint based modelling approaches [1] and own developments. To infer gene regulatory networks, we already developed a very efficient method that uses gene expression profiles of the investigated cellular context and ChIP binding information from several databases [2-4]. For pattern analysis, we employ machine learning methods [5], statistics, network analysis methods [6] aiming to determine polarization specific regulation and to identify specific regulators, such as transcription factors and miRNA for reprogramming the cells and to suggest treatment. Experimental validations can be performed by own people in the lab and cooperation partners in the German Cancer Research Center (DKFZ).

Your profile: If you are interested in the immune system, in systematically detecting functional patterns in networks or machine learning, have a degree in bioinformatics, biology, the medical sciences, bioengineering or related subjects, and you have a good working knowledge in English, we are looking forward to your application.

Jena University Hospital: Being the largest employer in the region, our around 5,000 employees working in 26 departments and clinics provide ambulatory care for around 280,000 patients and inpatient treatment for more than 55,000 patients each year. In addition, 2,300 students of medicine and dentistry are trained, and in 25 institutes, scientists from more than 25 nations do research to advance medicine. PhD students at Jena University Hospital can benefit from a wide range of offers that encourage individual health promotion at work.

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Genetically encoded voltage indicators for studying cell proliferation

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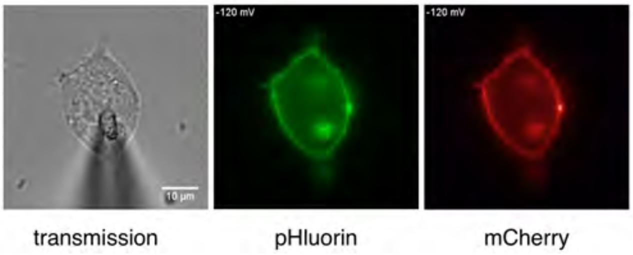
Keywords:
Molecular Physiology, Patch Clamp, Electrical Signaling, Fluorescence, Cancer

The electrical cell membrane potential is an important characteristic of the cell's state because it determines numerous physiological processes, such as electrical signaling as well as electrogenic import and export of molecules. It is even speculated that promotion of the cell cycle, i.e. the process leading to cell division, also requires a paradigmatic sequence of cell potential changes. This, however, has never been demonstrated directly because classical electrical experiments with cells are invasive and do not allow the assessment of very many cells. For the quantitative evaluation of, for example, cancer cells in culture, one would need to observe thousands of cells over a long period of time under cell culture conditions – a task not feasible with state-of-the-art electrophysiological methods.



(left) Transmission image of a HEK293 cell with an attached patch-clamp pipette in the whole-cell mode. (center, right) Florescence images illustrating the voltage-dependent green and the voltage-independent red fluorescence of the GEVI, here held at -120 mV.

We have therefore developed various fluorescent proteins that harbor transmembrane voltage-sensing protein moieties and that function as ratiometric genetically encoded voltage indicators (GEVIs). Using such fluorescent proteins and various modern methods of cell biology and biochemistry, including fluorescence microscopy, image analysis, FACS analysis, electrophysiology, and molecular biological manipulations of cancer cells, the PhD candidate will work on a project to address the following major aims:

(A) Develop and optimize ratiometric GEVI readout on an automated fluorescence microscope.
(B) Study the development of membrane potential during the cell cycle for various cancer cell types.
(C) Establish automated GEVI readout as a versatile tool for cell biological research and pharmacological applications.

The PhD candidate will be integrated into an active research environment, will receive coordinated PhD training, and has the chance to make major contributions to the understanding of how electrical cell membrane potential changes contribute to cell proliferation and, hence, how cancer cells might be targeted addressing this particular aspect.

Teaching and scientific conversation in the laboratory will be in English.

There is a close collaboration with the Shanghai Jiao Tong University, School of Medicine.

Cell signaling by intracellular labile heme

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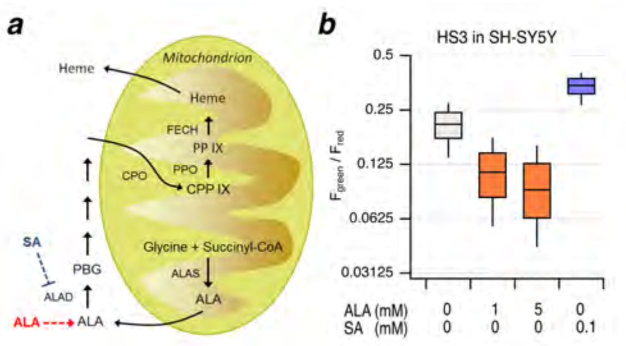
Keywords:
Molecular Cell Biology, Cell Signaling, Heme, Fluorescence, Porphyria

Meanwhile it is well established that heme is not only a tightly bound prosthetic group in proteins such as hemoglobin or cytochromes; it can also function as signaling molecule under physiological conditions and can exert adverse effects when present in excess. In this context several important knowledge gaps remain. Besides the requirements to understand the molecular mechanisms of heme-protein interactions via heme-regulatory motifs (i.e. with binding constants in the higher nanomolar range leading to cellularly available or "labile" heme), it is not clear how heme gradients over the plasma membrane are established or maintained. For example, it is by no means trivial to predict the concentration of biochemically active heme in the extracellular space following an insult of hemolysis, nor do we know the impact of elevated extracellular or intracellular heme levels on the physiological function of membrane proteins and intracellular signaling. The lack of detailed information is largely associated with insufficient experimental means of measuring and controlling the intracellular heme level.



a) Heme synthesis pathway highlighting experimental points of intervention by blocking (SA) or promoting (ALA) heme synthesis. b) FACS analysis of neuronal cell expressing a fluorescent heme sensor indicating the dependence of labile heme on SA and ALA.

However, we have successfully developed fluorescence proteins that are suited to monitor free intracellular heme in a ratiometric, i. e. quantitative manner (see Figure). Using these tools and various cell biological and biochemical methods, the PhD candidate will work on a project to address the following major aims:

(A) What are the molecular mechanisms linking the HO-1/Keap1/Nrf2 stress axis to an imbalance of intracellular heme?
(B) How do potential heme transporters affect heme redistribution and function of human cells?
(C) Optimize and automate measurements of free extracellular and intracellular heme levels.

The PhD candidate will be integrated into an active research environment, will receive coordinated PhD training, and has the chance to make major contributions to the understanding of how the indispensable cell stressor heme affects cell function and how it contributes to human disease conditions.

Teaching and scientific conversation in the laboratory will be in English.

There is a close collaboration with the Shanghai Jiao Tong University, School of Medicine.


Research Position in MR Spectroscopy / Neuroimaging

The Medical Physics Group at the Jena University Hospital invites applications for a research scientist position in the field of MR spectroscopy and (functional) MRI.

As part of an interdisciplinary project between the Medical Physics Group and the Department of Psychiatry and Psychotherapy, modulating effects of emotion-regulating psychotherapy on brain function and functional circuits, especially in fronto-limbic networks, are investigated by MR spectroscopy (MRS) and functional MRI methods to study neurotransmitter metabolism and functional connectivity.

The research is carried out in a cooperative and highly interdisciplinary working environment with many opportunities for independent scientific work. Candidates should have a keen interest in MRS and fMRI. A degree in (medical) physics, biomedical engineering, biophysics, computer science, neuroscience, or a related discipline *with a strong background in magnetic resonance imaging and explicit prior experience in MRS* is preferred.

The successful candidate should have preferably experience and considerable interest in

- Hands-on experience of spectroscopic and imaging data acquisition
- Reconstruction and processing of MRS data, data post-processing and analysis
- Expertise in MATLAB, FSL, and FreeSurfer
- Clinical studies in neuroscience/psychiatry
- Strong written and oral English communication skills

Experience in pulse sequence programming with IDEA would be an added bonus. MRI measurements will be conducted on a state-of-the-art, whole-body 3T MRI system (Prisma Fit, Siemens Healthineers) dedicated exclusively to research.

Jena University Hospital https://www.uniklinikum-jena.de/en/) is an equal opportunity employer. Women, minorities and individuals with disabilities are encouraged to apply. More information about the Medical Physics Group can be found on https://www.uniklinikum-jena.de/idir/Arbeitsgruppen+im+IDIR/AG+Medizinische+Physik.html

Applications should include a letter of interest, a curriculum vitae, a list of publications, a list of grants if applicable, a summary of past research experience and future research interests (max 2 pages); PhD, Bachelor/Master and High School certificates and respective transcripts; PDF copy of most recent thesis or 3 most important papers and three references (contact details only).

All materials should be sent **electronically as a single PDF** file to Prof. Jürgen R. Reichenbach, Head of Medical Physics Group, Department of Diagnostic and Interventional Radiology, Jena University Hospital, Germany, juergen.reichenbach@med.uni-jena.de.


Research Position (PhD) in Musculoskeletal Magnetic Resonance Imaging (MRI)

The Medical Physics Group at the Jena University Hospital invites applications for a research scientist (PhD) in the field of musculoskeletal magnetic resonance imaging (MRI).

As part of an interdisciplinary project between the Medical Physics Group and the Research Group of Motor Skills, Pathophysiology and Biomechanics, morphofunctional parameters of back muscles will be determined from MRI image data sets in volunteers and will be correlated with electrophysiological parameters (surface electromyography, EMG). Within the project, MRI techniques will be developed and applied to perform high spatial resolution tissue segmentation (e.g., muscle, fat, ligaments, connective tissue, and bone). The program includes 3D ultra-short-time (UTE) MRI methods for quantifying longitudinal and effective transverse relaxation time constants (T_1 and T_2*) by dynamic detection of echo time and flip angle series.

The research is carried out in a cooperative and highly interdisciplinary working environment with many opportunities for independent scientific work. Candidates should have a keen interest in MRI. A degree in (medical) physics, biomedical engineering, biophysics, computer science, or a related discipline *with a strong background in magnetic resonance imaging and explicit prior experience in MRI* is preferred.

The successful candidate should have preferably experience and considerable interest in

- Hands-on experience of imaging data acquisition
- Sequence programming
- Reconstruction and processing of MRI data, data post-processing and analysis
- Expertise in MATLAB
- Strong written and oral English communication skills

Experience in pulse sequence programming with IDEA would be an added bonus. MRI measurements will be conducted on a state-of-the-art, whole-body 3T MRI system (Prisma Fit, Siemens Healthineers) dedicated exclusively to research.

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Research Position (PhD) in Musculoskeletal Magnetic Resonance Spectroscopy (MRS)

The Medical Physics Group at the Jena University Hospital invites applications for a research scientist (PhD) in the field of musculoskeletal magnetic resonance spectroscopy (MRS).

As part of an ongoing project, exercise-induced lactate changes in human muscle will be quantified *in vivo* by implementing an improved measurement volume selection using adiabatic refocusing pulses (sLASER method) into an existing lipid-nulling spectroscopic sequence. The sequence will be used in in vivo measurements of the calf muscles of a group of healthy volunteers to directly examine local dynamic lactate changes in the loaded muscle, which provides valuable insight into the anaerobic metabolism in muscles.

The research is carried out in a cooperative and highly interdisciplinary working environment with many opportunities for independent scientific work. Candidates should have a keen interest in MRI/MRS and muscle physiology. A degree in (medical) physics, biomedical engineering, biophysics, computer science, or a related discipline *with a strong background in magnetic resonance imaging and explicit prior experience in MRS* is preferred.

The successful candidate should have preferably experience and considerable interest in

- Hands-on experience of spectroscopic and imaging data acquisition
- Sequence programming
- Reconstruction and processing of MRI data, data post-processing and analysis
- Expertise in MATLAB
- Strong written and oral English communication skills

Experience in pulse sequence programming with IDEA would be an added bonus. MRI measurements will be conducted on a state-of-the-art, whole-body 3T MRI system (Prisma Fit, Siemens Healthineers) dedicated exclusively to research and equipped with the necessary coils. In addition, the Sequence Development Environment (IDEA) with pre-built source code from the manufacturer is available.

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FRIEDRICH-SCHILLER-UNIVERSITÄT JENA

UNIVERSITÄTSKLINIKUM jena

Research Position (PhD) in Quantitative Susceptibility Mapping

The Medical Physics Group at the Jena University Hospital invites applications for a research scientist (PhD) in the field of quantitative susceptibility mapping.

Quantitative susceptibility mapping (QSM) is the most recent technique to assess magnetic susceptibility of tissue in absolute terms. QSM has become possible by new approaches for solving the challenging inverse source problem to derive the underlying susceptibility distribution from the magnetic field perturbations. The main tasks for the candidate in this project encompass implementation and testing of QSM mapping techniques, development of programs for image reconstruction and calculations of parameter maps as well as development of image processing pipelines to apply these tools to clinical MRI data of patients with neurodegenerative diseases.

The research is carried out in a cooperative and highly interdisciplinary working environment with many opportunities for independent scientific work. Candidates should have a keen interest in MRI and mathematical problem solving in relation to QSM. A degree in (medical) physics, biomedical engineering, computer science, applied mathematics, or a related discipline *with a strong background in magnetic resonance imaging, explicit prior experience in MRI and a strong mathematical background* is preferred.

The successful candidate should have preferably experience and considerable interest in

- Hands-on experience of MRI data acquisition
- Ill-posed inverse problems and their solutions
- Reconstruction and processing of MRI data, data post-processing and analysis
- Expertise in MATLAB
- Strong written and oral English communication skills

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All materials should be sent **electronically as a single PDF** file to Prof. Jürgen R. Reichenbach, Head of Medical Physics Group, Department of Diagnostic and Interventional Radiology, Jena University Hospital, Germany, juergen.reichenbach@med.uni-jena.de.