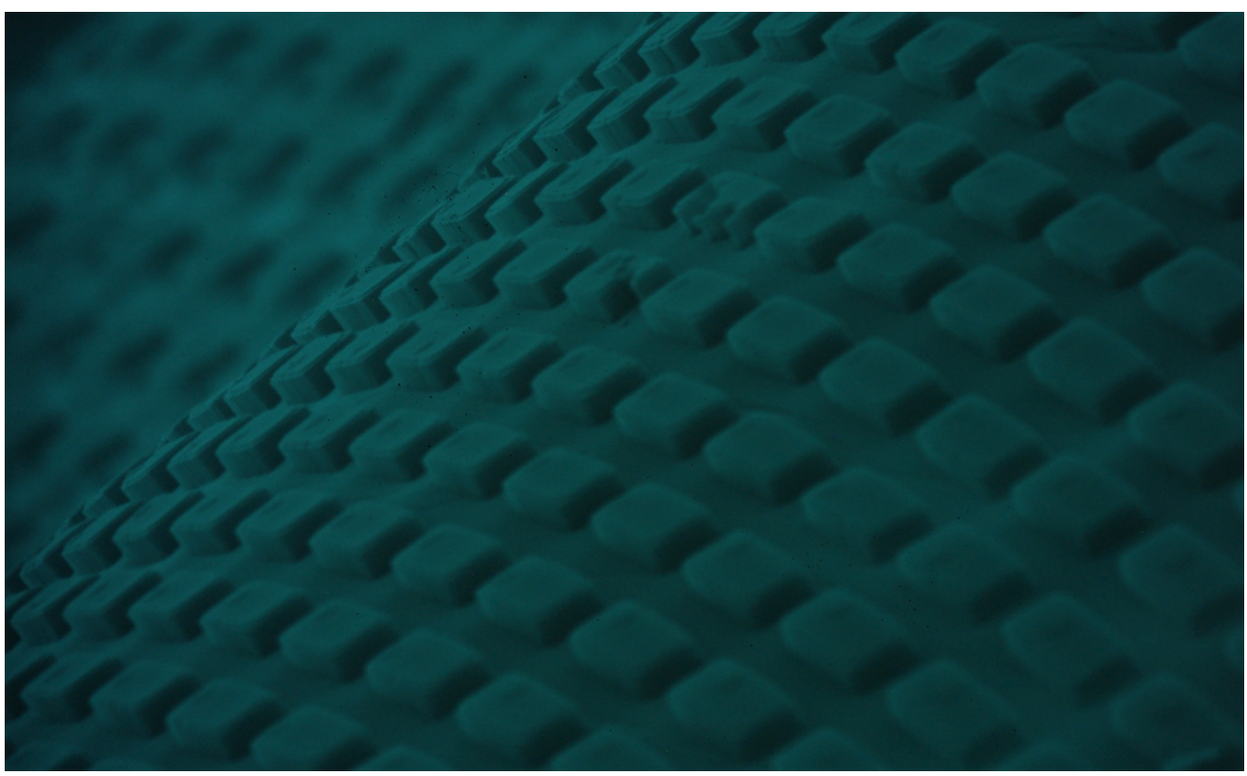
CINSaT

Center for
Interdisciplinary Nanostructure
Science and Technology

Newsletter No. 10 (June 2021)



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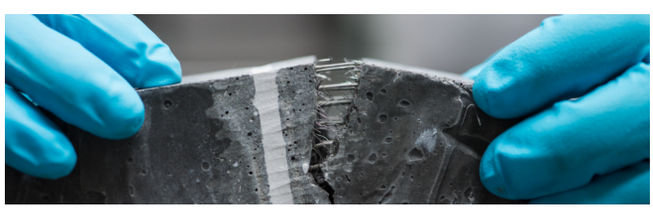

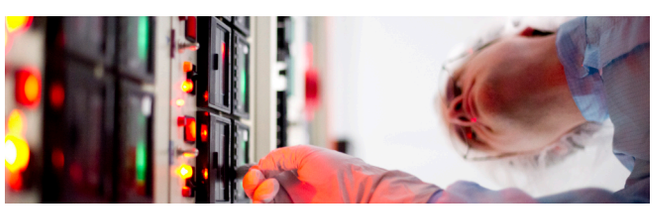

Cover Image

Burhan Kaban, Technical Electronics:

Structuring of a AZOPD-polystyrene mixture via nanoimprint lithography. The material is provided by AG Fuhrmann-Lieker (Sekvan Bagatur) and processed in the INA. The film shows 1x1 µm² quadratic structures, but the film has detached from the glass substrate and became wavy.

Preface

Dear reader,

welcome to the first CINSaT newsletter of 2021. The third newsletter published in the wake of the still ongoing SARS-CoV-2 pandemic. All meetings of CINSaT committees and the 2021 CINSaT spring meeting were held virtually. Despite the circumstances, the spring meeting was well received and a success in its unique realization, which you can read about in the Latest Reports section. Nevertheless, we all hope that the next spring meeting will be held like it was used to be, with exciting talks given in front of a live audience and interesting face to face talks. In consideration of the recent developments in the first half of 2021, I think this is not an unreasonable thought.

First, let me address the recent personnel changes. As of April 2021, two respected members left the CINSaT management to advance their careers in new directions. Prof. Dr. Bernd Witzigmann took a position at the University of Erlangen-Nürnberg. His tasks as a member of the CINSaT executive board are assumed by Prof. Dr. Thomas Niendorf. Executive Manager Dr. Nina Felgen will stay at the University Kassel, but in a new position as member of the Research Service. Her replacement is Daniel Merker, currently a PhD student at the Technological Physics Department, who is just in his final stage of thesis preparation, which he may defend end of the year.

We were once again able to create an interesting newsletter thanks to the numerous contributions of our members. Prof. Dr. Kilian Singer will present the Peer Scope system that is designed to improve the human-human interaction in virtual lectures. Three research highlights from our members are presented, showcasing the broad spectrum of the CINSaT with reports from chemistry about the synthesis of lanthanide complexes with possible application as quantum bits (Prof. Dr. Pietschnig), theoretical physics about ultrafast nonthermal NV center formation in diamond (Prof. Dr. Garcia), and measurement technology about virtual instruments for interference microscopy (Prof. Dr. Lehmann). Additionally, a new DFG project is presented by Prof. Dr. Schaffrath that aims for the functional analysis to resolve the potential role of the tRNA binding protein *Kti12*.

Furthermore, we are fortunate to welcome two new full memberships at the CINSaT adding new perspectives, capabilities, and expertise. Both give a short introduction about their work in the New Members section:

Prof. Dr. Stefan Böhm is the leader of the Department of Separating and Joining Manufacturing Processes (tff) with research focus on welding, bonding, and laser cladding.

PD Dr. Susanne Neupert is part of the Department of Animal Physiology, head of the research project “Single cell analysis within neuronal circuits” and a recognized expert in single cell mass spectrometry.

To round off this issue long-term member Prof. Dr. Ehresmann is presenting the field of research of his group, which is organized in the two subgroups “Functional Thin Films”, that is working on functionalization of magnetic thin films and “Physics with Synchrotron Radiation”, about the investigation of fundamental ionization processes induced by synchrotron or free electron radiation.

Like always, I hope you enjoy the reading of this issue and stay healthy!

General

Latest information from the CINSaT management

Here we report briefly about major issues from the CINSaT committees any major discussion results in their meetings

(a) Steering Committee

The last meeting of the steering committee was held on 25th February 2021 via video conference. The following issues were discussed:

- Prof. Dr. Bernd Witzigmann is leaving the University of Kassel and CINSaT on 1st April 2021 to take on a new position at the University of Erlangen-Nürnberg. The members of the steering committee regret the loss of a valuable member of the steering committee and wish Prof. Witzigmann the best for his new endeavors. Possible successors for the position were discussed.

- Dr. Nina Felgen announced that she is leaving the position as Executive Manager of the CINSaT on 15th March 2021 to take on a new position at the Research Service of the University of Kassel. The steering committee thanks Dr. Felgen for the excellent work over the years and wish her the best for the new position.

- The idea of an image film for the CINSaT is further discussed regarding financing. The possibility of a sponsoring should be evaluated.

(b) Member Meeting

The members met twice in 2021: 19th January and on 1st June. In the following, main issues discussed, and decisions are briefly listed, which are of general interest:

- Prof. Dr. Demekhin is the new speaker for the focal point “Chiral Systems”. Prof Dr. Baumert proposed to turn the position over to Prof. Dr. Demekhin. The proposal was accepted.

- Two application for full memberships were accepted in January. After approval by the Presidium in March we can welcome PD Dr. Susanne Neupert and Prof. Dr. Ing. Prof. h.c. Stefan Böhm to the CINSaT as full members. Furthermore, Dr. Arne Senftleben changed status from associate to full membership.

- The idea of a new CINSaT image film is discussed in relation to the upcoming 20th anniversary of the CINSaT. The idea is met with good responses by the members and will be further planned.

- Prof. Dr. Thomas Niendorf was elected as a new member of the executive board of the CINSaT on 1st June 2021 substituting the previous member Prof. Witzigmann. .

- The members voted for an extension of the CINSaT regulations (Ordnung des CINSaT) with an additional paragraph §4(12), which enables voting by mail or suitable digital procedures in urgent matters that require approval by the members. With decision of the presidium on 18th June 2021 the revised CINSaT regulations came into effect on 19th June 2021.

- The continuation of the “Seed Money” is discussed due to the fact that a long-term financial support by the institutional assistance funds of the University of Kassel is still uncertain. Discussions about a future university support is on the way. However, the continuation of the “Seed Money” is ensured for another round in 2021 and is approved by the members.

- Daniel Merker is announced as the new Executive Manager of the CINSaT from 16th April 2021. He will replace Dr. Nina Felgen. However, Dr. Felgen will be still available and will support the transition period.

Education

Innovative teaching during the pandemic

We managed to even improve the quality of lecture during the corona pandemic by using a new technology where the students have the feeling to follow the lecture behind an intelligent glass screen. This system optimizes human-human interaction using a see-through interaction screen. Users feel like they are sitting directly across from each other, connected via eye contact, interacting in a more human way. There is never any possibility to obscure the writing, gaze directions and gestures are authentically connected to the presentation. Peerscope lets you share your screen in a more natural, more human way. By including non-verbal gestures, eye and hand movements, you can make your presentations more lively and your message clearer. This project was awarded in 2019 by the North Hessian Business Association as part of the UNIKAT Idea Award. This project is now a spin-off of the University of Kassel, supported by the BMWi and European Social funds for Germany, via the funding programs WIPANO and EXIST.

The students were enthusiastic about the presence and quality of the lecture „Experimental Physik III - Relativitätstheorie, Quantenphysik, Kern- und Teilchenphysik“ (https://www.youtube.com/kiliansinger) and nominated the lecture for the Ars-legendi teaching award.

Also collaborating is like standing on the opposite side of a piece of glass, where you can manipulate the same content on your touchscreen, whilst looking your collaborator directly in the eye! Peerscope was developed with the help of a lot of students and a great development team funded by the WIPANO project. My group has also contributed essential patches to the open source community. Today's use of Moodle with lots of images, video integration and complex computer algebra tasks would be unthinkable without our essential contributions to the moodle core. For secure face-to-face exams during the Corona pandemic, our team has developed and successfully used a video exam system to test students in distributed lecture halls in

peerscope system

such a way that we can advise each student on questions regarding assignments, queries are possible at any time, but also cheating attempts can be excluded. The software could also be used from home due to complete data security safety as no data are stored and all servers are hosted at university. As a particularly attractive possibility for students to deepen the teaching content, we have started to offer the possibility e.g. to create own teaching videos on deepening topics using the "Peerscope" video technology.

Further information

https://peerscope.de

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Research Highlights

Virtual instruments and transfer characteristics

In practical applications the measurement uncertainty of an instrument plays an important role. Virtual instruments have been built, which enable an estimation of the measurement uncertainty without performing any real measurement. Simulation based virtual instruments are used in measurement technology in the same way as “digital twins” in mechanical engineering.

One of the most used principles in optical three-dimensional (3D) surface topography measurement is interference microscopy. According to the current state-of-the-art measurements are performed on a sample object in order to check whether a certain instrument is capable or not. As this procedure is time-consuming and expensive, there is a need for virtual topography measuring instruments.

However, due to the complicated physics behind optical topography measurement the development of virtual instruments is not straightforward. In the Measurement Technology Group we recently achieved some progress in modeling measurement processes in coherence scanning interference microscopy (CSI). The modular models consist of two independent steps: the light-surface interaction and the transfer characteristics of the instrument.

Although the light-surface interaction is typically based on elastic scattering mechanisms, diffraction at surface structures needs to be considered. In this context there are two options: Analytical models going back to Kirchhoff’s diffraction theory are computationally efficient but they are only approximative solutions. Rigorous simulations such as FEM are directly related to Maxwell’s equations but even today suffer from computational burden and the results may be affected by numerical artefacts. In both cases the 3D conical illumination in a microscope needs to be considered. Moreover, polarization strongly affects measurement results obtained from edges of surface structures. These subjects are addressed in our paper published in Optics Express [1].

For the modeling of the transfer characteristics, the transfer function of the optical instrument needs to be known. 3D microscopes typically perform a through-focus scan along the optical z-axis in order to gain the depth information of an object. The camera records an image stack consisting of numerous microscopic images of the intensity depending on the xy image coordinates. As a consequence, a 3D transfer function of the spatial frequency coordinates qx, qy and qz results. The 3D spatial frequency representation is closely related to the Ewald

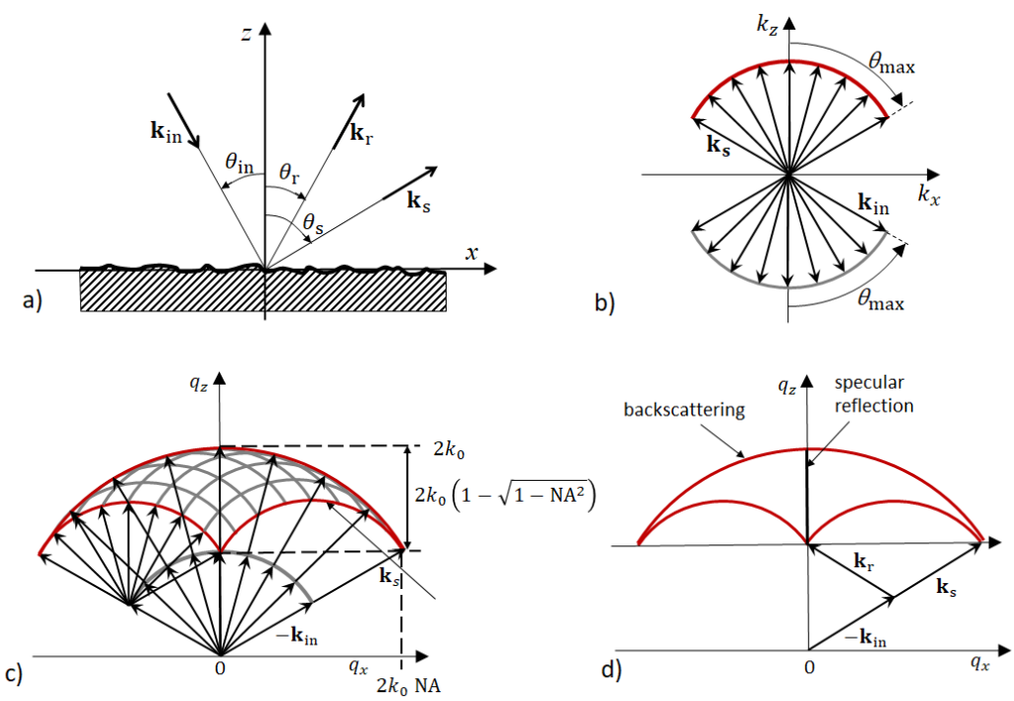


Fig. 1: Construction of the transfer range of a microscope of given NA in reflection mode

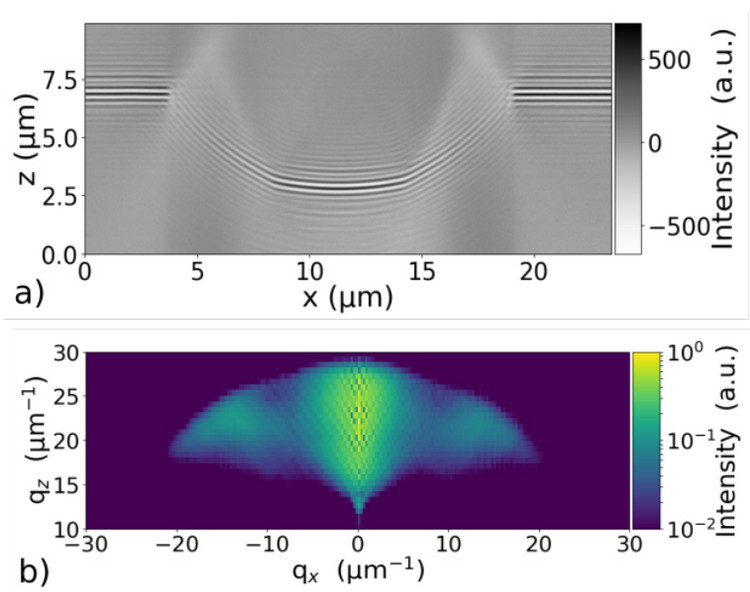
sphere construction known from x-ray diffraction. Any point contributing to the image formation is given in q-space by the difference of the wave vector of the scattered wave minus the wave vector of the incident wave. However, interference microscopes are typically based on reflection. Thus, the angles of wave vectors are limited by the numerical aperture of the objective lens and only a portion of the Ewald sphere will contribute. Mathematically, this equals a convolution of all possible incident wave vectors, which are combined with all possible vectors of scattered light. The big advantage of the q-space representation is that each plane wave propagating in space leads to a Dirac function. Based on this concept we recently developed a model describing the transfer characteristics of CSI instruments [2].

Further information

[1] T. Pahl, S. Hagemeier, M. Künne, D. Yang and P. Lehmann, “3D modeling of coherence scanning interferometry on 2D surfaces using FEM,” Opt. Exp. 28 (26), pp. 39807-39826 (2020)

[2] P. Lehmann, M. Künne and T. Pahl, “Analysis of interference microscopy in the spatial frequency domain,” J. Phys. Photonics 3 (2021) 014006

Fig. 2: Cross section of a measured interference image stack and the corresponding 3D spatial frequency representation for a concave silicon mold fabricated using deposition, lithography and etching at INA (Hillmer group). The structures are used as molds in Nanoimprint Lithography.



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Azido Functionalized Aromatic Phosphonate Esters in ^{R}POSS Cage-Supported Lanthanide Ion (Ln = La, Nd, Dy, Er) Coordination

Exciting lanthanide ions: Very recent results from the Hybrid Materials group at the Institute of Chemistry, in collaboration with researchers from the INA, presenting the synthesis of nano scale ^{R}POSS-cage- and phosphonate ester-supported lanthanide complexes with azide-based anchoring units for subsequent evaluation of their photoluminescence (PL) properties aiming at a potential future application in surface immobilized optically switchable isolated molecular quantum bits.

Owing to their outstanding photoluminescence properties, lanthanide ions play a central role in lighting, sensing, and display technologies. Furthermore, they are promising candidates for application in quantum-based information storage on an atomic and molecular level. In comparison to their carboxylic acid counterparts, the advantage of phosphonate esters arises from their lower vibrational frequencies, resulting in reduced nonemissive excited-state quenching and improved quantum yields. Owing to their higher stability, aryl azides have attracted broad industrial interest and found application, for example, as photoresistor cross-linkers, in conducting polymers, and for light-induced polymer surface activation. The 4- or 4′-azido functionalized phosphonate esters shall function as anchoring groups for future immobilization of these complexes on (In/Ga)P semiconductor surfaces and subsequent evaluation of their potential as optically switchable isolated molecular quantum bits. The rigid POSS-cage (polyhedral oligomeric silsesquioxane) structure in combination with the phosphonate esters is assumed to enhance the excited-state lifetimes of the metal centers, paving the way for potential future molecular data storage and manipulation.

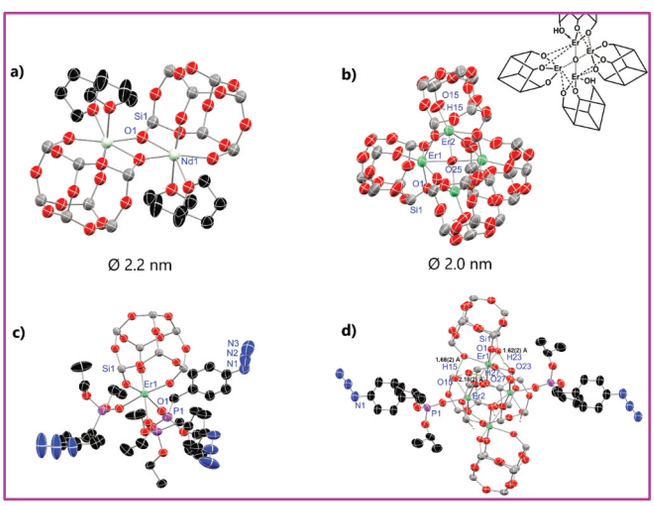


*Figure 2: SCXRD structures with aggregate diameter (Ø) of: **a)** [Nd{^{Ph}POSS}(THF)$_2$]$_2$; **b)** [Er$_4${^{iBu}POSS}$_2${^{iBu}POSS$_{Si-OH}$}$_2$(μ_4-O)]; **c)** [Er{^{Ph}POSS}(**L1**)$_3$]; **d)** [Er$_2${T$_7$(O)$_3$}{T$_6$(OH)$_2$(O)$_2$}[μ_3-OH](**L2**)]$_2$. iBu and Ph substituents as well as hydrogen atoms are omitted for clarity.*

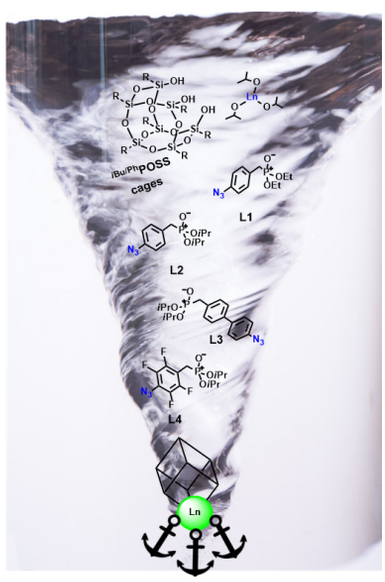
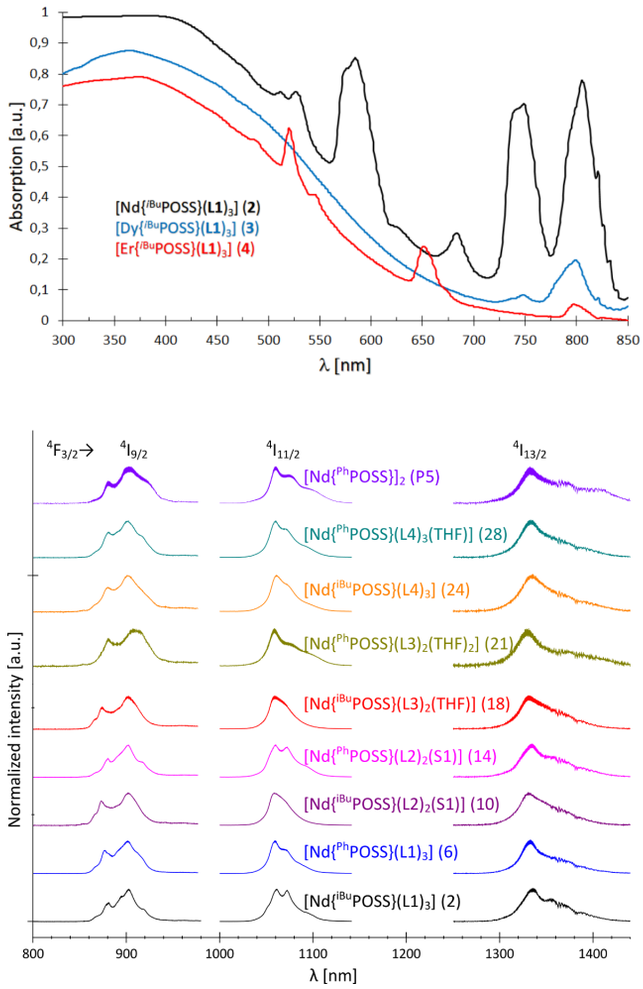


Figure 1: Schematic preparation of ^{R}POSS-(R = iBu, Ph) and phosphonate ester-supported lanthanide complexes.

In our work recently published in ***Inorganic Chemistry***, we presented protocols for the preparation of 4-, or 4′-azido substituted phosphonate ester ligands (**L1**−**L4**) featuring different aromatic backbones. In combination with our expertise in POSS cage chemistry, these ligands were then applied in ^{R}POSS-cage supported (R = *i*Bu, Ph) Ln^{3+} ion (Ln = La, Nd, Dy, Er) coordination of POSS-lanthanide precursors under retention of the N_3 substituent, as demonstrated in more than 30 different complexes (Figure 1). In this context, an azido functionalization at the 4- or 4′-position of **L1**−**L4** is expected to be the most suitable to avoid steric congestion between a semiconductor surface and the rest of the POSS cage-supported complexes. Single crystal x-ray diffraction (SCXRD) data revealed the lanthanide precursors to form di- and tetramers while the phosphonate ester supported POSS-lanthanide target complexes preferably form monomers in the solid-state. A reaction of the latter with airborne water as well led to the formation of well-defined tetrameric species. The SCXRD structures show the complexes to form nano scale aggregates in a range of 1.9−2.7 nm (Figure 2). Preliminary ^{1}H-diffusion ordered spectroscopy NMR (DOSY-NMR) corroborate that the mono- and dimeric solid-state structures most likely are



retained in solution. Infra-red (IR) investigations revealed the ligands as well as the complexes to show an anomalous splitting of the asymmetric and symmetric N_3 stretching modes due to Fermi interactions with combination tones including the symmetric N_3 or C−N stretching mode and other low-lying frequencies. Moreover, the PL properties of the obtained compounds were examined. The absorption spectra of all the presented complexes exhibit the anticipated metal-centered absorption bands in a range of 300−850 nm of the Nd^{3+} ($\lambda_{abs,max}$ = 586 nm), Dy^{3+} ($\lambda_{abs,max}$ = 802 nm), and Er^{3+} ($\lambda_{abs,max}$ = 521 nm) cations, respectively (Figure 3, top). The µ-PL room temperature spectra of the different Nd^{3+} complexes show three expected metal-centered emission bands in the NIR region of relative weak intensity corresponding to the $^4F_{3/2} \rightarrow {}^4I_{9/2}$, $^4F_{3/2} \rightarrow {}^4I_{11/2}$ and $^4F_{3/2} \rightarrow {}^4I_{13/2}$ transitions (Figure 3, bottom). Observed emission band splitting features have been attributed to electrostatic orbital interactions of Nd^{3+}-centered f-states and ligand-centered states at the oxygen donor sites.

Further information

Ingo Koehne, Miriam Gerstel, Clemens Bruhn, Johann P. Reithmaier, Mohamed Benyoucef and Rudolf Pietschnig, Inorg. Chem. (2021), 60, 7, 5297- 5309
https://doi.org/10.1021/acs.inorgchem.1c00266

Figure 3: Top: Exemplary absorption spectra of a Nd^{3+} (black), Dy^{3+} (blue), and Er^{3+} complex (red) at rt exhibiting typically sharp metal centered absorption bands. Bottom: Stacked room temperature µ-PL emission spectra (λ_{exc} = 750 nm) of different Nd^{3+} complexes presented in this work showing metal centered emission bands. There are three emission bands in the NIR, corresponding to the $^4F_{3/2} \rightarrow {}^4I_{9/2}$, $^4F_{3/2} \rightarrow {}^4I_{11/2}$ and $^4F_{3/2} \rightarrow {}^4I_{13/2}$ transitions. The spectra are normalized to the emission band maximum of each recorded transition.

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Ultrafast nonthermal NV center formation in diamond

Proof of concept for a fully the nonthermal formation of color centers in diamond upon femtosecond-laser irradiation

Reliable and stable quantum computers have the potential to revolutionize many activities in the world since they are able to solve problems which are impossible to handle by classical computers. They consist of so-called quantum bits (qubits) that can be prepared in superposed and entangled states in contrast to classical bits. Among the most suitable candidates to represent solid-state qubits, nitrogen-vacancy (NV) centers in diamond are the most promising ones due to their unique properties and the stable environment.

Ideally, NV centers are created deterministically at defined regions in an isotopically pure diamond substrate. The nuclear spin of a color center can then be used as long-lived qubit, which allows for multiple readouts so that fidelity quantum devices are feasible. Color-center manufacturing technologies should therefore be able to provide a controllable ensemble of NV centers. The development of such a well suited technique is of current fundamental interest. Widely used approaches mainly consist of two-step process. First, the color center components are implanted into the diamond environment. The second step consists in the formation of the NV centers.

The implantation step is commonly realized by ion bombardment of the target diamond crystal, by deterministic single ion implantation or by N-insertion during the diamond crystal growth process. Usually, all manufacturing techniques produce nitrogen atoms and crystal vacancies which are well separated from each other in the diamond crystal. Therefore, after implantation, structural rearrangement processes and migration must occur, so that a relatively high and uniformly distributed density of NV centers can arise. This last step is mostly achieved through thermal annealing of the diamond environment. By the thermal heating of the crystalline system the atoms gain kinetic energy, so that their mobility is increased and they can diffuse through the host crystal until stable NV centers are formed.

In our work recently published in **Carbon** we propose a new and fully nonthermal method to induce the formation of color centers providing the necessary formation energy by ultrashort laser pulses (see schematic illustration in the upper panel of Fig. 1). Femtosecond-laser pulses can directly access the bonding properties of the solid without disturbing the atomic system directly, which makes them an ideal tool to address NV center formation in an already implanted diamond crystal.
We performed simulations of a femtosecond-laser induced NV center formation in a diamond environment using the in-house electronic-temperature-dependent DFT code CHIVES (**C**ode for **H**ighly exc**I**ted **V**alence **E**lectron **S**ystems). Our results show, yielding a proof of concept, that femtosecond-laser pulses could be used to controllably produce NV centers nonthermally on a timescale less than 250 fs after the excitation for a laser-induced electronic temperature of T_e = 47 366.6 K. At this high electronic temperature about 11 % of the valence electrons are excited. We were able to resolve the underlying mechanisms of the diffusion

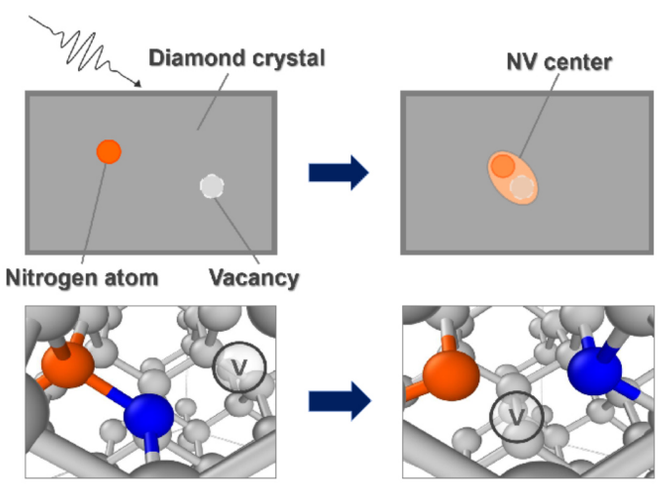

Figure 1: (top) Schematic illustration of the femtosecond-laser induced nonthermal NV center formation in diamond. The laser energy is used to merge the initially separated nitrogen atom with the crystal vacancy with low impact on the surrounding crystal. (bottom) Closeups of our simulation cell near the nitrogen impurity (orange) and the crystal vacancy (transparent). The carbon atom in between (blue) changes its position with the vacancy within 250 fs of the simulation.

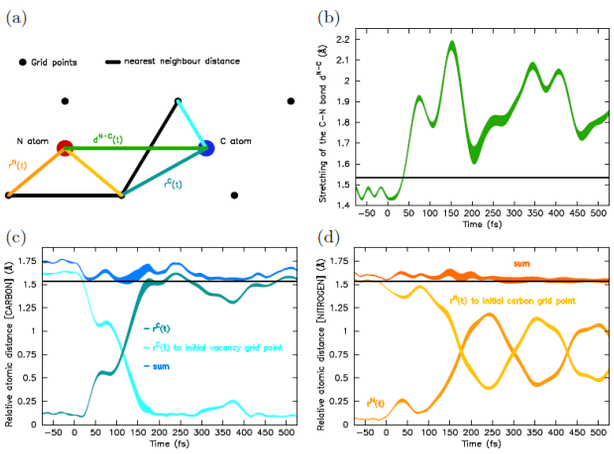

Figure 2: Relative atomic distances for selected atoms and grid points. (a) Sketch of the relative atomic distances of the nitrogen atom and the interstitial carbon atom for an arbitrary time after the femtosecond-laser excitation. The color coding is used in the following graphs. The horizontal black line indicates the distance between grid points in the diamond crystal, here 1.5325 Å. (b) Interatomic distance between the interstitial carbon atom and the nitrogen impurity as a function of time. (c) Time evolution of the relative atomic distance of the carbon atom to its initial grid point rC(t) (turquoise), to the initial vacancy grid point (light blue) and the sum of both distances (blue) for a laser induced electronic temperature of Te = 47 366.6 K. About 150 fs after laser excitation the carbon atom is located close to the initial grid point of the vacancy. (d) Relative atomic distance of the nitrogen atom to its initial grid point (light orange), to the initial carbon grid point (yellow) and the sum of both distances (orange).

process by following the atomic pathways during and after the excitation, as shown in Fig. 2. The ultrashort-laser pulse induces a change in the interatomic bonding which leads to an oscillatory behavior of the nitrogen atom. This behavior is fundamentally different to the thermal case where the nitrogen atom remains close to a grid point. The above mentioned oscillations can be explained by performing static computations of the electronic free energy in dependence of the atomic displacements, which reveals that the diamond grid points do not longer correspond to a minimum in the potential energy surface at the considered excitation strength. Those computations furthermore indicate that the energy minimum defining the NV center configuration changes in dependence of the laser strength. Potentially, this behavior could be used to produce customer designed NV centers in diamond with different properties.

Further information

M. Kempkes, T. Zier, K. Singer, M. E. Garcia, Carbon 174, 524-530 (2021), https://doi.org/10.1016/j.carbon.2020.12.062

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New Projects

Functional analysis of the tRNA binding protein Kti12 (DFG SCHA750/25-1)

In eukaryotes, Kti12 enables carboxymethylation (cm^5) of transfer ribonucleic acids (tRNA) by the Elongator complex. The modification is located inside the anticodon of tRNA and supports correct translation via improved base pairing during decoding of messenger RNA (mRNA). Interestingly, either down or upregulation of Elongator have been associated with neurodegenerative disease and diverse cancer in humans.

The DFG project focusses on the tRNA binding protein Kti12 (Fig.1) and its role in Elongator regulation, thereby contributing to the fast growing field of epitranscriptomics. The central dogma of molecular biology describes the production of proteins from DNA. During this process, tRNAs play a key role as they translate the mRNA triplet codon within the ribosome and attach the corresponding amino acid to the growing polypeptide chain. Diverse chemical modifications have evolved in nature to ensure proper folding and decoding of tRNA.

The Elongator complex consists of six protein subunits and carboxymethylates uridines (cm^5U_{34}) located inside the anticodon of tRNA. Thereby, cm^5U_{34} modifications play an important role during decoding of the mRNA and were found to be essential in higher eukaryotes. The research group of Prof. Schaffrath makes use of baker´s yeast *Saccharomyces cerevisiae* as a model eukaryote in order to study the effects of cm^5U_{34} loss to the organism. Surprisingly, the modification activity of Elongator was revealed to be dependent on a tRNA binding protein called Kti12. However, the exact function of Kti12 remains elusive to the scientific community.

Structurally Kti12 can be separated into an N-terminal ATP hydrolysing domain (NTD) and a C-terminal tRNA binding domain (CTD) connected via a flexible linker region (Fig.1).

Our previous study revealed the ATP hydrolyzation by Kti12 to be dependent on the $tRNA^{Sec}$ species *in vitro*. Yet, it remains unclear which tRNA could activate Kti12 *in vivo* since $tRNA^{Sec}$ is not natural to baker´s yeast. We further showed the CTD of Kti12 to be mainly involved in tRNA binding (Fig.2A). Specific substitutions at the C-terminus did additionally decrease the tRNA affinity *in* vitro as well as Elongator function *in vivo* (Fig. 2B).

Since the affinity of Kti12 was found to be independent of the presented tRNA species, our results suggest a discrimination between tRNA species by the N-terminal ATPase function of Kti12 which in turn might regulate Elongator (Krutyhołowa *et al.* 2019). Both domains in conjunction are required for *in vivo* function of the Elongator complex as dissections or amino acid substitutions that disrupt either the ATP binding pocket or tRNA binding of Kti12 lead to phenotypes indicative for Elongator loss (Fig.2B).

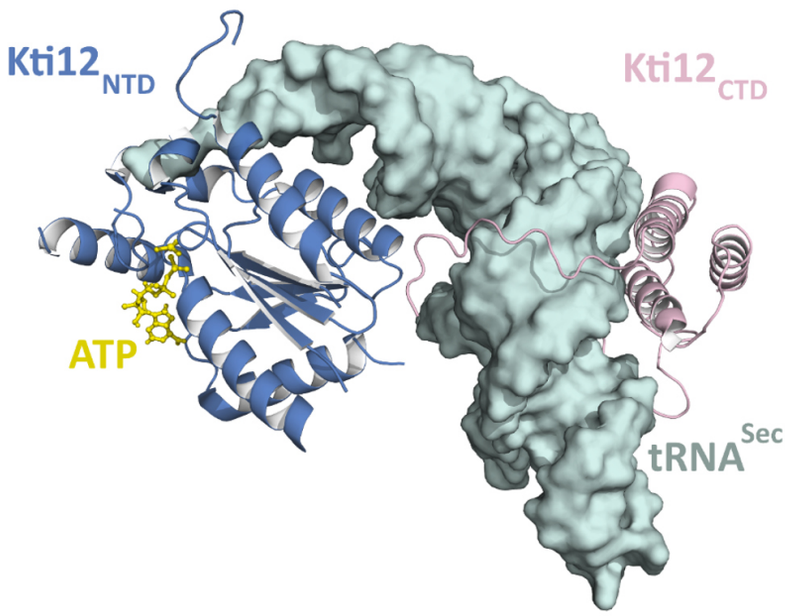

Fig.1: Structural model of the Elongator partner protein Kti12 during ATP hydrolysis induced by $tRNA^{Sec}$. The NTD of Kti12 exhibits an ATP binding pocket which allows cleavage of the nucleoside triphosphate in dependency of bound tRNA, whereas the CTD of Kti12 was identified as the main tRNA interacting domain. The structural model was calculated via the obtained crystal structure of $Kti12_{NTD}$ from Chaetomium thermophilum (PDB ID 6qp0, Krutyhołowa et al. 2019) and homology to the O-phosphoseryl-tRNA kinase (PSTK; PDB ID 3adb).

Within the DFG project, we aim to further investigate the unanswered questions of both Kti12 domains *in vivo* as well as *in vitro* with regards to Elongator activity as a tRNA modifier. Our previous work allows us to selectively turn off the ATPase or tRNA binding function of Kti12 via characterized mutations. With assays such as UV-Clip, TAP purification, immuno-precipitation we aim to further clarify Elongator´s need for Kti12 dependent ATP hydrolysis, as well as whether Kti12 is distinguishing between different substrate tRNA species. Additionally, we are interested in the phospho-regulation of the Elongator complex via the Elp1 subunit which has been shown to be dependent on Hrr25 kinase recruitment by Kti12.

In summary, our DFG project aims to resolve the potential role of Kti12 as a regulatory Elongator protein. The gained information could be utilized as a means to target Elongator associated disease syndromes in future.

Further information

Krutyhołowa R., Hammermeister A., Zabel R., Abdel-Fattah W., ReinhardtTews A. et al. 2019. Kti12, a PSTK-like tRNA dependent ATPase essential for tRNA modification by Elongator. Nucleic Acid Res. 47(9): 4814-4830 https://doi.org/10.1093/nar/gkz190

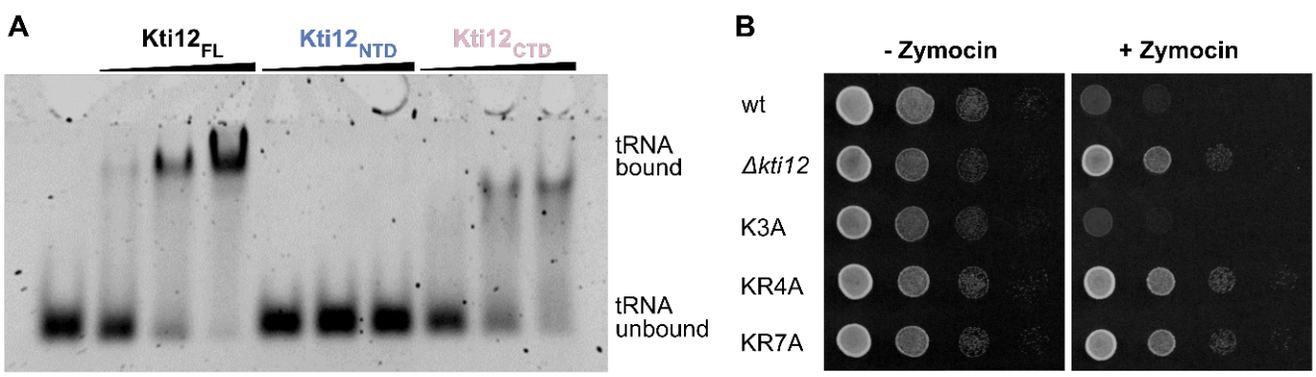

Fig.2: The C-terminal domain of Kti12 mediates tRNA binding and Elongator function. (A) Recombinant full length (FL), N-terminal (NTD) or C-terminal (CTD) Kti12 was incubated with bulk tRNA from yeast and subjected to an electrophoretic mobility shift assay (EMSA). The interaction between protein and nucleic acid leads to a decrease in phoretic mobility when compared to tRNA alone, thereby resulting in a shift of tRNA signal during electrophoresis (Krutyhołowa et al. 2019). (B) Substitutions of tRNA binding residues in the CTD of Kti12 (K3A, KR4A, KR7A) lead to phenotypes indicative for Elongator function loss. The strains KR4A and KR7A phenocopy a kti12 deletion strain as they grow on media containing zymocin, a tRNAse toxin that specifically cleaves Elongator modified tRNA, thereby leading to cell death in wildtype (wt) yeast strains.

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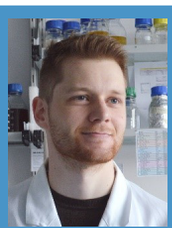

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New Members

Prof. Dr.-Ing. Stefan Böhm

FACHGEBIET

TRENNENDE UND FÜGENDE

FERTIGUNGSVERFAHREN

Prof. Dr.-Ing. Stefan Böhm studied electrical engineering at Darmstadt Technical University, specializing in control and data technology. For his doctorate, he moved to RWTH Aachen University, where he completed a dissertation on the simulation of electron beam welding in mechanical engineering in 1999. After his dissertation, he became a senior engineer at the Department of Adhesive Bonding Technology at RWTH Aachen University. In 2003, he was appointed junior professor at the Technical University of Braunschweig in the Department of Microjoining. In 2009, he became an full professor at the Department of Packaging and Interconnection Technology. In 2010, he moved to the University of Kassel, where he has been serving as the head of the Department of Cutting and Joining Processes (tff) ever since.

Foto: Holger Jenss & Nicolas Wefers

The tff is part of the Faculty of Mechanical Engineering (FB 15) at the University of Kassel. The "cutting processes" at tff include sawing, drilling and milling, the "joining processes" include welding, bonding and (generative) laser cladding (LMD).

The research focus of Prof. Dr.-Ing. Stefan Böhm in the field of welding is on laser beam welding (also hybrid) and laser cladding, magnetic pulse welding, electron beam welding and friction stir welding. In all processes, the process-microstructure-property relationships play a major role.

In the field of bonding, Prof. Dr.-Ing. Stefan Böhm's research focuses on the process chain. Examples are bonding and debonding "at the push of a button", aging-resistant bonding on stainless steels or titanium, pretreatment processes to improve bondability, minimum quantity dosing or adhesive-integrated markers for lifetime prediction.

In both adhesive bonding and welding, in-process as well as post-process non-destructive testing of the joints is a major issue, which Prof. Dr.-Ing. Stefan Böhm addresses with research on the use of structure-borne sound analysis, thermographic methods and shearography.

Research activities in the field of welding and bonding are also taking place outside the classic mechanical engineering applications. For example, research into the use of titanium and titanium shape memory alloys is underway in the field of medical technology, particularly in implantology. Examples of this are bonded titanium-based dental implants and nitinol-stainless steel joints in surgical

instruments, which are formed by means of welding and bonding.

In the field of machining, Prof. Dr.-Ing. Stefan Böhm's research focuses primarily on sawing using band saws and circular saws, the cutting of mineral materials and composites, and the machining of hard wear-resistant coatings with geometrically determined cutting edges.

The research work of Prof. Dr.-Ing. Stefan Böhm is related to CINSaT because of the nanoscale nature of various parameters that determine the properties of the processes mentioned.

In the field of welding of similar and dissimilar metals, the tff is working on optimizing the properties of the joints and their characterization. The property-determining parameters are on nanoscale size.

In adhesive bonding, tff considers a variety of material classes (e.g. metals, plastics, ceramics) as substrates. In addition to the physical, chemical and, in some cases, mechanical adhesion mechanisms acting on a nanoscale, which are influenced at tff by various methods (e.g. plasma polymerization, nano-laser structuring and deposition of usually monomolecular adhesion promoter layers), the modification and activation of adhesives is also the focus of research activities at tff. For example, carbon nanotubes (CNTs) are used to strengthen adhesives and improve conductivity. Other, largely microscale fillers are functionalized to optimize bonding to the polymer matrix of the adhesive.

In cutting, the surface of the rake and flank face of the tool, but also the cutting edge itself, is decisive for the quality of the cutting process and its efficiency. For this reason, cutting mate-rials are coated at tff by processes such as CVD or by using laser implantation of micro- or nanoscale particles to minimize friction or increase hardness. Likewise, cutting edges are rounded in the submicrometer range to realize particularly efficient cutting processes.

Further information

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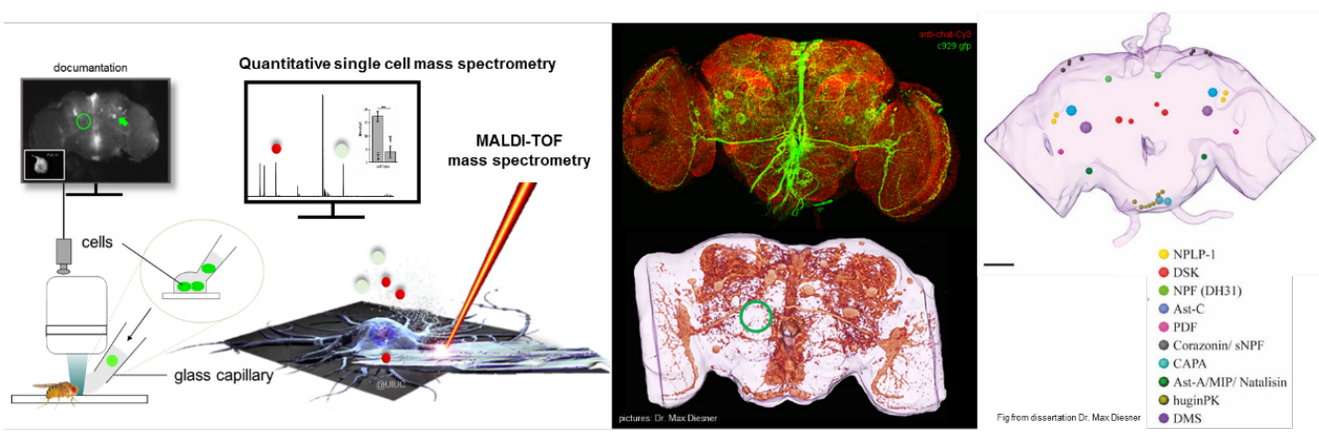
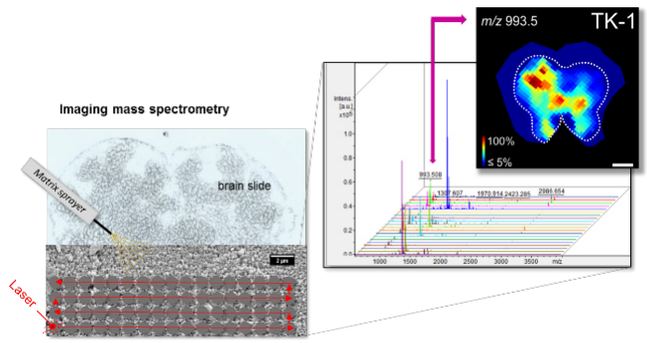
PD Dr. Susanne Neupert

PD Dr. Susanne Neupert is a young research group leader at the Department of Biology, Animal Physiology at the University of Kassel. She is an internationally recognized expert in single cell mass spectrometry. She heads the research project “Single cell analysis within neuronal circuits” at the graduate school “clocks”. Dr. Neupert is member of CINSaT since March 2021. Her team’s interdisciplinary projects bridge neurochemistry, entomology, neuroscience, and neuroethology. Focus of her research is the structural and functional analysis of neuropeptides and biogenic amines in insect brains, controlling feeding behavior, circadian rhythms of rest/activity, and responses to environmental stress. General neurotransmitters such as acetylcholine are synthesized and released at synaptic sites, signaling at the scale of milliseconds. In contrast, neuropeptides are specifically transported to and released at various non-synaptic release sites within a neuropeptidergic cell. Neuropeptides signal at a time scale of seconds to hours via volume transmission affecting far apart neuronal circuits in the brains of insects and mammals, alike. Their wide-spread occurrence, structural diversity and spatial localization in the nervous system reflect their influence in an extensive variety of physiological processes, neural dysfunctions and behavioral patterns. Neuropeptides appear to signal in concerted actions with biogenic amines that belong to the reward system in mammals and insects. To understand their cooperation and functions in the control of behavior is a major, timely task of neuroscience.



Analysis and mapping of neuropeptides and biogenic amines. Single cell preparation procedure for subsequent qualitative and quantitative MALDI-TOF mass spectrometrical analysis (left) and immunocytochemistry (top right). After isolation of an individual soma from an intact brain, the brain is photographed (top left) and prepared for 3D brain reconstruction (right below) to evaluate the neuroanatomy of the analyzed neuron. Peptidergic map of neurosecretory cells of the adult D. melanogaster brain (right) (Diesner, Predel, Neupert S. [2018] Neuropeptide Mapping of Dimmed Cells of Adult Drosophila Brain. J ASMS 29:890-902.)

Dr. Neupert's research team is working with the fruit fly *Drosophila melanogaster* with an ample genetic toolbox available. Furthermore, larger insect species such as the cockroaches *Periplaneta americana* and *Rhyparobia maderae* that are pest-insects are employed, which offer advantages for cellular analysis. Basic features of central nervous systems are evolutionary conserved in vertebrates and invertebrates. Thus, the less complex brains of insects offer many experimental advantages. Next to employing molecular and genetic techniques, her team's main expertise is high-sensitive mass spectrometry such as matrix assisted laser desorption/ionization (MALDI) time-of-flight (TOF) mass spectrometry at the single cell level. In addition, single cell transcriptomics and immunocytochemical studies are employed to determine single cell functions in complex neuronal circuits. Thereby, Dr. Neupert´s team explores: (1) the equipment of mature neuropeptides (neuropeptidome) and their potential co-transmitter of individual cells; (2) potential post-translational modifications of neuropeptides, (3) differential processing events of neuropeptides that are encoded on a single precursor gene; (4) co-localizations of neuropeptides that are encoded by different precursors, and (5) peptidergic and aminergic maps of neuronal circuits with single cell-resolution. Her team also explores which mechanisms determine neuropeptide/biogenic amine release at the single cell level. Next to basic research, Dr. Neupert thrives at further improving and developing new mass spectrometry techniques to maximize resolution.



Imaging mass spectrometry investigates the spatial distribution of neuropeptides in single tissue sections to examine release (Habenstein, Schmitt, Liessem, Ly, Trede, Wegener, Predel, Rössler, Neupert. [2021] Transcriptomic, peptidomic, and mass spectrometry imaging analysis of the brain in the ant Cataglyphis nodus. J Neurochem. doi: 10.1111/jnc.15346.)

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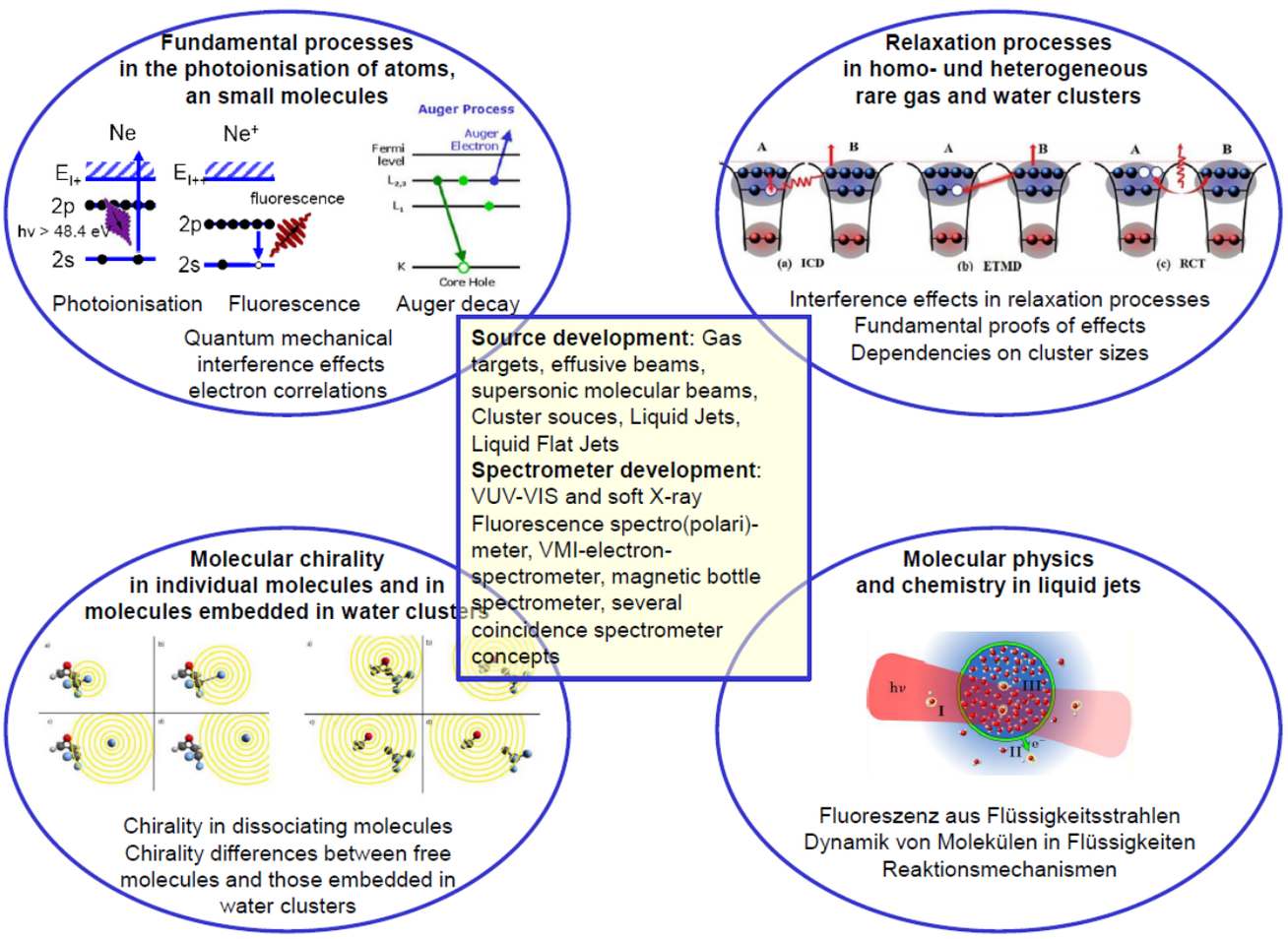
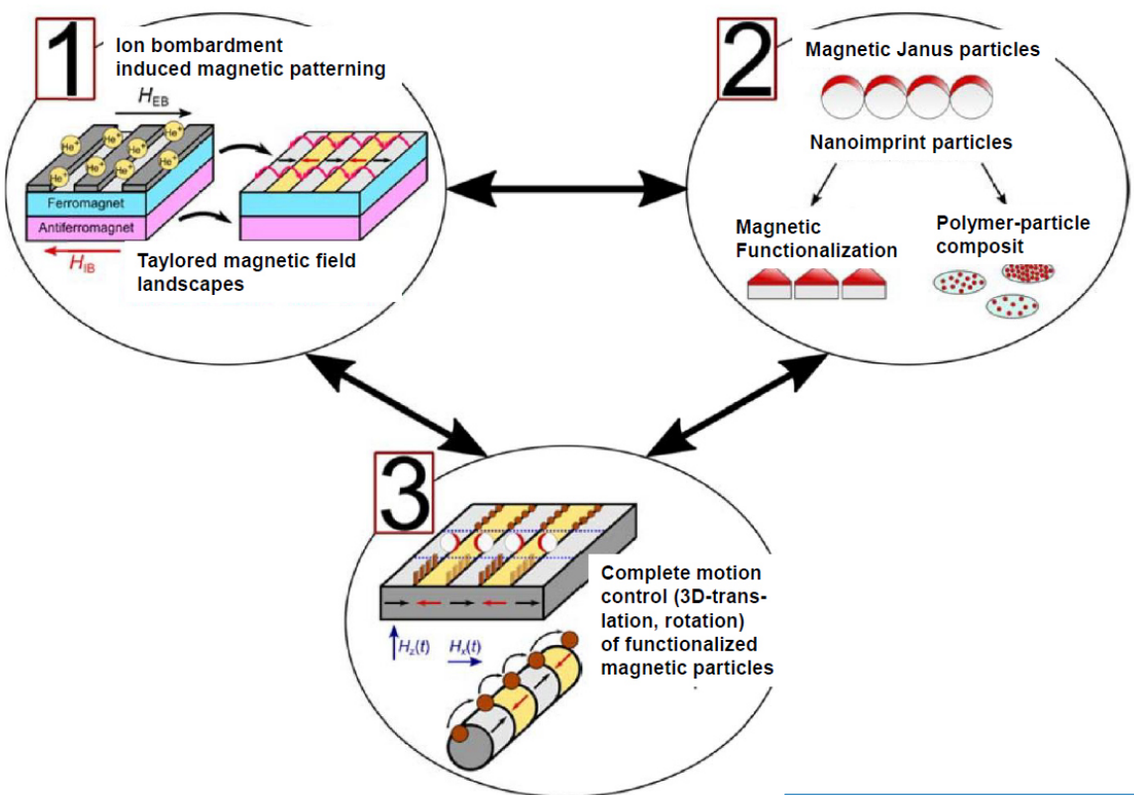
Research Groups

Functional Thin Films and Physics with Synchrotron Radiation (FTFPSR)– Faculty 10

FTFPSR is organized in two subgroups, “Functional Thin Films (FTF)” and “Physics with Synchrotron Radiation (PSR)”. The activities of PSR focus on investigations of fundamental photoionization processes induced by short wavelength synchrotron and free electron laser radiation from the vacuum ultraviolet down to the x-ray range. Scientific questions to be answered here are, how quantum mechanical interference effects and electron correlations (Interactions between electrons in atoms, molecules, clusters, and liquids) do modify photoionization probabilities upon interaction with one or more photons. In particular, we currently investigate how quantum mechanical entanglement between atoms and molecules and their constituents in weakly bound clusters and liquids determines relaxation and charge transfer processes, hitherto unknown. These recently discovered processes are discussed as a missing link to understanding the processes induced by ionizing radiation on the human body and as possible mechanisms relevant to astrochemistry on dust and icy grains. Another scientific focus is the investigation of molecular chirality by photoelectron circular dichroism, exploiting the asymmetric scattering of photoelectrons during their way out at the nuclear backbone of a chiral molecule. Here we use the possibility to atomic-site selectively emit photoelectrons by addressing specific photoionization thresholds and resonances. The corresponding enabling experimental stations are developed in our group and are used at the synchrotron and free electron laser facilities in Berlin and Hamburg and at the facility for antihydrogen and ion research (FAIR) in Darmstadt.



The FTF part of the group investigates the modification of magnetic thin film systems by light non-magnetic ions. Besides corresponding fundamental investigations on how the ions induce modifications in the magnetic system we develop a technology for domain engineering by a combination between lithography and light-ion bombardment. This technology has been used to develop sensor concepts, like angular and magnetic field sensors. Engineered magnetic domains lead to engineered magnetic field landscapes (MFLs) above the domains. These MFLs, superposed by a dynamically varying external magnetic field have been used for a full motion control of magnetic particles. Presently motion types of magnetic Janus particles are investigated, non-magnetic spherical particles covered by a magnetic cap of defined magnetic characteristics and plans are at hand to fabricate micro-particles with a defined 3D geometry. We intend to use these particles in lab-on-chip applications for the development of diagnostic devices. The developed technology includes machine learning algorithms and the exploitation of liquid mediated particle-surface interactions addressing the detection of disease markers.



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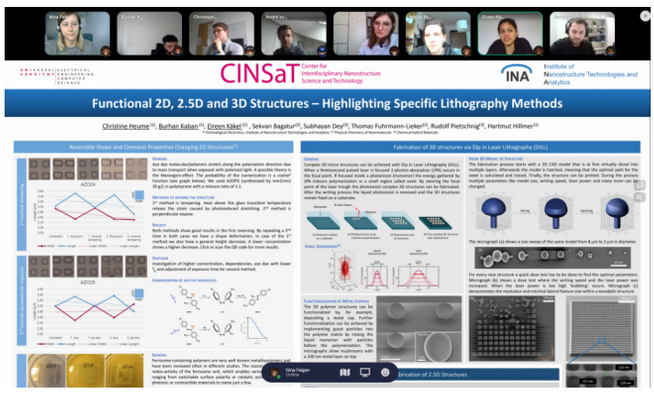
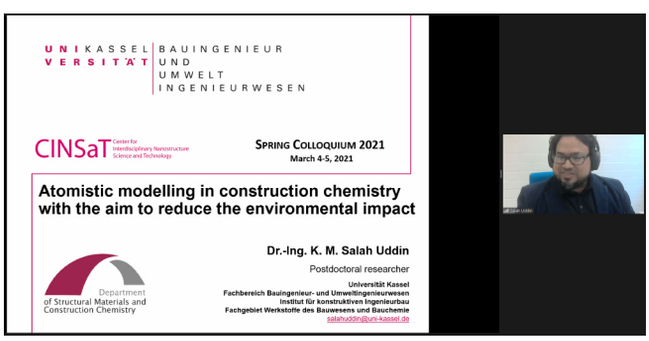
Latest Reports
Spring Meeting 2021

CINSaT uses internal virtual retreat for thematic sharpening of scientific foci and internal exchange

On March 4 and 5, 2021, as every spring, CINSaT had invited to the internal closed meeting to shed light on current research foci, to further develop thematically and to plan joint projects. An important contribution to this is made by the PhD students of the individual disciplines, who fill the meeting with life through their contributions and thus help to create a wide-ranging discussion platform. Unlike usual, the event did not take place in the AHORN Berghotel in Friedrichroda, but virtually via ZOOM as a lecture platform, as well as Gather Town as a platform for the poster session.



Online-Postersession realized with gather.town



Presentation by Dr.-Ing. K. M. Salah Uddin.

After the warm welcome and opening by the CINSaT speaker, Prof. Dr. Johann Peter Reithmaier, Prof. Philipp Demekhin as the new focus speaker “Chiral Systems” gave an overview of the past and planned activities in the SFB ELCH. This was followed by the session on Nanostructures in Science, Engineering and Art”, where first Prof. Bernhard Middendorf and afterwards Prof. Thomas Niendorf gave overview of activities in the field of materials science. The session was rounded off by the contribution of Dr. Salah Uddin, who gave an entertaining talk on atomistic modeling in construction chemistry to reduce environmental pollution. After a short break, the focus on “Photonics” formed the last block of the lecture series for the first day. In addition to the overview lecture by Prof. Peter Lehmann, Tobias Pahl (AG Lehmann) and Julia Heupel (AG Popov) provided contributions from this focus.

This year, participants again had the opportunity to present their poster contributions in one-minute poster flash sessions before and after the lunch break, thus drawing attention to their research topic in advance. Due to circumstances during the last CINSaT Fall Colloquium no poster prizes were awarded, so this was made up for during the Spring Colloquium. The jury consisted of Prof. Thomas Fuhrmann-Lieker, PD. Susanne Neupert, Prof. Kilian Singer, and Prof. Thomas Kusserow.

The poster session, which was realized via Gather Town - a videoconferencing tool as a virtual world in the style of 2D video games of the 80s - was very well received by the participants and the choice of the platform offered numerous opportunities for discussion and exchange, so that conversations continued even after the official end of the event. The diverse research activities of CINSaT were presented in an impressive and creative way on a total of 39 posters and provided an excellent basis for further discussions.

The second day started with the session on “Quantum Technology”, about which its speaker, Prof. Kilian Singer, gave a good overview first, before Mirali Gheibi and Jayanta Ghosh (both AG Baumert) gave an exciting talk on “Observation of long-lived electronic coherence in lanthanide complexes at room temperature”. The session was followed by a talk from Prof. Hartmut Hillmer, who presented the activities in the focus area “3-dimensional nanostructures”, and a contribution by Lukas

Wetterau (AG Witzigmann) on “Micromagnetic modeling of a low-noise GMR sensor”. The lecture block was concluded by Prof. Arno Müller with an overview of the activities in the focus “Multiscale Bioimaging”, which included the workshop together with the focus “Photonics”, as well as contributions by Mostafa Aakhte (AG Müller) and Jenny Plath (AG Stengl).

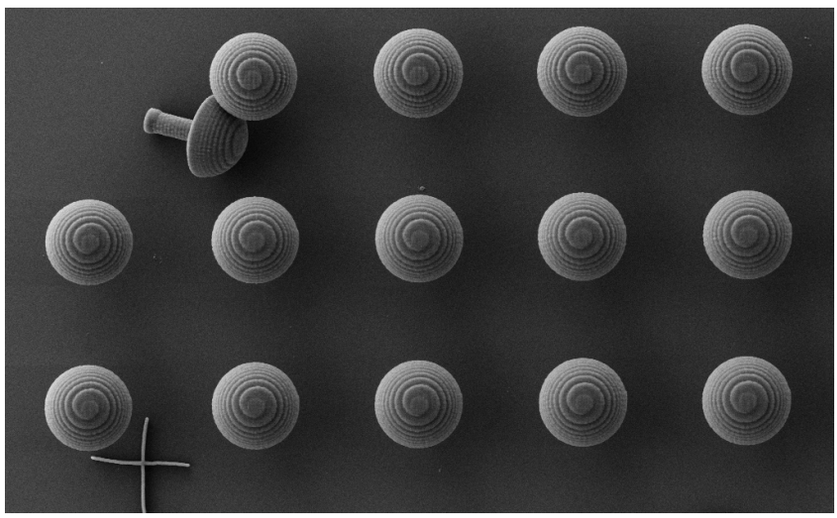
After lunch, the participants went into individual focus sessions, between which they could switch at will thanks to the virtual platform, to have the opportunity to perceive other topics and identify possible points of contact.

At the end of the event, the winners of the poster prizes were announced: First place went to Tianyu Fang (AG Singer, poster title: Examine molecular chirality with optical forces), second place to Meike Reginka (AG Ehresmann, poster title: Magnetic textures in 3D hollow hemispheres) and third place to Eric Kutscher (AG Demekhin, poster title: Photoelectron circular dichroism of fenchoone induced by broadband laser pulses).

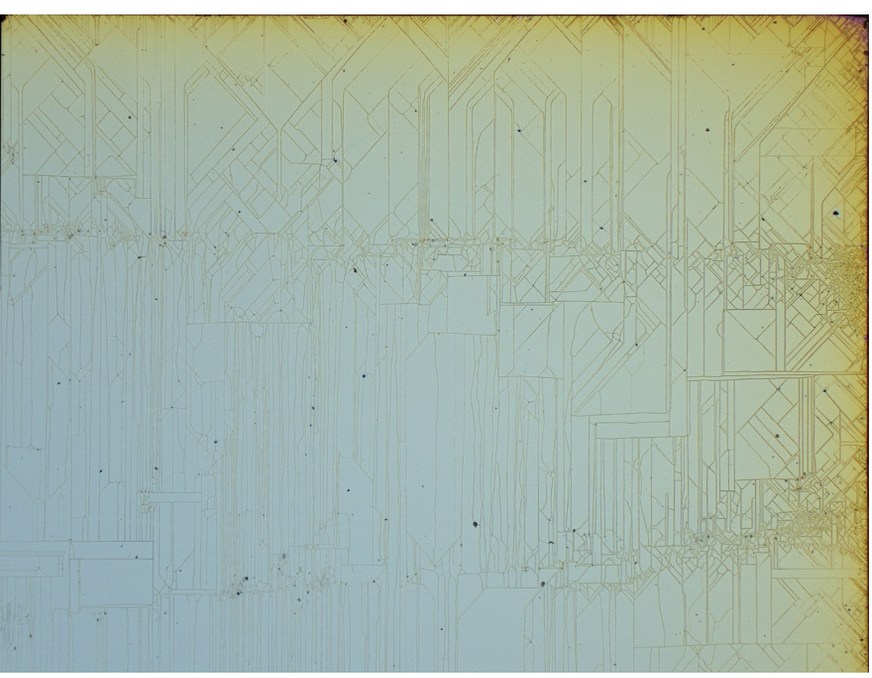
The new formats and the implementation of the poster session were very well received by all participants. A convivial exchange is not so easy to realize virtually, but creative ideas (coffee break kits for the participants and hidden gimmicks in the Gather Town) have consoled well over the set circumstances. With 110 participants the colloquium was a great success. Nevertheless, we hope to be able to hold the next spring colloquium again in presence, because not only socializing activities and group photo are missing, but also the sociable face-to-face exchange, where still the best ideas arise

Poster prize winners, left: Tianyu Fang on 1st place, middle: Meike Reginka on 2nd place, right: Eric Kutscher on 3rd place

Nano Arts



Christine Heume, Technical Electronics:
The mushroom-shaped particles were created by dip-in laser lithography (DILL) via two-photon-polymerization in IP-Dip 2 resist from the manufacturer Nanoscribe. The shield of the mushroom has a diameter of under 10 µm.



Sabine Dück, Technical Physics:
A 150 nm thick silicon nitride layer was treated in a Rapid Thermal Annealing setup at 680 °C. This caused crack formation in this peculiar manner.

Photo: Campus Heinrich-Plett-Straße, Press and Public Relations Office University of Kassel, Studio Blåfield

Imprint

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Responsible according to press law (german: ViSdPR):
CINSaT executive board,
University of Kassel