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photo: Press and Public Relations Office University of Kassel, Studio Bläfield
Welcome to the first CINSaT newsletter in 2018

The time is passing quickly and I thought, I just finished the preface page for the last newsletter while Dennis Holzinger, our center executive manager, asks me again for the next one. However, I also very much enjoy it to see the articles for the new newsletter at first before all of you and see all the excellent and exciting work done by our members, postdocs, PhD, master and bachelor students.

This issue starts with some general summary report from the management as well as from different meetings taken place since the last newsletter. In the educational category, Thomas Kusserow (FB 16, INA) and Thomas Fuhrmann-Lieker (FB10, Chemistry) report on their participation in a summer school in Jyväskylä in summer 2017 (their Nano Science Center is partner of CINSaT since 2016), where both of them held a class together. There is also a vital student exchange in both ways and several students from Finland are currently in Kassel.

Two research highlights are reported this time by Arno Ehresmann and Iris Koch (FB10, Physics) about smart magnetic materials and by Peter Lehmann (FB16, Electrical Engineering) about a new type of optical microscopy based on high resolution interferometry followed by a report of Raffael Schaffrath and Cindy Brachmann (FB10, Biology) on a new DFG project called „Protein Urmylation in Yeast - Mechanism and Functional Relevance”. For non-biologists, if you want to understand the goals and challenges they have to deal with, I recommend to read their article.

The core part of CINSaT is to bring groups together from different disciplines to gain by additional synergy working together on a common goal. In this direction we are getting from year to year more successful. Therefore, I am proud that we can report this time about two coordinated projects. The first report is about the new collaborative research center (CRC) on „Extreme Light for Sensing and Driving Molecular Chirality” coordinated by Thomas Baumert (FB 10, Physics), the flagship under the coordinated projects in fundamental research. In the first round of a 4-years’ time frame, 9 CINSaT members together with 4 external partners are participating. In the second report, three CINSaT members, Hartmut Hillmer (FB16, INA), Rudolf Pietschnig (FB10, Chemistry) and Arno Ehresmann (FB10, Physics) explain their cooperative work on „Multi-functional Anisotropically Shaped Hybrid-Particles”.

In this issue, three CINSaT members present themselves and the research topic of their groups, which are the groups by Philipp Demekhin (FB10, Theoretical Physics) Martin Garcia (FB10, Theoretical Physics) and Mohamed Benyoucef (FB10, INA).

Finally, a report is given about the very successful spring meeting in Friedrichroda, which obtained again a new record number in participants, and announcements are made about the upcoming autumn colloquium and a Symposium organized by the PhosMorg consortium coordinated by Raffael Schaffrath (FB10, Biology). However, there is always a last thing after the last thing. So, please enjoy also the nano art pages before you close the newsletter and before you start waiting for the next newsletter.

Enjoy the reading of this issue.

Johann Peter Reithmaier
Here, we report briefly about major issues from the CINSaT committees and major discussion results in their meetings.

(a) Steering Committee
Since the last period, we had two meetings on the February 24th and May 11th of this year. The next meeting is scheduled to July 7th. The following major issues were discussed and decided by the steering committee:

- Potential name change for the priority topic „biosensing” to „molecular dynamics cellular signal paths”. This point was also intensively discussed at the spring meeting. The steering committee expects a final approval, at latest during the next member meeting in fall of this year.
- It was decided that the current formal problems to hire an assistant should be solved on a short time scale by hiring student assistants before a general solution will be found.
- An Erasmus agreement is planned with the Heriot-Watt University in Edinburgh for Nano Science students. After visits of colleagues from Edinburgh in Kassel, a reverse visit is planned with some colleagues from Kassel University.
- This summer, the first 2-3 students came from Jyväskylä (Finland) to Kassel within the Erasmus program.
- CINSaT is now mentioned in the DAAD data base as partner for the nano science program of the University of Kassel.

(b) Research Coordination Committee
The steering committee had a joined meeting with the priority speakers on February 6th of this year. In this meeting, the priority speakers reported briefly for the first time about their initiatives and progress in coordinated projects. It was agreed that each priority group will meet separately with the related members to discuss opportunities to work together. The spring colloquium was used to get information about the different initiatives in the priority topics in a very compact form. However, the spring colloquium cannot substitute individual meetings also due to the time overlap.

The next meeting date is June 20th, 2018 at INA library (3rd floor).

(c) Member Meeting
The last member meeting took place on May 18th. The major issues that were discussed, the info that was given and the decisions that were made are as follows:

- The financial report for the year 2017 was presented. The CINSaT executive manager and the CINSaT speaker were released.
- Arne Senftleben (FB10, Experimental Physics III) was elected as a new associated CINSaT member.
- The members were informed that according to the presidential decision the advisory board needs 5 board members and not 4 as originally discussed. The selection of a female colleague out of a pre-approved list of 3 potential candidates is on the way. Inputs for a potential fifth female board member, who should be located out of Germany, should be sent to the CINSaT office until beginning of the upcoming winter semester.
- The speaker also informs that he is invited to an international meeting of about 20 speakers of nano science centers around the world, which will give an impression on how organizational and institutional problems are solved in different universities and countries and how our center may have to change its organizational form to get internationally competitive.
In 2016 the collaboration between the Nano Science Center in Jyväskyla and CINSaT was established and the possibility for ERASMUS funding of students, teachers and researchers exchange was announced. In the following months, both of us had the idea to apply for a course in the next summer school in Jyväskylä. After a short discussion we came to the conclusion that it would be a great idea to combine our plans and hold a class on “Materials for Nanophotonic Application” together. This would give the students the opportunity to learn about material properties and applications from the point of view and the experiences of different fields. After sending a short proposal to the organizers of the summer school and the international office of our university, we received very positive feedbacks and the plan for the course was fixed.

The sessions of the course were scheduled to fill the whole second week of the summer school with focused sessions in the morning and afternoon on fundamentals of optical properties, nanophotonic structures, lasers and waveguides (all regarding inorganic and organic materials) as well as devices, characterization methods and special materials, like liquid crystals, biophotonic and heterogeneous materials. Additionally, two practical labs on transfer matrix simulations and ellipsometry were included to offer the students a chance to directly apply the new topics.

During application and planning of the summer school course, the international office in Kassel and the organizers in Jyväskylä helped us in every possible way to minimize the impact of any red tape. Therefore we could mainly concentrate our work on preparing the lectures and the lab and planning our visit.

The bridge over Jyväsjärvi connecting the Nano Science Center with the other campus and the city (photo: Summer School Team Jyväskylä).
On August 13, we arrived in Jyväskylä and were picked up at the airport by Jussi Toppari, our main contact in the Nano Science Center. Our course started the next day with 20 students awaiting to learn more about optical properties of different materials. During the breaks, in the evenings and at social activities, it was quite easy to get into good discussions with students, other teachers or the research staff in Jyväskylä. After the courses, most of the days the organizers offered an additional program including a get-together evening with barbecue, a bike ride around the lake, a dinner and a farewell party (named “Rock after Research,” with bands having members of the Nano Science Center) and a visit to Lethisaari Island (with barbecue, swimming and sauna).

Since we had already some contacts to Jyväskylä due to the CINSaT fall colloquium, we used every available free time to meet and discuss with researchers to find possible topics for future research work. This led to some ideas with the groups of Mika Pettersson and Jussi Toppari which were pursued since last summer. Also some time was found to have a lab tour and an informative meeting for students in Jyväskylä which are interested to come for an ERASMUS exchange to Kassel.

The one week at the summer school was filled with great experiences, be it working with our class, meeting other teachers or finding new contacts to researchers in Jyväskylä. We really appreciate the funding from ERASMUS and especially all the help we received from the organizers of the summer school and our international office. Finally, we can only recommend to consider an exchange as teacher or researcher to other CINSaT members.
In our modern world, devices using optical output in the form of displays are omnipresent. Therefore, researchers are constantly looking for new ways to improve the existing technology. Recently, a collaboration between the University of Kassel and the ISC Fraunhofer Institute in Würzburg led to new findings in the field of remotely switchable optical surfaces.

The ISC Particle Technology group is specialized in synthesizing micro- and nanoparticles with silica backbone. In this case, the particles are composed of superparamagnetic iron oxide nanoparticles that are “glued” together with silicon dioxide, resulting in plate-like microrods with unique reflection and scattering properties. If these particles are present in a liquid environment – in this case water – they are able to freely rotate and, therefore, change their spatial alignment upon application of external magnetic fields. This leads to a change of reflectivity and diffraction of incoming light in the so-called magneto-optical fluid. Yet, the particles are randomly distributed throughout the fluid. In order to align the particles in defined structures, a simple permanent magnet is not sufficient. This is where the Experimentalphysik-IV group comes into play. The scientists are able to fabricate topographically flat substrates that exhibit a well-defined magnetic pattern. The shapes of the magnetic microstructures can be arbitrarily set by a combination of photolithography and helium ion bombardment on exchange bias thin film systems and are stable at room temperature.

For this project, magnetic parallel stripe patterns with stripe widths in the range of a few micrometers were fabricated and used as a magnetic template for the alignment of the superparamagnetic microrods. A fluid cell of 100 µm thickness containing the magneto-optical fluid was built on top of the magnetic mold. Thereby, a grating-like structure is created that can serve as a reflective diffraction grating for visible light. If external magnetic fields of only a few mT are applied perpendicular to the substrate surface, the grating constant can be doubled due to a change of the magnetic potential energy landscape of the microrods, i.e., the particle favor every second magnetic stripe border. Upon application of an external field parallel to the surface plane and large enough to magnetically saturate the substrate (= 100 mT) the defined alignment can be suppressed and, hence, the diffraction effect turned off. Both procedures are completely reversible and the diffraction effect is stable as long as the fluid does not run dry. The obtained results are very promising considering their potential application in smart surfaces with remotely switchable properties.

Research Highlights
Smart surfaces - magnetically switchable light diffraction

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Further Information
The lateral resolution in two-dimensional microscopic imaging is subject to the fundamental limit published by Ernst Abbe in 1873 and, in principle, this limit even holds in 3D interference microscopy.

White-light interferometry (WLI) as one of the most used techniques for optical 3D measurement of micro- and nano-structures is based on interference microscopy employing temporally low coherent light. Consequently, WLI signals captured by a single camera pixel during a continuous decrease or increase of the optical path difference between the reference and the measurement arm of an interferometer consist of a high frequency interference contribution and a low frequency coherence envelope, as shown in Fig. 1. Signal processing in WLI determines the position of the coherence envelope’s maximum as well as the phase of the interference contribution with respect to the phase of a synthetic reference signal generated numerically.

We call the resulting topography either ‘coherence’ or ‘phase’ topography, depending on whether it is obtained from the envelope position or the phase. The spectrum of a measured WLI signal equals the spectrum emitted by the light source weighted by the spectral sensitivity of the camera. However, this is no longer correct for high NA (numerical aperture), e. g. for our Linnik interferometer equipped with objective lenses of NA = 0.9. In this case, the well-known NA effect becomes relevant leading to an increased interference fringe spacing, which results in a longer effective wavelength of the measured signals. Spectral analysis shows that additional lower frequency contributions occur at high NA. These are related to oblique angles of incidence and appear even if a light source of narrow bandwidth is used. This broadening in the spectral domain leads to a limited longitudinal spatial coherence, which is independent of the temporal coherence of the light source. Motivated by strange measurement results obtained in a previous DFG project, we studied the consequences of these effects with respect to transfer characteristics and lateral resolution capabilities of WLI instruments at high NA.
Using a blue LED as a light source, we basically observed three phenomena (see Fig. 2):

- The coherence topography seems to provide superior lateral resolution compared to the topography obtained from phase, although phase analysis enables better axial resolution. This has to do with nonlinear transfer characteristics related to the position of the coherence envelope.

- If the lateral dimensions of the surface structure are close to the lateral resolution limit of the microscopic imaging system, the coherence topography will be inverted, i.e. the measured height values will change their signs, compare Fig. 2 (a) and (c). This is another consequence of nonlinear transfer characteristics in case of diffraction.

- Third, the lateral resolution with respect to the phase topography can be improved if WLI signals are analyzed at longer wavelengths. This seems to contradict the theory of microscopic imaging where shorter wavelengths provide better lateral resolution. However, the light employed throughout our study originates from a blue LED with a center wavelength of 460 nm. What is changed is the evaluation wavelength, which corresponds to the wavelength of the synthetic reference signal shown in Fig. 1. Longer wavelength components can be interpreted as effective wavelengths \( \lambda_{\text{eff}} = \lambda / \cos \theta \). For our signals, the maximum angle \( \theta_{\text{max}} = \arcsin(\text{NA}) \) results in a maximum wavelength contribution of the WLI signal of \( \lambda_{\text{eff}} = 1055 \text{ nm} \).

Fig. 2 shows the 3D structure of a rewritable Blu-ray disc and demonstrates the phenomena mentioned above. In Fig. 2 (c) the groove structure can be recognized, although the topography looks noisy. This results from the fact that the signal contribution at a wavelength of 900 nm is quite low. All results discussed here could be confirmed by numerical simulations based on either Kirchhoff diffraction theory or by an extended Richards-Wolf model.
New Projects

Protein Urmylation in Yeast - Mechanism and Functional Relevance (DFG SCHA750/15-2)

The Division of Microbiology, led by Professor Schaffrath, uses the budding yeast Saccharomyces cerevisiae as a model to study protein and RNA modification pathways that influence mRNA translation, protein synthesis and cell growth. One of the protein modifications the group is interested in is the so-called urmylation. Here, the protein Urm1 is transferred to a target protein (e.g., Ahp1) via a conserved signal cascade which finally leads to a covalent bond between both proteins. The function and fate of urmylated proteins is still unclear, which requires further investigation.

Glutathione peroxidases and peroxiredoxins ensure maintenance of cellular redox homeostasis and are thus crucial for the protection of cells against oxidative stress. This importance is further evidenced by disease formation and premature aging in humans associated with defects in thiol peroxidases. Ahp1 (alkyl hydroperoxidase 1) is a 2-Cys peroxiredoxin from yeast that maintains two redox-active thiols (C31, C62) (Fig. 1) critical for reactive oxygen species (ROS) detoxification. During catalysis, Ahp1 forms a homo-dimer and reduces ROS with its peroxidatic Cys (CP: C62) residues that get oxidized to a sulfenic acid (-SOH). Next, the sulfenylated CPs are disulfide-linked to the resolving Cys (CR: C31) residues from opposite Ahp1 subunits to form the oxidized dimer (Fig. 1). Upon reduction, which involves disulfide exchange onto the thioredoxin system (Trx2), the Ahp1 homo-dimer gets repaired (Fig. 1) for another peroxidatic cycle.

Interestingly, redox stress triggers post-translational modification of Ahp1 including urmylation, a conjugation to the ubiquitin-like protein Urm1 (Fig. 1). Urm1 not only modifies proteins but also acts as a sulfur-donor for tRNA-thiomodification. Together with the Elongator (a multifunctional complex involved tRNA-modification, transcription, signaling, and others) pathway, this generates 5 methoxy-carbonyl-methyl-2-thio modifications at anticodon wobble uridines (mcm5s2U34) of certain tRNAs. Importantly, tRNA-thiolation and ROS dependent Ahp1 urmylation both require Urm1 to be thiocarboxylated (Urm1-COSH) by Uba4, an E1-like activator enzyme. This suggests that the two Urm1 functions are linked by S-transfer coupling both to oxidative stress. Consistently, several groups including our own have shown that redox stressors (H2O2, diamide) trigger protein urmylation, and among Urm1 targets (identified from yeast, flies and human cells) are factors of the oxidative stress response.

Nonetheless, a specific function for urmylation of Ahp1 remains elusive. Apparently, Urm1 is not a (ubiquitin-like) tag for degradation but may otherwise affect localization, interaction or structure of the peroxiredoxin. In line with this, it was shown that Ahp1 is urmylated at Lys residue K32, which is next to the redox-active CR (C31) (Fig. 1). Hence, Urm1 conjugation may interfere with Ahp1 through conformational changes near the thiol centre critical for catalysis and dimerization (Fig. 1).

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Further Information
DFG SCHA750/15

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A. Jüdes et. al., Urmylation and tRNA thiolation functions of ubiquitin-like Uba4•Urm1 systems are conserved from yeast to man, FEBS Lett 589, 904-909 (2015) doi 10.1016/j.febslet.2015.02.024

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Microbiology Division Professor Schaffrath (home page)
https://www.uni-kassel.de/fb10/institute/biologie/fachgebiete/mikrobiologie/
Having established tools and protocols (SCHA750/15-1) for the diagnosis of urmylation and for URM1 pathway analysis, we will clarify mechanistic aspects of the urmylation pathway and the relevance of Urm1 conjugation for the cell. How exactly sulfur (Urm1-COSH) is used during the urmylation reaction is unclear, making it crucial to study its fate post-urmylation. Also, whether and how urmylation of Ahp1 may affect the thiol-based redox-active switch, which is important for the peroxiredoxin to function in the response to ROS, are key questions in need for answers. In particular, we aim to clarify the following ill-defined aspects of the urmylation pathway:

- the role of the activated sulfur in Urm1-COSH for the Urm1 conjugation pathway,
- the fate the activated S-species derived from Urm1-COSH faces post-urmylation,
- the role of Ahp1 urmylation for the performance of a thiol-based redox switch in the ROS response.

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Fig. 1. Structural context and urmylation of the peroxiredoxin Ahp1. (A) Overview of reduced Ahp1 (Ahp1red) subunits (beige/green) (PDB: 4DSR) with details on the urmylation site (Lys-32, blue) and the cysteine (red) based thiols (yellow) in CR (Cys-31) and CP (Cys-62). Urmylation uses a highly conserved di-glycine motif of Urm1 (orange) (PDB: 2QJL) forming a covalent isopeptide bond with Lys-32 of the respective Ahp1 subunit. The interface Phe residues (dark green), which provide the hydrophobic interactions (dotted line) between the two subunits, are highlighted. (B) After oxidation of Ahp1 (Ahp1ox), the dimer (PDB: 4DSQ) undergoes a conformational change and a disulfide (yellow) is formed between the CP of one (beige) and the CR of another (green) Ahp1 subunit. It has been shown that the hydrophobic Phe side chains bring the two subunits into the correct orientation to each other, regardless of the redox status. Crystal structures: J Biol Chem 287: 17077ff. Illustration created with The PyMOL Molecular Graphics System, Version 1.8 Schrödinger, LLC.
New Coordinated Projects

SFB/CRC 1319 ELCH

The DFG funded Collaborative Research Center (CRC) / Sonderforschungsbereich (SFB) 1319 ELCH (Titled: “Extreme Light for sensing and driving molecular CHirality”) started successfully at the Universität Kassel in January 2018 coordinated by Prof. Dr. Thomas Baumert.

Handedness, a common everyday experience termed chirality in science, has fascinated scientists as well as philosophers for centuries. Molecular chirality is widely recognized for its relevance to the building blocks of life and its vital role for medicine and health. The CRC 1319 ELCH focuses on a completely different but equally fundamental aspect, namely on a microscopic quantum mechanical understanding of individual chiral molecules in the gas phase under perfectly defined experimental conditions. It employs the most advanced tools of experimental and theoretical gas phase atomic, molecular, and optical/quantum optical (AMO) physics for control and manipulation of chirality on the single-molecule level. With the help of extreme light (Fig. 1), covering all relevant excitation regimes in terms of energy, intensity, and temporal resolution, it addresses the full chiral quantum system of electrons and nuclei in each individual molecule. The CRC 1319 ELCH will provide a purely light-driven gas phase research center for chiral molecular physics, which is unprecedented, despite the importance of chiral molecules for practical applications in chemistry and life science and their potential for fundamental physics research. In fundamental physics, chiral molecules can serve as versatile probes due to their inherent connection to tunneling – as discovered by Hund in the early days of quantum mechanics and their pronounced sensitivity to parity violating interactions.

The tremendous attention paid to individual aspects of gas phase single-molecule chirality in the current scientific discussion attests to the timeliness of our CRC. The principal investigators of our consortium are among the drivers of this development, with several ground-breaking contributions in recent years (Fig. 2). This CRC brings together these renowned theorists and experimentalists with world-leading technologies, who join forces in order to understand, as the main scientific goal, single-molecule chirality and the electronic response of chiral molecules to electromagnetic radiation.

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This understanding will provide the basis for controlling chirality on the single-molecule level. Within our CRC, we will develop advanced and light-based methods for the analysis, separation, cooling, trapping, manipulation and control of chiral molecules. Our specific long-term goals are the efficient determination of absolute configuration on the single-molecule level in the gas phase, chiral purification, i.e., the complete light-driven conversion of a sample of molecules with mixed handedness into a sample with only one handedness, and to perform fundamental physics experiments with chiral molecules.

Fig. 2: Three recent breakthroughs by our CRC members on single-molecule chirality sensing. Left: forward/backward electron emission with respect to the light propagation is the basis of photoelectron circular dichroism (PECD), which, after resonance-enhanced multiphoton ionization (REMPI), is accessible via velocity map imaging (VMI). Here, the three-dimensional electron momentum distribution is obtained with tomographic methods [1]. Middle: cold target recoil ion momentum spectroscopy (COLTRIMS) reveals the absolute configuration of a small chiral molecule by Coulomb explosion. [2] Right: opposite enantiomers have the same rotational constants and the same magnitude of dipole moment components, but the sign of the combined product of the molecule-fixed dipole moment components is distinct for each enantiomer allowing for enantiomer-specific detection of chiral molecules via microwave three-wave mixing spectroscopy (M3WM). [3]

Besides our scientific aims, we will pursue three further key goals within this CRC. The strategic goal is to establish an internationally leading research center for light-driven chiral molecules in the gas phase. The core activities at Universität Kassel (ten research projects (RPs)) will be closely linked to the participating institutions Universität Frankfurt (three RPs), Universität Marburg (one RP) and DESY (one RP), invigorating existing collaborations and establishing new ones. The CRC can build on a 15 year focused hiring policy in AMO physics at Universität Kassel and on a four year funded collaborative project on chiral molecules between the Hessian partners through the Excellence Initiative of the State of Hesse (LOEWE ELCH) (Fig. 3).
The educational goal is to provide the best possible training for students and PostDocs in this promising new area of AMO science and give the initial boost for their later career. Science education will be complemented by a dedicated outreach program, with measures that span from kindergarten via the high school level to the general public. Our gender equality goal is to take advantage of the already high-level infrastructure at Universität Kassel and substantiate it by physics specific components that will encourage female scientists to advance to senior ranks of research.

Fig. 3: The timeline towards the CRC 1319 ELCH started with a fundamental research project first proposed as a contribution of Kassel to an EU RTN Network „Imaging and control in chemistry“ in 2005 and a first publication in 2012 [1] funded by the Universität Kassel. This and other excellent research projects paved the way to the LOEWE excellence initiative funded by the Hessian state from 2013 for four years. In 2017 the Universität Kassel installed a Bridge-Funding to be prepared for the possible start of the DFG funded CRC 1319 ELCH in 2018. Since January 2018 the CRC 1319 ELCH is running.

Fig. 4: PIs of the CRC 1319 ELCH: From left to right: Prof. Dr. Singer (KS), Prof. Dr. Giesen (KS), Dr. Reich (KS), Dr. Dawkins (no PI, KS), Prof. Dr. Baumert (KS), Dr. Braun (no PI, KS), Prof. Dr. Demekhin (KS), Prof. Dr. Dörner (F), Dr. Sentfleben (KS), Prof. Dr. Schnell (HH), Dr. Knie (KS), Prof. Dr. Koch (KS), Prof. Dr. Ehresmann (KS), Prof. Dr. Pietschnig (KS), Prof. Dr. Berger (MR), Dr. Schöffler (FR).

References
Tomographic data:
MASH - Multifunctional Anisotropically Shaped Hybrid-Particles

“MASH: Multifunctional Anisotropically Shaped Hybrid-Particles” is a joint research project, within the internal funding initiative „Zukunft“ of the University of Kassel, coordinated by Prof. Dr. Hartmut Hillmer in collaboration with the CINSaT members, Prof. Dr. Arno Ehresmann and Prof. Dr. Rudolf Pietschnig.

Polymer micro- and nanoparticles have a wide variety of applications in liquid environments, such as molecular transporters, microsensors or contrast agents in medical diagnostics. For these types of applications and many others, the particles are chemically functionalized by reactive molecular groups on their surface, which serve as binding sites for analytes. In general, spherically shaped particles are more widely encountered than geometrically more complex shapes, due to the fact that most fabrication techniques are bottom-up approaches mostly driven by thermodynamic interactions, where the most energetically favorable outcome is a sphere. From a modeling point of view, the system also becomes increasingly more complicated the more parameters/asymmetries are added to it. However, it has been shown that the spherical shape of the particles brings about numerous limitations when used in a confined hydrodynamic environment. Here, the anisotropic non-spherical particles reveal advantages in terms of wall-interactions and adhesion, amongst others, which give access to more degrees of freedom of the particle movement. From this idea, a project focused on the development of multifunctional anisotropically shaped hybrid-particles, in short MASH, that combine several defined physical and chemical properties has been created. Three CINSaT groups from different disciplines (Hillmer: Engineering, Pietschnig: Chemistry, Ehresmann: Physics) combine their expertise in their fields to investigate fundamental aspects of the production and applications of such micro- and nanoparticles, adding to the university’s already existing interest in nanostructures.

![Diagram](image)

Fig. 1: Schematic representation for functionalization combinations.

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The goal of this joint consortium is to manufacture three-dimensionally defined MASH-particles using Nanoimprint lithography (NIL) as one of the main fabrication techniques and to integrate different functional elements into the particles. Their multifunctionality is then used as a tool to address multiple tasks within the same system, providing advantages like time efficiency and adaptability with highly tailored hydrodynamic properties. The project plans to investigate how chemical modifications of the guest particles change functionality or whether chemical or physical surface modifications lead to the desired multifunctionality. Furthermore, the interaction between different functionalizations is an important part in the material choice, as well as how the end result depends on the shape of the MASH-particles.

The combination of photoluminescence and magnetic properties in micro- and nanoparticles is promising, as these allow versatile applications of the particles as contrast agents on one hand and microtransporters on the other. In a previous collaboration, the three CINSaT groups worked on embedding europium(III)oxide guest nanoparticles with fluorescent and magnetic properties into polymer microfibers using the high resolution structuring process, NIL, for the fabrication of particles possessing an accuracy of spatial dimensions in nanometer range. In the publication that resulted from this, they characterize and optimize the fabrication parameters, as well as the materials involved.

Fig. 2: Left: SEM image of flexible AMONIL microfibers with imbedded Eu$_2$O$_3$ nanoparticles. Middle: Surface functionalized triangle structures with an Exchange-Bias thin film layer. Right: Surface functionalized zig-zag structures with an Exchange-Bias thin film layer.

The variation of shape, combined with the testing of different polymers, with focus on organosilicon and phosphorus compounds, is the next step in the research within this joint collaboration. During the next two years, further cooperation with other groups (e.g. Fuhrmann-Lieker and Lehmann) are planned to extend the repository of material manipulation and characterization platforms. Above all, the collaboration is based on the cooperation of doctoral candidates who bring together the scientific expertise of the subject areas within the interdisciplinary CINSaT platform.

Further information
Research Groups
Theoretical Atomic and Molecular Physics – Faculty 10

Prof. Dr. Philipp Demekhin studied physics at the Rostov State University (Russia) and obtained there a PhD degree in 2000. After that, he made postdoctoral research at the Rostov State Transport University (Russia), Technical University of Kaiserslautern (with an Alexander-von-Humboldt fellowship), University of Kassel (with an EU Marie Curie fellowship), and University of Heidelberg. In 2013, he obtained a Junior Professor position at the University of Kassel, where he established the Theoretical Atomic and Molecular Physics group. Since 2014, he is an associated member of CINaT.

The development of theoretical and computational approaches for ab-initio description of the electronic continuum spectrum in molecules with applications to angle- and time-resolved electron and fluorescence spectroscopy are among the main scientific research expertizes of the group. Thereby, the Theoretical Atomic and Molecular Physics group is entirely integrated in the consortium of scientists aiming at the investigation of electron dynamics of chiral systems. During 2013-2016, this consortium acquired financial support from the state’s Hessen Initiative for the Development of Scientific and Economic Excellence (LOEWE).

In 2018, this consortium of scientists established in Kassel a new DFG collaborative research center SFB-1319 ‘Extreme light for sensing and driving molecular chirality’. In this CRC-project, the Theoretical Atomic and Molecular Physics group plays one of the central roles in the theoretical description of the photoelectron circular dichroism (PECD), observed by experimental cooperation partners in the angle-resolved photoionization and fragmentation spectra of chiral molecules. This activity of the Theoretical Atomic and Molecular Physics group is a part of the CINaT main topic ‘chiral systems’.

Photoelectron circular dichroism as a function of the photoelectron emission angle $\theta$ and the molecular orientation angle $\beta$ after O 1s-ionization and subsequent dissociation of the R(+) methyloxirane into CH$_3^+$ and C$_2$H$_2$O$_+^+$ fragments (Tia et al., J. Phys. Chem. Lett. 8, 2780 (2017)).
Professor Dr. Martin E. Garcia is the head of the group Theoretical Physics II and also member of CINSaT since 2004. The main research efforts of the group were initially focused on the areas of Ultrafast Phenomena in Solids, with European and German funding, through a Research Training Network and different DFG Priority Programs, and transport properties of deposited nanostructures, also on the basis of DFG grants. Later on, the group acquired experience in the theoretical description of Laser Processing of Materials and started research in Biophysics. The group actively collaborates with many Universities and Institutes within Germany and also in the United States, Japan, China, France, Spain, Italy, Portugal, Sweden, Switzerland, Russia, Argentina, Colombia and Mexico.

The interaction of intense femtosecond laser pulses with solids gives rise to a variety of exciting new phenomena, that are initiated by the fact that electrons can rapidly be heated up to temperatures of several ten thousand Kelvin, i.e., far above the temperature at the surface of the sun. The resulting transient nonequilibrium state drives ultrafast structural phase transitions in different materials along pathways that are inaccessible under thermodynamic conditions. The group has developed a computational code called CHIVES (Code for Highly excited Valence Electron Systems) for performing ab-initio molecular dynamics simulations of laser excited solids. CHIVES is the fastest existing code for this purpose and has allowed Prof. Garcia’s group to explain and predict different laser induced nonthermal phenomena, like thermal phonon squeezing, transient fractional diffusion, anisotropic energy transfer and anomalous pre-melting. On the other hand, the group is running ultralarge-scale atomistic-continuum simulations (including up to hundreds of millions of atoms) to describe, on the same time and space scales as in experiment, laser ablation of films, laser nanostructuring of surfaces in vacuum and under a layer of water. The biophysical research activities of the group started with the description of protein folding in cages and under the influence of external electric fields. Electric-field induced conformational changes were predicted. Recently, the group analyzed conformational changes induced by microwave electromagnetic radiation on proteins involved in neurodegenerative diseases. Moreover, the group was able to explain different electrophysiological experiments on exocytosis in secretory and synaptic cells. Prof. Garcia’s group is involved in the joint interdisciplinary projects PhosMOrg and “Biological Clocks”, aimed at investigating biological problems funded by the University of Kassel.
Priv.-Doz. Dr. Mohamed Benyoucef has received his PhD from the University of Bristol (United Kingdom) and his Habilitation from the University of Kassel. He is the head of the Nano Optics group, which was established in 2010 in the Institute of Nanostructure Technologies and Analytics. Prior to working in Kassel, he was the Head of Optical Spectroscopy at the IFW Dresden and Max Planck Institute for Solid State Research, Stuttgart. His research group focuses on the development of novel and advanced single semiconductor nanostructures fabricated on Si, GaAs, and InP substrates using molecular beam epitaxy system and studies their specific aspects of quantum optics.

Quantum dots (QDs) have provided huge opportunities for physical research and technological applications, including quantum information and optoelectronics. QDs are often called “artificial atoms” because they locally confine single charges in discrete energy states analogous to the orbital energy levels of natural atoms. However, QDs can be tuned during production by controlling its properties to emit any colour of light wanted. His group has recently developed and demonstrated nearly perfect single-photon emission from single QDs emitting at telecom wavelengths, reported high quality single QDs at telecom C-Band with vanishing fine-structure splitting, and developed telecom wavelengths InP-based photonic crystal microcavities with embedded QDs to be used as efficient single-photon sources for long-distance quantum information. The group has recently also realized for the first time bright light emission from single QDs directly grown on Si; this could allow a direct combination of photonics and electronics on the same chip.

He has engaged in several projects dealing with quantum information such as projects on quantum communication funded by the BMBF and EU Flagship program on Quantum Technologies. He is also an active member of the national initiative for Quantum Technology-Fundamentals and Applications “QUTEGA.” Current collaborative projects within the CINSaT include the submitted LOEWE project application on Molecular Quantum Systems (with M. Baumert, C. Koch, R. Pietschnig, J. R. Reithmaier, K. Singer, B. Witzigmann) and theoretical investigation of the photonic nanostructures (with B. Witzigmann).

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(a) Telecom single-photon emission from single InP-based QDs. The inset shows corresponding µ-PL spectrum and AFM image of low dot density. (b) InAs QDs embedded in defect-free silicon matrix. (c) Telecom wavelengths InP-based photonic crystal microcavities with embedded QDs. (d) Site-controlled quantum dots.
As in previous years, CINSaT invited its members to participate to the internal science colloquium taking place at the Ahorn Berghotel in Friedrichroda at the end of February 2018. The internal colloquium is an important forum to communicate current research activities within the focus topics of CINSaT. At the same time, unique possibilities are offered to the members to debate about the future development of the focus topics as well as planning coordinated joint projects. A key ingredient to ensure a broad and diverse discussion platform relates to the active contribution of the members’ PhD students. With around more than 80 participants, the colloquium could follow up the pleasantly high participation rates of the past two years. These numbers once again emphasize the positive development of CINSaT during the recent years.

The colloquium opened with a warm welcome speech given by the head of CINSaT Prof. Dr. Johann Peter Reithmaier. The spokesman emphasized that the constructive feedback from the past colloquia was used to introduce two structural changes in the program: Besides the regular series of talks within the context of CINSaT’s focus topics, for the first time, individual focus topic meetings were held for substantial discussions. In addition, this session was intended as a kick-off event for further development and intensification of cooperation within the focus topics. Therefore, individual implementation strategies were worked out during these meetings. As a second improvement, a hiking tour was organized to offer an opportunity for a relaxed exchange of views and to get to know each other. Framed by the wintery scenery, this event was experienced as enrichment for the colloquium.

Conference room during the focus sessions.

Impressions of the hiking tour.
Within the scope of the focus sessions, the scientific staff of the participating departments again impressively presented latest research results stemming from the world of nanostructures. The interdisciplinary collaboration between the different departments was highlighted as an important foundation for the achieved results. The diversified program was enriched by the introduction talk of Dr. Arne Senftleben (Department for Femtosecond Spectroscopy and Ultrafast Laser Control) within his application for associated membership within CINSaT.

To intensify and deepen the scientific exchange, the scientific program was again complemented by the evening poster session. The numerous research activities within the CINSaT focus topics were presented on 60 posters, with no limits concerning the participants’ creativity for visual presentation, e.g., presenting movies of experimental findings on tablet devices. Based on the positive experiences of the last colloquium, the poster session was again scheduled open-end and could therefore provide a fertile ground for the planning of future joint projects.

Scientific discussions during the evening poster session.

Group photo of the participants.
Announcements

Phosphoregulation of Biomolecules:
from Mechanisms to Organisms

1st Symposium

11th of June 2018
Bootshaus, University of Kassel

Anne Jantschke, Dresden
Armin Geyer, Marburg
Sebastian Glatt, Krakau
Stefanie Kellner, München
Stefan Knapp, Frankfurt/Main
Christof Lenz, Göttingen
Andreas Wodarz, Köln
<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title/Abstract</th>
</tr>
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<tbody>
<tr>
<td>08:20</td>
<td>R. Schaffrath (PhosMOrg Coordinator)</td>
<td>Welcome by PhosMOrg Consortium</td>
</tr>
<tr>
<td>08:30</td>
<td>F. W. Herberg / S. Pautz (PhosMOrg)</td>
<td>Phosphotransfer basics, kinetics, modelling and detection</td>
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<tr>
<td>09:00</td>
<td>C. Lenz (Göttingen)</td>
<td>Mass spectrometry in phosphoproteomics</td>
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<tr>
<td>09:30</td>
<td>S. Knapp (Frankfurt/Main)</td>
<td>Selective targeting of protein kinases</td>
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<td>10:00</td>
<td></td>
<td>Coffee break / Poster</td>
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<tr>
<td>10:30</td>
<td>M. E. Garcia / B. Reuter (PhosMOrg)</td>
<td>Session II – Mechanisms/Organisms</td>
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<tr>
<td>11:00</td>
<td>T. Fuhrmann-Lieker / B. Mohr (PhosMOrg)</td>
<td>Biomolecular phosphorylation relevant for NanoScience</td>
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<tr>
<td>11:30</td>
<td>A. Jantschke (Dresden)</td>
<td>The relevance of phosphorylation/phosphate in biomineralization</td>
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<tr>
<td>12:00</td>
<td>A. Geyer (Marburg)</td>
<td>The chemistry of diatoms: Synthetic silaffins for silica precipitation</td>
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<td>12:30</td>
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<td>Lunch</td>
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<tr>
<td>14:00</td>
<td>R. Schaffrath / M. F. Landrock (PhosMOrg)</td>
<td>Session III – Organisms</td>
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<tr>
<td>14:30</td>
<td>S. Glatt (Krakau)</td>
<td>Phosphoregulation of protein and tRNA function <em>in vivo</em></td>
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<tr>
<td>15:00</td>
<td>S. Kellner (München)</td>
<td>Lost in translation: tRNA modifications protect the proteome</td>
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<td>15:30</td>
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<td>Application of NAIL-MS in the diagnosis of RNA modification dynamics</td>
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<tr>
<td>16:00</td>
<td>H. A. Müller / V. D’Angelo (PhosMOrg)</td>
<td>Coffee break / Poster</td>
</tr>
<tr>
<td>16:30</td>
<td>A. Wodarz (Köln)</td>
<td>Regulation of actomyosin contractility at adherens junctions</td>
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Autumn Colloquium 2018

CINSaT cordially invites you to join the annual autumn colloquium, which takes place on Wednesday, the 24\textsuperscript{th} of October 2018, between 13:00-18:00, at the lecture hall 282, Campus Heinrich-Plett-Straße. The spirit of the colloquium is to provide current research issues within the interdisciplinary framework of nanostructure science to a broad audience in order to find a common language for research.

The program is organized in a way that invited external speakers were chosen to represent current and future activities within the scope of CINSaT’s scientific key topics. The event is completed by a poster session in which the participators have the opportunity to hold scientific discussions and informal exchanges about current activities within the CINSaT. Note that the physical well-being of the participants is ensured.

We are pleased to welcome you to the colloquium and look forward for your participation!
Nano arts

In this section, artistically appealing images from the CINSaT groups will be presented. If you obtained any kind of visually appealing and fascinating data during your experiments with focus on micro- and nanometer length scales, you are cordially invited to submit your contribution to the editors.

In this edition:

Exchange bias capped magnetic Janus particles imaged by helium ion microscopy.

photo: AG Ehresmann, Functional Thin Films, HIM picture provided by Kai Arstila, University of Jyväskylä, Department of Physics is gratefully acknowledged.
The amazed Damsel: 500 nm silica beads assembled in mono- and multi-layers, observed through a white light microscope.

photo: AG Ehresmann, Functional Thin Films.

Dark field microscope image of a nanoimprint stamp made of polyvinyl alcohol.

photo: AG Hillmer, INA

„The amazed Damsel“: 500 nm silica beads assembled in mono- and multi-layers, observed through a white light microscope.

photo: AG Ehresmann, Functional Thin Films.
Imprint

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